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REPORT

United Kingdom Nuclear Science Forum

Progress Report

Data Studies During 2001 and 2002

Edited by T.D. MacMahon

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NPL 
National Physical Laboratory

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Centre for Acoustics and Ionising Radiation
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ABSTRACT

The United Kingdom Nuclear Science Forum (UKNSF) meets once per year to discuss items and issues of direct relevance and importance to forum members, and to review nuclear data for applications in the UK nuclear industry. Links are maintained throughout the year, mainly through e-mail, the postal system and the UKNSF website: (www.npl.co.uk/uknsf). Work of primary interest includes the measurement and evaluation of decay data (e.g. half-lives and gamma ray emission probabilities), fission yields and neutron cross sections. All known studies within the UK are summarised in this report. Specific applications and international links of relevance are also described.

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Approved on behalf of the Managing Director, NPL
by Dr. M. Sené, Head, Centre for Acoustics and Ionising Radiation.

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1. Introduction

The United Kingdom Nuclear Science Forum (UKNSF) provides an appropriate means of encouraging technical discussions of the measurement and evaluation of nuclear data. Membership ranges across approximately 30 UK organisations. The Forum has the support of the Health & Safety Executive (Nuclear Installations Inspectorate), and acts as the communication network for matters relating to the NEA Data Bank and the IAEA Nuclear Data Section.

The 2001 meeting of the UKNSF was held at Harwell on 3rd May (Chairman, A.L. Nichols, AEA Technology, Future Technologies, Harwell; Secretary, R.J. Perry, Serco Assurance, Winfrith).

The 2002 meeting was held at BNFL London Office on 25th June (Chairman, S.M. Judge, NPL; Secretary, R.J. Perry, Serco Assurance, Winfrith).

UKNSF members have assisted the NEA Nuclear Science Committee and the IAEA Nuclear Data Section during these two years to formulate and progress programmes of work and define data file priorities.

A.L. Nichols relinquished his position as chairman of the UKNSF at the end of September 2001, after being appointed Section Head of the IAEA Nuclear Data Section, Department of Nuclear Sciences and Applications, Vienna, Austria.

The Radionuclide Metrology Group at the National Physical Laboratory now provides the secretariat for the UKNSF, and the Forum is chaired by R.A. Forrest, UKAEA Fusion, Culham.

2. Measurements

2.1 Insights into the Neutronics of Moderating Materials in a Fast Spectrum Reactor

P. Morris (BNFL/CEA, Cadarache), D.R. Weaver (University of Birmingham) and G. R. Rimpault (CEA, Cadarache)

In support of higher actinide and fission product (nuclear waste) transmutation studies, a number of critical experiments have been performed in the MASURCA fast spectrum test reactor at the Cadarache Nuclear Research Centre, France. These experiments were designed to investigate the neutronic characteristics of fast reactor cores containing various localised neutron moderator materials including boron carbide and zirconium/calcium hydrides. Analysis of these experiments, for the purpose of code validation and the investigation of unforeseen physics phenomena, has been progressing since September 1999, using a combination of deterministic and Monte-Carlo methods and data.

Recently, some notable discrepancies were found, between deterministic calculation and experiment, within the moderated target region of the hydride moderated cores. These discrepancies were thought to originate from an inadequate treatment of thermal neutron incoherent scattering from bound hydrogen by the deterministic scheme. In order to confirm this hypothesis, Monte Carlo (MCNP) calculations were performed utilising both the elastic and inelastic components of the incoherent scattering cross section. These calculations proved conclusive for the ZrH_2 case, and the effect was quantified with a significant reduction in (C-E)/E type discrepancies.

No such scattering data was found to be available for CaH_2 and a neutron scattering experiment was performed at ILL, Grenoble to enable the generation of such data. A subsequent analysis of the CaH_2 moderated core under review has concluded that the same incoherent scattering effects are not as strong for the CaH_2 case and discrepancies between calculation and experiment are not significantly reduced by the use of the correct low energy scattering data. Relatively close agreement between Monte Carlo and deterministic codes when using the same data suggest that the residual discrepancies are possibly due to experimental (or systematic) errors in measurement.

2.2 Nuclear Materials Assay

P M Keates, D R Weaver (University of Birmingham), and S Holloway (AWE)

Quality assurance objectives, associated with the non-destructive assay and sentencing of radioactive wastes containing fissile material, require a detailed understanding and assessment of the total measurement uncertainty. The assay techniques employed to measure such wastes, which primarily detect and analyse both passive and induced neutron and gamma-ray signatures, can be modelled with a variety of simulation (e.g., Monte-Carlo based) computational tools.

