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Report

UK Nuclear Science Forum

Progress Report: Data Studies During 1998

A report produced for the IMC

Milestone M1 of
Contract TE/G/00521/Z(IMC/RPS/GNSR/5002)

Edited by A L Nichols

The running of the UK Nuclear Science Forum is financed by the Industry Management Committee (IMC) comprising Nuclear Electric Limited, Scottish Nuclear Limited and British Nuclear Fuels Limited and their successor companies.

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Executive Summary

Nuclear data studies for commercial applications in the UK are formulated, monitored and reviewed through the UK Nuclear Science Forum (UKNSF). This work involves the measurement and evaluation of decay data (eg half-lives and gamma-ray emission probabilities) and fission yields; all known UK studies in 1998 are summarised in this document. Applications developments and international links of relevance in the field of nuclear data are also described.

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1. INTRODUCTION

The UK Nuclear Science Forum (UKNSF) is the main body for technical discussions within the UK of the measurement and evaluation of nuclear data (e.g., neutron cross sections, decay data and fission yields). Membership ranges across approximately 20 different organisations, including nuclear plant operators, vendors, regulators, non-energy applications, academia, and various data measurers and evaluators. The Forum also has the support of the UK Department of Trade and Industry and the nuclear-based Industry Management Committee (IMC) to act as the communications network for all matters relating to the NEA Data Bank/Nuclear Science Committee and the IAEA-Nuclear Data Section.

Two meetings of the UKNSF were held in 1998 on 21 May and 19 November (Chairman, A L Nichols (AEA Technology, Harwell) and Secretary, R W Mills (BNFL plc)). UKNSF members have also assisted the NEA-Nuclear Science Committee and the IAEA-Nuclear Data Section during the year to formulate new programmes and define data-file priorities.

2. MEASUREMENTS

2.1 Radionuclide Standardisation and Measurement of Nuclear Decay Data

(contact: S A Woods (Radioactivity Measurement Group, Centre for Ionising Radiation Metrology, National Physical Laboratory, Teddington))

Work has continued on the primary and secondary standardisation of radionuclides identified as being of importance to the UK measurement community, in parallel with studies of selected decay scheme parameters. NPL also provides recommended radionuclide decay data upon demand.

(a) Standardisations of ^{33}P, ^{169}Yb, ^{186}Re, ^{192}Ir, ^{210}Pb, ^{237}Np and ^{241}Am have been completed.

(b) Emission probabilities have been determined for selected gamma-ray transitions following the decay of ^{186}Re.

(c) Standardisations of ^{210}Po, ^{238}Pu, ^{239}Pu and ^{244}Cm are ongoing.

(d) The novel method of Digital Coincidence Counting has continued to be developed; custom built hardware and 32 bit data analysis software for real-time data collection and compression are being implemented and validated.

(e) Measurement techniques have been devised to facilitate the accurate assay of the activity of ^{81m}Kr gas used for medical diagnostic treatments.

Financial support is provided by the National Measurement System Policy Unit of the UK Department of Trade and Industry.

2.2 An Epithermal Neutron Beam for Use in Boron Cancer Therapy

(A Brown, T D Beynon, M C Scott and D R Weaver (University of Birmingham))

Work is underway to produce a well-characterised epithermal neutron beam for use with Boron Cancer Therapy (BCT). Efforts have concentrated on the production of a suitable target for high-power proton beams, and has involved both Computational Fluid Dynamics code modelling and prototype design testing.

Other projects on dosimetry, radiobiology and preparation of a patient treatment facility are in hand. Work is also on-going to upgrade the Dynamitron.

2.3 Fast Fission of ^{238}U

(M A Kellett and D R Weaver (University of Birmingham))

A thesis has been prepared on the findings of a series of measurements using three different samples (9.6g, 24g and 48g) of depleted uranium with a ^{238}U content of 99.7%. The same programme of measurement was also carried out for a sample of highly enriched ^{235}U (99.3% and 40g). Various mono-energetic neutron beams over the ranges 1.4 to 2.0 MeV and 4.2 to 5.7 MeV were used, along with timing cycles involving 20 and 40 second irradiation and count periods.

