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THE DATA LIBRARY UKACT1 AND THE INVENTORY CODE FISPACT

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Abstract: The library UKACT1 contains neutron induced cross-sections for 625 target nuclides in the GAM-II 100-energy group format. The targets include all stable nuclides and radioisotopes with half lives greater than 1 day and Z≤84. First and second isomers are included both as targets and as products of reactions. Approximately 8700 distinct reactions have data.

The inventory code FISPACT is a development of the existing FISPIN code which can read UKACT1 and the decay data library UKDECAY1 (covering 1314 nuclides) and produce output relevant to fusion. This includes the surface gamma-dose rate, bremsstrahlung contributions and biological hazards. In addition, a sensitivity routine enables the most important reactions in the production of specific nuclides to be identified and the errors of amounts of nuclides to be estimated.

Calculations of the arisings of irradiation of Ti and some elements as impurities in iron are given as examples.

(activation, nuclear data, inventory code, neutron-induced cross-sections, isomers, systematics, titanium)

Introduction

The widespread use of fusion reactors for electricity generation will involve the production of large amounts of activated material. In order to design suitable materials and plan operating scenarios, predictions of activation of a wide range of materials in fusion fluxes are required. This paper reports on progress in the continuing programme of work in the UK to improve both the nuclear data libraries and the associated inventory code.

The Data Library UKACT1

UKACT1 is an essentially complete library containing activation cross-section data for neutron induced reactions with thresholds up to 14.9 MeV. Most of the work on this library has been to ensure completeness rather than in trying to improve significantly the accuracy of the individual reactions. It contains cross-section data in 100-group GAM-II format for reactions on 625 target nuclides. These include all stable isotopes and radionuclides with half lives greater than one day and with atomic number ≤84. In addition, some nuclides with shorter half lives have been included where a product formed by a single reaction is a long lived nuclide, e.g. ^{45}Ti(n,2n)^{44}Ti where there is no other route for the production of ^{44}Ti. The target nuclides include 49 first isomers (m) and 4 second isomers (n). It is extremely important that all the relevant isomers for all elements are included because in some cases such as ^{178}Hf and ^{192}Ir the second isomers are very long lived (31 and 241 years respectively).

UKACT1 is developed from the REAC library produced by Mann et al[1]. This was modified by Gruppelaar et al[2] with the addition of some missing reactions and renormalisation of the reactions to the (then) best systematics. The following changes have been made to the interim library.

(a) Addition of reactions on 162 targets. These are calculated using the THRESH[3] code and the systematics given by Forrest[4]. The identification of m and n isomers in the interim library has been corrected (previously only a single isomer per nuclide was included) and many existing reactions have had to be split (by using a suitable isomer ratio) if the route to the isomeric product was missing.
(b) Many of the existing targets had no capture data or nearest neighbour data had been used. This was improved by using suitably processed data from the JEF1 library (for 176 nuclides) or the ACTL[5] library.
(c) Superelastic collisions have been included.
(d) To try and ensure that no non-zero reactions have been missed from the library a checking program was written. This uses information on all the targets and decay data on all nuclides to check that reactions to all products (including isomers) exist. This enabled many missing reactions to be identified.

Some calculations using UKACT1 are discussed below. UKACT1 is known to have weaknesses and a new library UKACT2 is in preparation. The main problems of UKACT1 are the unsatisfactory capture data and the use of very simple isomer ratios and THRESH generated cross-sections.

When UKACT1 was compiled it was anticipated that first wall spectra would be very hard and that consequently capture reactions would be of little importance compared to the threshold reactions. However, as shown in Figure 1, the DEMO[6] spectrum is much softer than the CTRIII[7] spectrum, and when considering NET this increase in low energy neutrons is even more pronounced. It is therefore necessary to put more effort into improving the capture data in the library.

The Decay Data Library UKDECAY1

In addition to the cross-section data for the target nuclides the inventory code also requires radioactive decay data for the target and short lived product nuclides formed either by