AWE is sponsoring a programme of work to utilise and develop such tools to aid in understanding the performance of a variety of neutron and gamma-ray based waste assay systems through a rigorous assessment of the total measurement uncertainty. Such waste

assay systems are an integral part of the overall AWE waste management strategy. This work will also directly benefit another AWE programme, initiated by the UK 1998 Strategic Defence Review, which seeks to examine the verification role of radiometric non-destructive assay technologies in establishing the effectiveness of any future nuclear weapon arms control agreements.

Work has progressed from the initial scoping calculations to simulating the response of generic passive/active neutron assay systems. In addition, preliminary experimental work has commenced to determine the feasibility of employing detector-detector cross (time) correlation signatures to establish the location of fissile material within (say) a waste drum. Such information is of relevance to minimising the geometrical component of measurement uncertainty.

2.3 Radioactivity Metrology and Radionuclide Decay Data

Radioactivity Metrology Group, Centre for Acoustics and Ionising Radiation, National Physical Laboratory, Teddington, Middlesex.

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 ^{60}Co , ^{89}Sr and ^{152}Eu have been completed.
- (b) Standardisations of ^{238}Pu and ^{241}Am are ongoing. An international collaboration, to investigate the problems with the standardisation of ^{204}Tl , under the auspices of BIPM continues.
- (c) The method of Digital Coincidence Counting is being extended to facilitate its use with atmospheric proportional counters.
- (d) Measurement of the alpha emission probabilities for ^{235}U has commenced (EUROMET Project 591).
- (e) The new Triple-to-Double Coincidence Ratio Liquid Scintillation counting system has been validated against existing standardisation methods for ^3H .
- (f) As part of an IAEA-CRP to provide internationally recommended radionuclide decay data, evaluations of the decay schemes of ^{56}Co , ^{85}Kr , ^{94}Nb , ^{103}Ru and $^{106}\text{Ru}/^{106}\text{Rh}$ are on-going.

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

3. Calculations

3.1 Safety and Environmental Assessment of Fusion Power Plant Conceptual Designs

R. Pampin-Garcia, D R Weaver (University of Birmingham) and N Taylor (UKAEA-Culham).

The conceptual design and performance analysis of fusion power plants is intended to provide insight on fusion physics and technology issues, and contributes to the optimisation of the design and material choices for future fusion power plants.

Under the European Power Plant Conceptual Study (PPCS) framework, four of these conceptual designs have been analysed, ranging from the very conservative (assuming only modest physics and technology extrapolations), to the more advanced and futuristic. The tasks performed at UKAEA-Culham include: (a) the estimation of the radioactive waste expected to be generated during the operation and decommissioning of the plant; and (b) a conservative evaluation of the worst consequences (doses to public) that could be derived following a postulated failure in the device leading to a release of activated material.

Detailed calculations of neutron spectra in all plant structures using Monte Carlo methods have been conducted, and an inventory code used to estimate the amount and characteristics of the neutron induced radioactivity. Finally, a FE analysis code helps in the evaluation of the decay heat driven thermal transient, following the worst hypothetical loss of coolant accident coupled to a confinement breach. Results have been presented throughout the last year, and a final overall report is expected by the end of 2003. They show that temperature excursions and doses to public are well within structural and regulatory limits, even for this bounding scenario, and that no radioactive waste would require permanent disposal 100 years after plant shutdown.

Work will follow on the detailed neutron transport and activation analysis of the divertor, a key component regarding plant performance and economic efficiency, which has shown only marginally acceptable activation and thermal behaviour.

4. Data Libraries: Evaluations

4.1 European Activation File development

RA Forrest (UKAEA-Culham)

The Euratom/UKAEA Fusion Association has continued the development of the European Activation File (EAF) under the Nuclear Data Task of the EFDA Fusion Technology Programme. EAF covers the neutron-induced cross sections and decay data libraries that are required as input to the FISPACT inventory code.

4.1.1 2001

During 2000 the development of the SAFEPQAQ-II application was completed. SAFEPQAQ-II is used to evaluate, select and process the activation cross section data, and has been installed at both JUKO Research (The Netherlands) and CEA Cadarache for use in the production and

testing of EAF-2001. An initial version of EAF-2001 has been prepared and will be released as part of EASY-2001 after testing in 2001.