The results provide further data on the ^{238}U delayed-neutron yield in the energy range up to 5.7 MeV. Sadly the loss of the Gayther fission chambers following their sale to Germany during the course of the project, coupled with the demise of the fission chamber used to normalise the bombarding neutron flux, has meant that the accuracy achieved was not as high as first hoped. However, the results have given some further insight into the variation of the ^{238}U delayed neutron-yield in the MeV region.

2.4 Plutonium Mass Measurements

(L Bourva (AEA Harwell Instruments Ltd) and D R Weaver (University of Birmingham))

Studies at Harwell Instruments Ltd to develop accurate methods for neutron coincidence counting have been applied to plutonium mass measurements. This work has led to the empirical determination of the Pu-240 effective mass coefficients for Pu-238 and Pu-242. A High Efficiency N95 Neutron Coincidence Counter was used to measure samples of high-purity Pu-238, Pu-240 and Pu-242 nuclides. Specific correction factors for the mass and neutron multiplication in each sample were adopted to derive N95-specific Pu-240 effective mass coefficients.

Work has been sponsored by EURATOM Safeguards.

3. DATA LIBRARIES: EVALUATIONS

3.1 Data Library Developments

The status of the UK Decay Data and Fission Yield Libraries is summarised in Table 1. Progress has been maintained in the evaluation of specific decay data (primarily activation and fission products). These studies have been undertaken to assist in the development of the Joint Evaluated Fission and Fusion Files (JEFF).

Activation and Fission Product Decay Data (A L Nichols (AEA Technology, Harwell))

Discussions were initiated in mid-1995 to focus the limited amount of UK evaluation effort on improving the quality of the decay data for a specific number of radionuclides of particular interest to the nuclear industry. Lists of problematic fission-product nuclides were formulated in 1994/95, along with a number of radionuclides of importance in decay-heat calculations for which no decay-scheme data have been measured. Decay-data evaluations have been undertaken from 1996 onwards (Table 2), along with the preparation of theoretical decay-data files for those nuclides lacking quantitative studies.

The decay data files of approximately 50 radionuclides within EAF (European Activation File) were also identified as problematic or incomplete when used for fusion-reactor applications, as shown in Table 3. Approximately 28 other radionuclides have been added to this list for completeness. One aim is to generate the recommended decay data files in ENDF-B6 format for use in JEFF-3.

As outlined above, the decay data for a number of fission- and fusion-based radionuclides have been evaluated during 1998:

^{17}N, ^{93}Rb, ^{94}Rb, ^{95}Rb, ^{114}Ag, ^{114m}Ag, ^{115}Ag, ^{115m}Ag, ^{141}Sb, ^{158}Ce, ^{178m}Hf, ^{178n}Hf, ^{180m}Hf, ^{185}Os, ^{190m}Os, ^{190}Ir, ^{190m}Ir, ^{190n}Ir, ^{199m}Hg, ^{201}Pb and ^{201m}Pb.

Some of these radionuclides have extremely complex decay schemes, and their evaluations have proved to be labour intensive (eg ^{94}Rb and ^{95}Rb). Theoretical decay-data files were also produced for approximately 30 short-lived fission products.

All of these data will be incorporated into UKPADD as highly consistent data files (1). Evaluations will continue in 1999 and 2000 to complete these fission- and fusion-based programmes of work.

Studies funded by British Nuclear Fuels plc and UK Atomic Energy Authority (Fusion Division).

Table 1: UKNSF Decay Data and Fission Yield Libraries - Status Table, December 1998

Data	Present status	File development
Fission product decay data	UKFPDD-2 evaluations (ENDF/B-V format) were submitted for JEF-1.1 and partially included. Some of these evaluations have been carried through to JEF-2.2.	None, but see UKPADD-6 below.
Activation product decay data	UKPADD-6 library (ENDF/B-VI format) has been completed: comprehensive decay-scheme data for 446 activation products and specific fission products have now been evaluated for this library.	Decay data for further sets of radionuclides (mainly activation products) are being evaluated, as agreed through the NEA Data Bank (see Section 3.1).
Heavy element and actinide decay data	UKHEDD-2 evaluations (ENDF/B-VI format) have been submitted and absorbed into JEF-2.2.	UKHEDD-2.2 includes recommended decay data for Pa-234g, Pa-234m and Th-234.
Fission yields	UKFY-2 was submitted and accepted for JEF in 1990. After minor modifications (to achieve consistency with JEF-2.2 decay data and to allow for missing decay data), a final version of UKFY-2 was incorporated into JEF-2.2. A new draft evaluation was produced in 1994 (UKFY-3), maintaining consistency and continuing to allow for missing decay data.	An update is envisaged when JEFF-3 decay data become available (ensuring consistency with JEFF-3 decay data, and including fewer approximations for missing decay data); this updated file will be submitted for inclusion in JEFF-3.