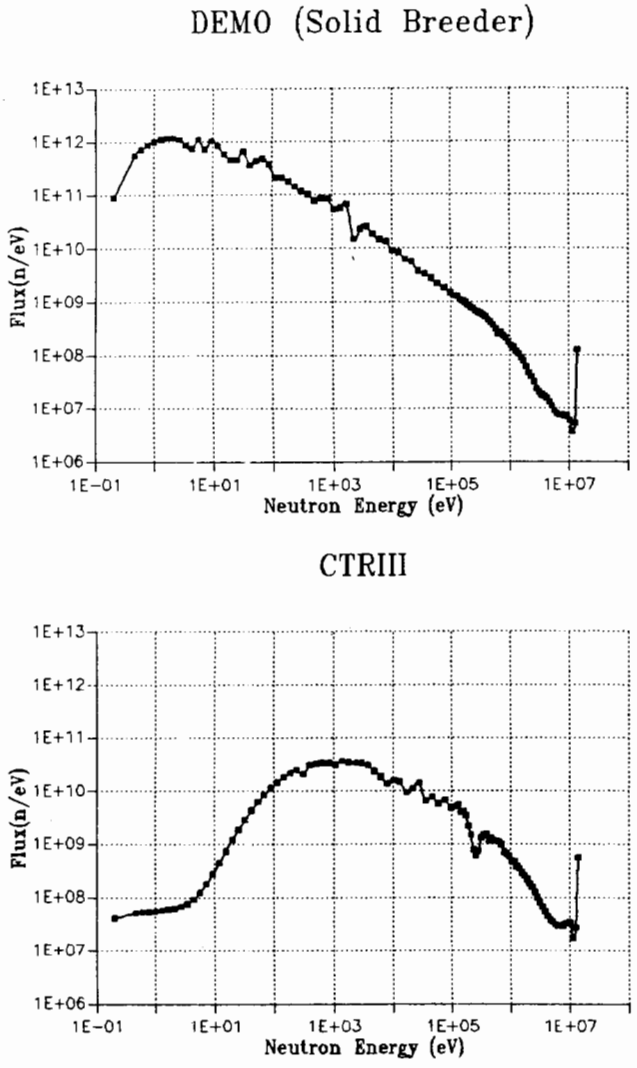

Figure 1 Neutron spectra for the CTRIII and DEMO fusion reactors.

reactions or by decay. FISPACT reads the decay data in ENDF/BV format and it is therefore possible to use existing JEF1 evaluations for most of the nuclides. In all 1314 nuclides require data, although for the 266 stable isotopes only identifying information is needed. Where data are not available in the JEF1 library, data were extracted by hand from the handbook Table of Radioactive Isotopes[8].

For these constructed ENDF/BV files no spectral data are included, as these nuclides are expected to be of limited importance. However, the spectral data are estimated by FISPACT so that dose rates from the 420 nuclides are not ignored. If subsequent inventory runs indicate that any of these nuclides contribute significantly to the total dose rate, then spectral data can be input or other evaluations used.

One change has been made to the data in UKDECAY1, the amendment of the half life of ^{91}Nb. In the original JEF1 file a value of 9993 years was used, but this has been amended to 680 years following the experimental results of Nakanishi and Honda[9]. A further addition has been to include the fictitious isotope ^{51}Fe in the library for reasons described below.

The Inventory Code FISPACT

The code FISPACT is a development of the UKAEA code FISPIN[10] which is used for fission applications. FISPACT uses the same calculational method, but has new routines and larger storage area because of the increased size of the data libraries. In addition a sensitivity option allows the calculation of the coefficients $(dN_i/N_i)/(d\sigma_j/\sigma_j)$ for specified nuclide N_i and cross-section σ_j. These coefficients enable the most important reactions in the production of a nuclide to be identified and also error estimates of the amount of the nuclide to be made. FISPACT can read directly the ENDF/BV format of the decay data and can collapse the 100-group cross-sections and neutron spectrum to a suitable 1-group library. Important indices for judging acceptability of various irradiated materials in addition to activity are the surface gamma-dose rate and ingestion and inhalation doses. These are calculated by the code and suitable graphical output is also available. Documentation is available on the use of the program in reference 11. Most emphasis so far on the use of the code and the validation of the data has been for long term activation.

Results

Inventory runs using pure natural titanium were carried out using a DEMO first wall spectrum at a wall loading of 5.0 MW m^{-2} for 2.5 years. Figure 2 gives the activity (Bq kg^{-1}) as a function of cooling time after the irradiation has finished. The isotopes which contribute significantly to the activity at various times are shown. The value where the nuclide is plotted on the x-axis corresponds to the half life, and the y-value corresponds to its activity at zero cooling time. Figure 3 is a similar plot showing the dose rate (Sv h^{-1}) as a function of cooling time. Dose rate refers to the dose from the gammas at the surface of an infinite slab of the material. This uses an approximation detailed in reference 12 and only gammas with energy above 100 keV are considered.