EAF-2001 contains new data evaluations (Ni-58, Ni-60, Be-9) and new model calculations for 35 capture reactions. A great deal of the development work has involved the use of new experimental data (now held in the SAFEPAQ-II relational databases) for branching and renormalising the reactions. Existing integral data can be used by SAFEPAQ-II for adjustment. There are a total of 12,470 reactions and these are available in both point-wise and multi-group format.

EAF-2001 also benefits from the ongoing decay data evaluations carried out by Nichols [1]. It should be noted that SAFEPAQ-II enables consistency between the various EAF files, thus the nuclide spins in the decay data library are automatically used as required when constructing the cross section library.

Following the production of the documentation, EASY-2001 will be released during the first quarter of 2001 for testing and validation.

4.1.2 2002

The final version of EAF-2001 has been released as part of EASY-2001 following testing. A major activity during 2001 has involved the validation of EAF-2001 using the experimental measurements made by three European Groups over the last few years. The results are presented in a comprehensive report [2]; in summary sixty-five reactions are considered, with 35 validated (agreement between experiment and calculations are within the uncertainties) and 25 recommended to be improved for EAF-2003.

Work has continued on collecting new experimental data and evaluations. New features have been added to SAFEPAQ-II (application used to produce the EAF libraries). These are being used in the development phase of EAF-2003 that is expected to be available at the beginning of 2003. EAF-2003 will also benefit from the ongoing decay data evaluations carried out by Nichols.

Preliminary work of the extension of energy of the EAF libraries to 55 MeV has begun. These higher energies are required for design calculations on IFMIF, a proposed materials testing facility.

4.2 Data Library Developments

A. L. Nichols (AEA Technology, Harwell; now with IAEA Nuclear Data Section)

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

Table 1: UKNSF Decay Data and Fission Yield Libraries – Status Table, December 2001.

Data	Current status	File development
Fission product decay data	UKFPDD-2 evaluations were submitted for JEF-2.2 and partially included.	None, but see UKPADD-6.3, below.
Activation product decay data	UKPADD-6.3 library has become the officially released version, containing comprehensive decay-scheme data for 474 activation products and selected fission products.	Decay data for further 24 radionuclides have been evaluated (mainly activation products), as agreed within the EAF Fusion programme (see Section 4.2.1).
Heavy element and actinide decay data	Decay data have been re-evaluated for the Th-228 decay chain, U-235, U-235m, U-238, Pu-239, Pu-241, Am-241, Cm-242 and Cm-244.	Decay data for the selected actinides and some of their decay products will be introduced into UKHEDD and JEFF-3 (see Section 4.2.2).
Fission yields	UKFY2 has been incorporated into JEF-2.2. A new evaluation was completed in December 2001 (UKFY3.4).	UKFY3.4 fission yield library will be submitted for inclusion in JEFF-3.

4.2.1 Activation and Fission Product Decay Data

An extensive exercise was initiated in 1999/2000 to assess the contents of the decay-data files for approximately 180 radionuclides within EAF-99 [3]. The aim was to produce a comprehensive list of nuclides that require more detailed evaluations of their discrete decay data. These studies revealed evidence for discrepant and erroneous decay data within EAF [4]. Three forms of recommendation were given: no further action; undertake a new evaluation; adopt existing decay-data evaluations from other sources. A rigorous, computer-based test procedure was also recommended to determine the consistency and completeness of any decay-data library. Radionuclides with inadequate decay-data files were evaluated in 2001 (see Table 2), as part of an improvement project funded through UKAEA Fusion by the UK Department of Trade and Industry, and Euratom.

As listed in Table 2, the recommended decay data exhibit good consistency when Q-values and branching fraction data are compared with the discrete emission data. Note that Ho-163 has a particularly small Q-value of only 2.650(28) keV which mitigates against the prescribed calculation of consistency within the UK processing code (COGEND) – recommended decay data for Ho-163 exhibit closer absolute agreement than implied by the % Deviation. These decay-data files have been assembled in ENDF-6 format for insertion into the Joint Evaluated Fission and Fusion library (JEFF-3) of the NEA-OECD.

Studies have been funded by the UK Atomic Energy Authority (Fusion Division).

Table 2: Decay Data of Activation Products Evaluated in 2001 – Consistency of Recommended Data.

