

NPL REPORT
DQL-RN 014
UKNSF(2006)P198
INDC(UK)-0090 Distr. G

**United Kingdom Nuclear
Science Forum**
Progress Report
**Data Studies During 2003
and 2004**

Edited by N P Hawkes

NOT RESTRICTED

MARCH 2006

United Kingdom Nuclear Science Forum

Progress Report

Data Studies During 2003 and 2004

Edited by N P Hawkes
Quality of Life Division

ABSTRACT

The United Kingdom Nuclear Science Forum (UKNSF) meets once per year to discuss items and issues of 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 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.

© Crown copyright 2006
Reproduced with the permission of the Controller of HMSO
and Queen's Printer for Scotland

ISSN 1740-0953

National Physical Laboratory
Hampton Road, Teddington, Middlesex, TW11 0LW

Extracts from this report may be reproduced provided the source is acknowledged and
the extract is not taken out of context.

Approved on behalf of the Managing Director, NPL
by Dr David Thomas, Head, Neutron Metrology Group

Contents

1	Introduction.....	1
2	Measurements	2
2.1	Insights into the Neutronics of Moderating Materials placed in a Fast Spectrum Reactor for the Transmutation of High Level Nuclear Waste.....	2
2.2	Nuclear Materials Assay	2
2.3	Radioactivity Metrology and Radionuclide Decay Data	3
2.3.1	<i>Validation and Demonstration of Equivalence for Measurement Standards</i>	<i>3</i>
2.3.2	<i>Primary Radioactivity Standardisations.....</i>	<i>4</i>
2.3.3	<i>Acknowledgement</i>	<i>4</i>
3	Calculations	5
3.1	Safety and Environmental Assessment of Fusion Power Plant Conceptual Designs.....	5
4	Nuclear Data Libraries and Data Evaluations.....	6
4.1	European Activation File development during 2003.....	6
4.2	European Activation File development during 2004.....	6
4.3	Fission Product yield evaluations, 2003 - 2004.....	7
4.4	Nuclear decay data evaluations.....	7
5	References.....	9
6	Acknowledgement.....	9

1 Introduction

The United Kingdom Nuclear Science Forum (UKNSF) encourages 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 2003 meeting of the UKNSF was held at BNFL London Offices on 21st May (Chairman, R Forrest, UKAEA, Culham; Acting Secretary, T D MacMahon, NPL).

The 2004 meeting was held at HSE London Office, Rose Court on 3rd June (Chairman, R Forrest, UKAEA, Culham; Secretary, T D MacMahon, NPL).

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.

The Radioactivity and Neutrons Team 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 placed in a Fast Spectrum Reactor for the Transmutation of High Level Nuclear Waste

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, using a combination of deterministic and Monte-Carlo methods and data, has been performed between September 1999 and September 2002.

Driving this work was the fact that some notable discrepancies were been found between deterministic calculation and experimental results 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, Monte Carlo (MCNP) calculations were performed utilising both the elastic and inelastic components of the incoherent scattering cross section. These calculations proved conclusively that for the ZrH_2 case the inclusion of the incoherent elastic component of the total scattering cross-section has a significant effect on the calculated reaction rates within the moderated target for isotopes with large, low-lying fission resonances, such as ^{239}Pu and ^{241}Am . This effect was quantified with a significant reduction in (C-E)/E type discrepancies for cores containing ZrH_2 moderator.

No multi-component thermal scattering data were found to be available for CaH_2 and a neutron scattering experiment [1] was performed at ILL, Grenoble to enable the generation of such data. A subsequent analysis of the CaH_2 moderated core under review using this new data has revealed that the same incoherent elastic 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 seem to provide evidence that the residual discrepancies found are likely due to experimental (or systematic) errors in the measurements themselves.

2.2 Nuclear Materials Assay

P M Keates and 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's 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.

A Thesis for submission for the Degree of PhD is in preparation.

2.3 Radioactivity Metrology and Radionuclide Decay Data

Radioactivity Metrology Group, Quality of Life Division, National Physical Laboratory

2.3.1 *Validation and Demonstration of Equivalence for Measurement Standards*

An extensive programme of measurements took place over the two years to demonstrate equivalence with other National Measurement Institutes as required under the International Mutual Recognition Arrangement. NPL has participated in eight BIPM Key Comparisons (^{241}Am , ^{125}I , ^{192}Ir , ^{54}Mn , ^{32}P , ^{204}Tl , ^{90}Y and ^{65}Zn). Reports of all BIPM comparisons can be found on their website <http://www.bipm.org/en/scientific/ionizing/>.