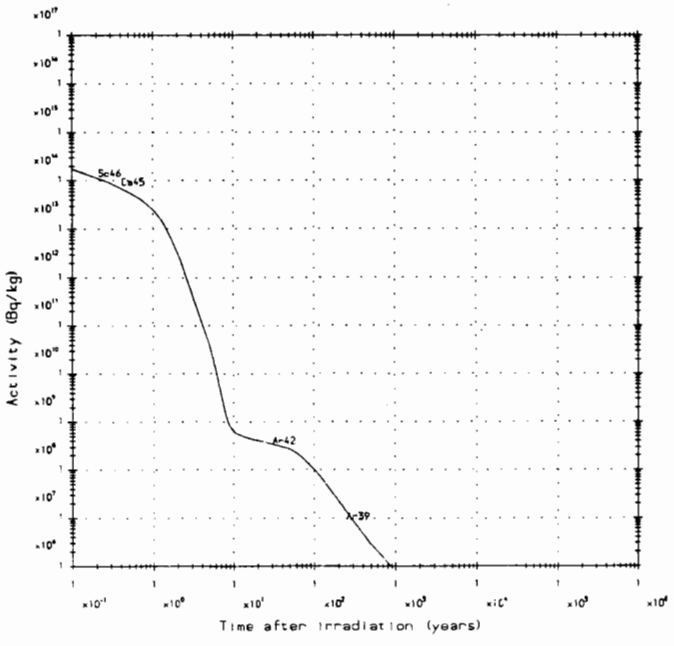

Figure 2 Activity as function of cooling time after irradiation of natural titanium

Also included is the correction due to bremsstrahlung from a set of selected nuclides. In this case the correction of about 10% is due to ^{42}K. The only nuclide shown in Figure 3 is ^{46}Sc, this is because the main dose rate at times of a few 10's of years is due to ^{42}K which is the short lived daughter of ^{42}Ar. The ^{42}Ar itself has no gamma-emission and so does not contribute to the dose rate, while ^{42}K has too small a half life to be shown on the plot.

An important feature of FISPACT is the determination of sensitivities. By this is meant the change in the amount of a daughter nuclide when a particular reaction cross-section is varied. The quantity calculated is the sensitivity coefficient S defined in equation (1)

$$S(N_i;x) = x/N_i . dN_i/dx \qquad (1)$$

For N_i representing ^{42}Ar and x representing reactions the values of S are shown below.

x	S (%)	fractional errors in cross-section
$^{46}Ti(n,\alpha)$	12.25	0.6
$^{43}Ca(n,2p)$	12.31	1.0
$^{48}Ti(n,\alpha)$	86.64	0.3
$^{45}Ca(n,\alpha)$	84.96	0.6
$^{49}Ti(n,\alpha)$	1.08	-
$^{46}Ca(n,n'\alpha)$	1.26	-

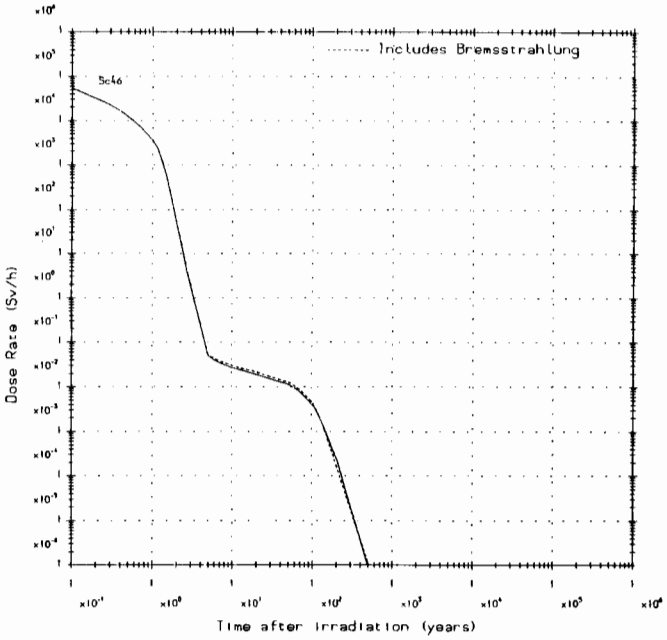

Figure 3 Dose rate as function of cooling time after irradiation of natural titanium

The production of ^{42}Ar from Ti is a two step process and the large (and almost equal) figures for the third and fourth reactions above indicate that the dominant route is $^{48}Ti(n,\alpha)^{45}Ca(n,\alpha)^{42}Ar$. A similar analysis for the production of ^{39}Ar indicates that the main route is $^{46}Ti(n,\alpha)^{43}Ca(n,n'\alpha)^{39}Ar$.

Table 1

Results of irradiation of 1 ppm of an element in an unreactive iron matrix. A first wall DEMO flux at 5 MWm^{-2} for 2.5 years and cooling times of 50 and 100 y are considered.