Table 2: Decay-Data Evaluations - Fission Products
Evaluations include related metastable states and daughter radionuclides when deemed appropriate (although not listed below).

Nuclide	Importance	Priority
45-Rh-106	Instrumentation for recycling	high
57-La-140	Fission product standard	high
62-Sm-147	Instrumentation for recycling	high
34-Se-79	Radiotoxicity	high
40-Zr-93	Radiotoxicity	high
50-Sn-126	Radiotoxicity	high
51-Sb-127	Reprocessing	medium
53-I-132	Reprocessing	medium
52-Te-132	Reprocessing	medium
53-I-138	Reprocessing/Delayed neutron emission	medium
59-Pr-143	Reprocessing	medium
59-Pr-144	Reprocessing	medium
65-Tb-161	Reprocessing	medium
35-Br-88	Delayed neutron emission	medium
35-Br-89	Delayed neutron emission	medium
35-Br-90	Delayed neutron emission	medium
37-Rb-94	Delayed neutron emission	medium
39-Y-98m	Delayed neutron emission	medium
53-I-137	Delayed neutron emission	medium
39-Y-99	Delayed neutron emission	low
51-Sb-135	Delayed neutron emission	low
53-I-139	Delayed neutron emission	low
35-Br-87*	Delayed neutron emission	low
35-Br-91	Delayed neutron emission	low
37-Rb-95	Delayed neutron emission	low
37-Rb-93	Delayed neutron emission	low
33-As-85	Delayed neutron emission	low

*Still undergoing evaluation (1999).

Table 3: Decay-Data Evaluations - Fusion Activation Products

Nuclide	Nuclide	Nuclide
7-N-17	(49-In-112m)	(76-Os-190m)
(25-Mn-58)	56-Ba-129	(76-Os-191m)
25-Mn-58m*	56-Ba-129m*	76-Os-195*
31-Ga-77#	58-Ce-147	77-Ir-187#
33-As-82#	59-Pr-143	(77-Ir-190)
(33-As-82m)#	59-Pr-144	(77-Ir-190m)
34-Se-79*	(59-Pr-144m)	77-Ir-190n
34-Se-79m	59-Pr-150	(77-Ir-191m)#
38-Sr-87m	(61-Pm-152)	77-Ir-191n**#
39-Y-96*	(61-Pm-152m)	(77-Ir-192)#
(39-Y-96m)	61-Pm-152n*	77-Ir-192m#
(39-Y-96n)(?)	(65-Tb-156)	(77-Ir-192n)#
41-Nb-100	65-Tb-156m*	77-Ir-197#
(41-Nb-100m)	65-Tb-156n*	77-Ir-197m**#
43-Tc-97*	67-Ho-160**	78-Pt-193*
43-Tc-97m	67-Ho-160m	(78-Pt-193m)
46-Pd-109	67-Ho-160n**	(78-Pt-197)#
(46-Pd-109m)	67-Ho-161	(78-Pt-197m)#
46-Pd-112	(67-Ho-161m)	(79-Au-192)#
(47-Ag-107m)	(67-Ho-170)#	79-Au-192m#
(47-Ag109m)	67-Ho-170m#	(79-Au-197m)#
(47-Ag-114)	72-Hf-178m	80-Hg-199m
47-Ag-114m*	72-Hf-178n	(82-Pb-201)
(47-Ag-115)	72-Hf-180m	82-Pb-201m*
47-Ag-115m*	75-Re-191*	83-Bi-208*
48-Cd-107	75-Re-192*	84-Po-208*
49-In-112	76-Os-185	

* No gamma lines in EAF/JEF library.
** No EAF/JEF data file.
# Still to be evaluated.
Nuclides in parenthesis have not been requested, but are included for completeness.