NPL played a leading role in two international comparisons; ^{18}F and ^{241}Am . The ^{241}Am comparison exercise was organised on behalf of the BIPM (see above). A solution of ^{241}Am was standardised and samples distributed to twenty laboratories. NPL also organised a comparison exercise for ^{18}F (a short lived positron emitting nuclide used for PET) where eleven laboratories worldwide took part. The participating laboratories standardised ^{18}F and compared the measured activity to the known activity of a long-lived ^{68}Ge check source.

NPL has also submitted samples to the BIPM SIR (international reference system): ^{18}F , ^{103}Ru and ^{51}Cr . The ^{18}F submission merits highlighting: in addition to demonstrating the equivalence of UK standards, the exercise links in standards from the other countries that participated in the successful comparison exercise organised by NPL.

2.3.2 *Primary Radioactivity Standardisations*

The provision of new standards of radioactivity in response to new developments in medical procedures and changing emphasis within the environmental measurement and radiochemical analysis user communities is an essential part of the National Measurement System.

This project provided new standardisations or primary measurements for radionuclides of interest in the medical, environmental and low-level fields of measurement and for use as yield tracers in radiochemical analysis. The actual standardisations carried out were decided in consultation with and in response to the needs of the user community.

A standardisation of ^{90}Y was completed to improve the accuracy of the response factors for the ionisation chambers to support the hospital calibration service. ^{90}Y was chosen as this nuclide is receiving increasing attention in the medical community for targeted radiotherapy (the first drug to use this technique was licensed by the FDA during this period).

A calibration factor for the NPL ionisation chamber was determined for the short-lived (13 seconds) gas $^{81\text{m}}\text{Kr}$. By using primary standards with low uncertainties to calibrate a γ -ray spectrometer, used as a transfer instrument, the uncertainty in the $^{81\text{m}}\text{Kr}$ activity determination was reduced.

For applications in environmental monitoring, $^{95\text{m}}\text{Tc}$ was standardised. ^{208}Po was also successfully standardised.

2.3.3 *Acknowledgement*

Financial support of the National Measurement System Policy Unit of the U.K. 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 (Univ. of Birmingham) and N Taylor (UKAEA Culham)

The design and performance analysis of fusion power plant conceptual designs intends to provide insight on fusion physics and technology issues regarding 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, spanning a range of assumptions from the very conservative to the more advanced in terms of physics and technology requirements.

The tasks performed at UKAEA-Culham include: (a) the estimation of the radioactive material expected to be generated during the operation and decommissioning of the plant; and (b) a conservative evaluation of the bounding consequences (maximum doses to the public) following a hypothetical worst-case scenario in which a release of activated material is postulated. 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 with a postulated confinement breach. Results show that temperature excursions and doses to the public are within structural and regulatory limits, even for this bounding scenario, and that no radioactive material would require permanent waste disposal 100 years after plant shutdown. A final overall report has been submitted to Euratom-EFDA.

Work has also been conducted on the study of alternative bounding scenarios, such as partial loss of cooling and others, and on exploring the potential for re-utilisation of the tritium breeder material during several plant cycles both from a breeding and from a regulatory (radwaste) point of view. Currently in progress is the design and performance analysis of a fifth PPCS plant model, whose characteristics include most of the favourable features found during the analyses of the previous plant models.

4 Nuclear Data Libraries and Data Evaluations

4.1 European Activation File development during 2003

R A 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 inventory code FISPACT.

EAF-2003 has been released and distributed as part of EASY-2003 [2]. A major activity during 2003 has involved the validation of the new data library using the experimental measurements made by three European Groups and data from Japan and the literature. The results are presented in a comprehensive report [3]; in summary 287 reactions are considered, with 171 validated (the agreement between experiment and calculations is within the uncertainties).

To realise the ultimate objective of fusion power it is necessary to extend the work on materials. To achieve the neutron fluences needed for production of radiation damage in materials an accelerator based testing facility such as the International Fusion Materials Irradiation Facility (IFMIF) will be required. This will produce neutrons of energy > 20 MeV, thus it is necessary to extend the energy range in the activation data library. EAF-2004 has been produced; this has an upper energy limit of 60 MeV and contains 62,860 reactions (a large increase over the 12,617 in EAF-2003). This version has not been distributed, but is an internal library for testing. An increase in the number of nuclides in the decay data library (extra 278) is also required. Changes to FISPACT have been made and calculations of the activation in an IFMIF spectrum carried out. Significant extensions to SAFEPAC-II (the application used to produce the EAF libraries), to treat data at the higher energies, have been added. Future work will complete the extension to higher energies and see the distribution of EASY-2005.

4.2 European Activation File development during 2004

R A 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 inventory code FISPACT.