Radionuclide	Evaluated Half-life	Consistency (% Deviation)
17-Cl-36	$3.07(3) \times 10^5$ y	0.0001
28-Ni-67	21(1) s	0.0093
34-Se-79	$1.12(12) \times 10^6$ y	0.0000
(34-Se-79m)	3.90(2) min	-0.0743
37-Rb-89	15.4(2) min	-0.0750
38-Sr-92	2.71(1) h	-0.0061
42-Mo-103	67.9(6) s	-0.0096
50-Sn-126	$2.42(14) \times 10^5$ y	0.0675
(51-Sb-126)	12.41(5) d	-0.0635
(51-Sb-126m)	19.1(2) min	-0.1708
(51-Sb-126n)	11(2) s	-0.5031
(52-Te-121)	19.16(5) d	0.0226
52-Te-121m	154(7) d	-0.1799
56-Ba-126	100(2) min	-0.1958
57-La-137	$6(2) \times 10^4$ y	0.0353
58-Ce-145	2.95(6) min	0.1188
67-Ho-163	4570(21) y	10.5087
(67-Ho-163m)	1.10(7) s	0.0373
68-Er-172	49.3(3) h	0.2611
79-Au-199	3.139(7) d	-0.0640
80-Hg-190	20.0(4) min	0.5330
80-Hg-205	5.2(1) min	-0.0431
81-Tl-193	21.8(7) min	-0.0502
(81-Tl-193m)	2.11(15) min	-0.0042

Radionuclides in parentheses have not been specifically requested, but their decay data have been evaluated because they are either related ground/metastable states or short-lived daughter nuclides.

Uncertainties in the half-life data are listed in the format 12.34(56), which represents 12.34 ± 0.56 ; these uncertainties are expressed at the 1σ confidence level.

4.2.2 Heavy Element and Actinide Decay Data

The decay data for an agreed set of actinides and some of their decay products have been evaluated (Table 3). This list of nuclides arose from a knowledge and assessment of decay-data measurements published over recent years (from mid-1980s onwards). Full decay-scheme evaluations have been completed, and the resulting data will be incorporated into UKHEDD-2.3.

Studies have been funded by British Nuclear Fuels (BNF plc), Sellafield.

Table 3: Evaluated Heavy Element and Actinide Decay Data – Consistency of Recommended Data.

Radionuclide	Consistency (% Deviation)
88-Ra-226 decay chain	references accumulated
90-Th-228	evaluated, awaiting data processing
88-Ra-224	evaluated, awaiting data processing
86-Rn-220	evaluated, awaiting data processing
84-Po-216	evaluated, awaiting data processing
84-Po-212	evaluated, awaiting data processing
83-Bi-212	evaluated, awaiting data processing
83-Bi-212m [†]	evaluated, awaiting data processing
82-Pb-212	evaluated, awaiting data processing
81-Tl-208	evaluated, awaiting data processing
92-U-235	-0.0040
92-U-235m	evaluated, awaiting data processing
92-U-236	-0.2605
92-U-238	-0.0051
93-Np-237	awaiting data publications
94-Pu-236	-0.0047
94-Pu-239	evaluated, awaiting data processing
94-Pu-241	evaluated, awaiting data processing
95-Am-241	0.2443
95-Am-242	0.0329
95-Am-242m	-0.5520
96-Cm-242	-0.0394
96-Cm-244	-0.0319

[†] evaluation of decay data for 83-Bi-212m impacts on recommended decay-data files for 84-Po-212m and 84-Po-212n (elimination of one of these proposed metastable states).

4.3 Fission Product Yield Evaluation

R. W. Mills (BNFL plc, Sellafield)

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

4.3.1 2001

During the year the collaboration concentrated on the analysis of data including high energy (>10 MeV) neutron and proton induced fission yield data to develop energy dependent models to estimate neutron and proton induced fission yield distributions.

Work on the Fission Product Yield Evaluation for JEFF-3 continued with the update of the UKFY3 experimental data in line with the review carried out in 2000. A draft version of the UKFY3 evaluated file was produced using the JEFF-3.T2 decay data file to calculate the cumulative yields and their uncertainties.

4.3.2 2002

During the year the collaboration concentrated on a set of benchmarks to compare the different empirical and theoretic models developed by the participants.

In March a fission product yield library, UKFY3.4, was submitted to JEFF-3. This used the draft JEFF3 decay data file, JEFF-3.T2, to produce cumulative yields.

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