3.2 Nuclear Data Project Team Competencies (S Franklin and S I Kafala (Imperial College), T D McMahon (DNST HMS Sultan, Gosport) and M C Moxon (Consultant))

While changes have taken place in the past year, the expertise and experience of the radionuclide metrology group at Imperial College has been maintained. The contract in place for 1997/98 from the IMC helped to develop the core-competency of the group, and saw the evaluation of the total, capture, elastic and inelastic scattering cross sections of ^{152}Sm over the incident neutron energy range of 10^{-5} eV to 2 MeV (2). Although the team is not currently together, the competencies are maintained, and the group can reassemble when required. Data evaluation is expected to play a more important role at Imperial College and DNST in future years.

The group has access to all the appropriate data sources, and to the Imperial College research reactor for cross-section experimental measurements across the water reactor spectrum.

3.3 Decay Data and Neutron Cross-Section Evaluations (T D MacMahon (Department of Nuclear Science and Technology, HMS Sultan, Gosport))

International Decay Data Evaluation Project: Participation has continued with collaborators at AEA Technology (UK), Idaho Falls, Brookhaven National Laboratory and Lawrence Berkeley Laboratory (USA), LPRI(France), PTB (Germany), CIEMAT (Spain) and Khlopin Radium Institute (Russia) to provide evaluated decay scheme data for the following:

(a) ENDSF,
(b) new Table of Radionuclides by LRPI/PTB,
(c) IAEA decay database.

3.4 Evaluation of Thermal and Low Energy Resonance Capture Cross Sections (S P Fox and D L Watson (Physics Department, University of York))

Thermal capture cross-sections and the resolved resonance parameters in the energy region up to approximately 150 eV are being evaluated for ^{95}Mo, ^{103}Rh, ^{109}Ag, ^{143}Nd and ^{145}Nd. The results of the new evaluation will be compared with the previous evaluations in BROND-2.2, EAF-97A, EFF-2.4, ENDF/B-VI.4, JEF-2.2, JENDL-3.2 and Mughabghab.

The evaluation is being carried out on behalf of the IMC.

3.5 JEFF-X (R W Mills (BNFL plc, Sellafield))

JEF-X is a graphical interface to the JEF2.2 evaluated file for use on X-windows-based workstations, which emulates and extends the functionality of JEF-PC. The code was developed by Ryan Evans under FORTRAN-77 using GKS graphics subroutines. The code ran originally under the SUNOS 4.1.X operating system on SUN workstations, but has now been ported and tested on Solaris 2.5 SUN workstations.

3.6 Fission Product Yield Evaluation (D J Hale and D R Weaver (University of Birmingham), and R W Mills (BNFL plc, Sellafield))

A PhD studentship on fission product yields at the University of Birmingham has been completed, defended and approved; the thesis by Darren Hale will be made available in 1999. These studies involved looking at different models, and the effects of the fissioning system and neutron energy upon the model parameters.

The UK group has continued international collaboration with colleagues in the USA, China, France, Germany, Japan, Netherlands, Russia and Sweden, through the forum of the IAEA-CRP on Fission Product Yield Data Required for Transmutation of Minor Actinide Nuclear Waste.

This work is being carried out with financial support from British Nuclear Fuels Ltd Research and Technology Nuclear Data Development Programme.

3.7 JEF-PC: A PC-computer Based Program to Display Data from the JEF-2.2 Library (D R Weaver (University of Birmingham) and M Konieczny (NEA Data Bank))

Version 2 of JEF-PC has been on sale during 1998, and 137 copies were sold (including a number of multiple-user licences). Discussions have taken place with a view to further developments of JEF-PC, but so far these have not been implemented. It is anticipated that any further evolution of the package may well involve a Windows or Internet format.

4. APPLICATIONS DEVELOPMENT

4.1 Reactor Physics, Shielding and Criticality Applications (N R Smith (AEA Technology, Winfrith))

JEF-2.2 data libraries are now used by the nuclear industry for reactor physics (WIMS), criticality (MONK), shielding (MCBEND) and inventory (FISPIN) applications. In some areas, the new libraries are being used in parallel with their predecessors whilst experience is built-up; in other areas, the libraries are increasingly used as the data of first choice due to the improved performance observed in benchmark studies. At a recent meeting of the Working Party on Criticality (WPC), agreement was reached that either the UKNDL or JEF-2.2-based library was acceptable for assessment purposes (subject to suitable evidence of validation being available).