EAF-2005 has been released and distributed as part of EASY-2005 [4]. The most important new feature in this version of EAF is the extension of the energy range from 20 to 60 MeV. The motivation for this change is the need to carry out activation calculations for the materials testing facility IFMIF. This is an accelerator based device with a significant number of neutrons with energies > 20 MeV.

EAF-2005 has been produced; this contains 62,637 reactions (a large increase over the 12,617 in EAF-2003). This version has now been distributed, and is fully documented

by six UKAEA reports (all documents can be downloaded from the web site <http://fusion.org.uk/easy2005>). Changes to FISPACT and SAFEP AQ-II (the application used to produce the EAF libraries), to treat data at the higher energies, have been added.

Using EASY-2003 a large number of activation calculations have been carried out on all the elements and the results are presented in the 'Activation Handbook' [5]. Much of the data are for fusion relevant neutron spectra, however for each element five importance diagrams are included. These are spectrum independent and cover the energy range from 0.05 eV – 20 MeV and show which nuclides contribute significantly at decay times from 1 s – 1 million years at these energies. Also presented are the pathways that produce the important nuclides. The handbook is relevant to many applications and provides a source of activation data without running inventory codes.

4.3 Fission Product yield evaluations, 2003 - 2004

R W Mills (BNFL, 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. The final report of this CRP is being edited by the IAEA and will soon be issued.

Feedback was received from the OECD / NEA Joint Evaluated File project on the UK Fission Product Yield File UKFY3.4. This feedback was considered and a new version of the file, UKFY3.5, issued to the NEA. The new file was examined and benchmarked by members of the JEFF community.

The UKFY3.5 file and preliminary JEFF-3 decay data (JEFF3T3ii) were benchmarked against various decay heat benchmarks. There were two comparisons chosen for this exercise. Firstly fission pulse calculations for thermal fission of U235, Pu239, Pu241 and fast fission of U238. The second comparisons were against the decay heat measured from PWR assemblies. These comparisons are described in a paper by Drs. Mills and Parker at the 2004 International Conference on Nuclear Data for Science and Technology. This paper was discussed at the UKNSF as paper UKNSF(2004)P186.

Following feedback, developments were made to the data and methods to produce an improved evaluation for issue in early 2005. This work was done in parallel with decay data developments co-ordinated by Mark Kellett of the CEA. The principal improvements concern helium and tritium yields, charge balance, estimates of yield uncertainty and yields of importance to thermal reactors.

4.4 Nuclear decay data evaluations

Radioactivity Metrology Group, Quality of Life Division, National Physical Laboratory

NPL participated in the International Atomic Energy Agency's Co-ordinated Research Programme 'Update of X- and Gamma-Ray Decay Data Standards for Detector Calibration and Other Applications'.

Half-lives for all 64 radionuclides included in the IAEA-CRP have been evaluated at NPL [6].

Gamma ray emission probabilities in the decays of ^{56}Co , ^{94}Nb and ^{106}Ru / ^{106}Rh have been evaluated for the IAEA-CRP.

The ^{56}Co evaluation was carried out in collaboration with the Lawrence Berkeley National Laboratory, U.S.A. and the complete decay scheme data for this radionuclide has been entered into the International Decay Data Evaluation Project (DDEP) database, http://www.nucleide.org/DDEP_WG/DDEPdata.htm.

Half-life data for the important radionuclides ^3H , ^{90}Sr , and ^{90}Y have been evaluated.

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

5 References

1. P. Morris, D. K. Ross, S. Ivanov, D. R. Weaver and O. Serot, *Inelastic neutron scattering study of the vibration frequencies of hydrogen in calcium dihydride*, Journal of Alloys and Compounds, **363** (2004) 85-89
2. R. A. Forrest, *The European Activation System: EASY-2003 overview*, UKAEA FUS 484, 2002
3. R. A. Forrest, M. Pillon, U. von Möllendorff, K. Seidel, J. Kopecky and J-Ch. Sublet, *Validation of EASY-2003 using integral measurements*, UKAEA FUS 500, 2003
4. R. A. Forrest, *The European Activation System: EASY-2005 overview*, UKAEA FUS 513, January 2005
5. M. R. Gilbert and R. A. Forrest, *Handbook of activation data calculated using EASY-2003*, UKAEA FUS 509, July 2004
6. M.J. Woods, S.M. Collins and S.A. Woods, *Evaluation of half-life data*, NPL Report CAIR 8 (January 2004)

6 Acknowledgement

This report was produced with the support of the HSE, Nuclear Safety Directorate, and represents edited contributions from members of the UK Nuclear Science Forum and their co-workers.