Recent work has focused on investigating key radionuclides where changes are being proposed for the JEFF-3 library. A JEFF-3 'starter file' is being assembled (JEFF-3T) which includes significantly updated evaluations (from JEF-2.2) for ^{235}U and Fe (amongst others). An IMC funded project has included benchmark studies using the JEFF-3T ^{235}U file for a range of criticality cases (AEAT-3981 - available through IMC).

The main conclusions were:

(a) JEFF-3T ^{235}U evaluation produces improved results compared with JEF-2.2 for both MONK(DICE) and MONK(WIMS) calculations of the harder spectrum systems analysed.
(b) Agreement between calculation and experiment for the JEFF-3T data is similar to that for JEF2.2 data over a small range of uranium solution experiments.
(c) Agreement for the traditionally more reliable lattice cases is generally worse than JEF-2.2, with significant under-predictions being observed for JEFF-3T calculations. Based on the experiments studied, this observation suggests that further evaluation activity is required before a file providing comprehensive improvements over JEF-2.2 can be made available.

JEFF-3T contains revised evaluations for Fe which take account of recent measurements at Geel. A programme of work is currently underway to evaluate the effects of the new data on shielding benchmark experiments.

Further JEF-2.2 benchmarking activity has taken place using MONK (joint AEA Technology/BNFL project), drawing on experiments from the OECD International Criticality Safety Benchmark Evaluation Project (ICSBEP). Studies have included:

(a) uranium oxide lattices - up to 10% ^{235}U enrichments, with some cases (~5% enrichment) including hafnium reflection,
(b) mixed oxide lattices - various Pu contents,
(c) low-enriched uranium solutions,
(d) uranium metal plate assemblies (water moderated) and uranium metal/polythene plates.

Further validation data have been produced as part of an HSE-funded project to support FISPIN for PWR fuel with Integral Gadolinia Poisoning.

4.2 Extensions to Product Data Libraries (C J Dean (AEA Technology, Winfrith))

A review of the WIMS JEF-2.2-based nuclear data library was held early in the year, and this led to an IMC project to enhance the library so that the contents included all relevant items from the 1986 library. The additions covered:

(a) Neutron group cross sections (at 293.16K) for the following nuclides, without burn-up or resonance shielding: ^{3}He, ^{4}He, ^{6}Li, F and natural Kr mixed from the six-component isotopes.
(b) Data for Mg and Cd (eight isotopes mixed to form the element) extended from 293.16 to 600 and 900K.
(c) Data for ^{107}Ag and ^{109}Ag extended from 293.16 to 600 and 900K.
(d) New data for In (^{113}In and ^{115}In combined by natural abundance) generated at 293.16, 600 and 900K.
(e) Response functions (absorption only) for $^{54}Fe(n,p)^{54}Mn$, $^{58}Fe(n,\gamma)^{59}Fe$,^{103}Rh (n,n') ^{103m}Rh and ^{176}Lu $(n,\gamma)^{177(g+m)}Lu$.
(f) Resonance shielding added for Co (as ^{59}Co) so that significant quantities found in magnets can be modelled.

(g) New data for ^{121}Sb and ^{123}Sb generated to model Sb-Be sources.
(h) New data with full burn-up added for Er, and data generated from BROND-2.2 as recommended for JEFF-3.0.
(i) A negative 1/V absorber included to allow steel measurements in Gleep to be studied.

Further work has also been performed (AEA Technology/BNFL) to add H in ZrH and Zr in ZrH data to both the MONK/MCBEND and WIMS data libraries and provide better modelling of TRIGA reactors.

5. INTERNATIONAL COOPERATION

5.1 European Activation File Development (R A Forrest and J-Ch Sublet (UKAEA, Culham))

Staff at UKAEA Fusion have continued the development of the European Activation File (EAF) under the Nuclear Data Programme of the Euratom Fusion Technology Programme. EAF covers the neutron induced cross sections and decay data libraries that are required as input to the inventory code FISPACT.

During the last year the new version of the EAF library and the FISPACT inventory code have been completed. The new version (EAF-99 and FISPACT-99) is fully documented (3-6) and is being distributed to users. Most of the effort in this program has been put into improving the neutron-induced cross sections in EAF-99, and about 750 reactions have been significantly changed. Details of the improvements are:

(a) New and improved systematic formulae are used for renormalisation.
(b) Data from newly available sources are used.
(c) A major validation exercise has been undertaken using data from EXFOR and several integral experiments (at European and Japanese laboratories (7)).
(d) Uncertainty data have been significantly extended and improved; results from the validation exercise, in conjunction with other sources of information and measurements, enabled the data for some important reactions to be improved.
(e) Use of an additional multi-group library (315 energy groups).
(f) Ability to use data relating to the clearance from regulatory control of activated material and to make calculations using these data.
(g) Changes to ensure year 2000 compliance (to ensure that the FISPACT code continues to work as expected once year 2000 is reached).
(h) Construction of an improved version of the EAF decay data library. New evaluations performed by Backhouse and Nichols (1) have been used for about 50 nuclides.

The EAF-99 cross-section data libraries (pointwise and groupwise) and the uncertainty file are available through OECD/NEA and RSICC.

5.2 JEFF Programme (C J Dean (AEA Technology, Winfrith), A L Nichols (AEA Technology, Harwell), D J Edens (BNFL Magnox, Berkeley), R A Forrest (UKAEA, Culham) and R W Mills (BNFL plc, Sellafield))

UK specialists continue to contribute to a number of OECD/NEA and IAEA programmes involving nuclear data development, particularly those undertaken as part of the JEFF Project.

(a) General Purpose Cross Section Library

Consolidation of benchmarking experience using JEF-2.2 resulted in UK contributions to three draft papers in the area of reactor physics (Rowlands), shielding (Avery) and criticality (Smith). These reviews assess the ability of JEF-2.2 to predict physics parameters and include indications of possible data improvements. A more formal data adjustment study has taken place in France, with some sensitivity input from Winfrith in the area of reactor shielding. A CEA draft paper by Fort is being studied, with the intention of forming a consistent overall indication of the quality of JEF-2.2 (Fort's work predicts potential cross section trends in 15 broad energy regions).

Definition of the content of the starter file for JEFF-3T has now been specified and agreed. Despite the initial aim of taking most data from EFF-3.0 and JEF-2.2, there are a fairly large number of evaluations taken from improved sources (mainly due to developments in other libraries where JEF-2.2 adopted earlier evaluations from the same generic source, eg. new JENDL-3.2 files become available for a JEF-2.2 evaluation based on JENDL-2). Assembly of JEFF-3T has run into two problems during 1998: staff changes at the NEA resulted in slow progress, and improved QA standards showed numerous problems in the existing files (such impacts need to be individually assessed as either important or trivial). NEA has injected extra staff, and is now coping well. The QA procedure includes generation of data in the 15 energy groups used in the JEF-2.2 assessment of Fort, which allows the project to review data trends at an early stage. Major aims are to make the files available for most clean-core benchmarking by September 1999, followed by the rest of the library before the end of the year. As noted elsewhere, the UK has been involved in testing the proposed ^{235}U and Fe evaluations as part of a policy of limited involvement where JEF-2.2 based libraries may need to be enhanced (see Section 4.1).

UK evaluators have assessed the quality of the data for a number of nuclides and made their results available to the JEFF programme. These studies include a number of fission products seen as important to specific aspects of the thermal reactor fuel cycle. Absorption of the results into JEFF-3 has proved difficult due to the lack of complete ENDF-B6 evaluations. UK industry is now sponsoring work leading to possible replacement evaluations in the thermal and resolved resonance regions where this exercise is judged to be worthwhile. The aim is to make avalable new files for ~10 fission products in 2000; when replacement thermal files are needed, they will be added to files recommended for fast reactor studies.

(b) Other JEFF-3 Libraries

UK contributions to decay data and fission yield evaluations are described elsewhere in this report (Sections 3.1 and 3.6). UK decay data libraries are normally issued each year, with UKPADD-6 expected to be available at the end of May 1999. The library includes

files from previous UKPADD releases and new files where appropriate. Although the quality procedures for assembly of JEFF-3 decay evaluations are yet to be fixed, data from this library are likely to be adopted for JEFF-3. A consistent energy balance is considered important, and the development of a code to perform this function is being considered.

The European Activation File has been developed for fusion studies, and has been adopted as the activation file for JEFF-3. Consistency of data for reactions common to this and the main JEFF-3 library is being sought.

Acknowledgement

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