	Activity ($Bqkg^{-1}$)			Gamma-dose rate (μSvh^{-1})		
	50 y	100 y	Dominant isotopes	50 y	100 y	Dominant isotopes
21-Sc	$2.89\ 10^{3}$	$2.05\ 10^{3}$	$^{39}Ar, ^{42}Ar, ^{42}K$	$4.03\ 10^{-2}$	$1.41\ 10^{-2}$	^{42}K
22-Ti	$2.72\ 10^{2}$	$1.0\ 10^{2}$	$^{39}Ar, ^{42}Ar, ^{42}K$	$1.15\ 10^{-2}$	$4.03\ 10^{-3}$	^{42}K
23-V	$4.98\ 10^{-2}$	$1.75\ 10^{-2}$	$^{42}Ar, ^{42}K$	$2.18\ 10^{-6}$	$7.64\ 10^{-7}$	^{42}K
24-Cr	$1.62\ 10^{-2}$	$5.63\ 10^{-3}$	$^{42}Ar, ^{42}K$	$6.9\ 10^{-7}$	$2.43\ 10^{-7}$	^{42}K
25-Mn	$7.34\ 10^{1}$	7.27	$^{53}Mn, ^{55}Fe$	$2.58\ 10^{-5}$	$2.09\ 10^{-6}$	$^{53}Mn, ^{55}Fe$
26-Fe	$2.12\ 10^{3}$	$5.52\ 10^{1}$	^{53}Mn	$1.0\ 10^{-1}$	$1.56\ 10^{-4}$	$^{60}Co, ^{53}Mn$
27-Co	$1.53\ 10^{7}$	$2.19\ 10^{4}$	$^{60}Co, ^{59}Ni$	$1.08\ 10^{4}$	$1.50\ 10^{1}$	^{60}Co
28-Ni	$1.25\ 10^{6}$	$8.37\ 10^{5}$	$^{63}Ni, ^{59}Ni, ^{60}Co$	$5.03\ 10^{1}$	$7.67\ 10^{-2}$	^{60}Co
29-Cu	$7.92\ 10^{6}$	$5.57\ 10^{6}$	^{63}Ni	$2.73\ 10^{1}$	$3.84\ 10^{-2}$	^{60}Co
30-Zn	$4.24\ 10^{5}$	$3.00\ 10^{5}$	^{63}Ni	$1.31\ 10^{-1}$	$2.04\ 10^{-4}$	^{60}Co
31-Ga	$3.18\ 10^{2}$	$2.25\ 10^{2}$	^{63}Ni	$5.78\ 10^{-8}$	$8.26\ 10^{-9}$	^{60}Co
32-Ge	$1.74\ 10^{1}$	$1.28\ 10^{1}$	$^{63}Ni, ^{79}Se$	$1.96\ 10^{-9}$	$4.11\ 10^{-10}$	^{60}Co
33-As	$1.76\ 10^{1}$	$1.76\ 10^{1}$	^{79}Se	$1.48\ 10^{-13}$	$1.48\ 10^{-13}$	^{81}Kr
34-Se	$5.65\ 10^{4}$	$5.63\ 10^{4}$	^{79}Se	$7.85\ 10^{-5}$	$1.90\ 10^{-5}$	$^{81}Kr, ^{85}Kr^{*}$
35-Br	$3.0\ 10^{4}$	$1.75\ 10^{4}$	$^{79}Se, ^{81}Kr, ^{85}Kr$	$1.64\ 10^{-2}$	$1.02\ 10^{-2}$	$^{81}Kr, ^{85}Kr^{*}$
36-Kr	$7.18\ 10^{6}$	$2.88\ 10^{5}$	$^{85}Kr, ^{81}Kr$	3.66	$1.48\ 10^{-1}$	$^{85}Kr^{*}, ^{81}Kr$
37-Rb	$3.13\ 10^{5}$	$1.23\ 10^{4}$	^{85}Kr	$1.60\ 10^{-1}$	$6.30\ 10^{-3}$	$^{85}Kr^{*}$
38-Sr	$3.63\ 10^{4}$	$1.48\ 10^{3}$	$^{85}Kr, ^{90}Sr, ^{90}Y$	$1.88\ 10^{-2}$	$8.48\ 10^{-4}$	$^{85}Kr^{*}, ^{90}Sr^{*}, ^{90}Y^{*}$
39-Y	$1.43\ 10^{3}$	$3.32\ 10^{2}$	$^{90}Sr, ^{90}Y$	$2.33\ 10^{-3}$	$6.58\ 10^{-4}$	$^{90}Y^{*}, ^{85}Kr^{*}, ^{90}Sr^{*}$
40-Zr	$2.04\ 10^{4}$	$7.08\ 10^{3}$	$^{90}Sr, ^{90}Y, ^{93}Zr, ^{93m}Nb$	$4.6\ 10^{-2}$	$1.90\ 10^{-2}$	$^{90}Y^{*}, ^{94}Nb, ^{90}Sr^{*}$

*indicates that the bremsstrahlung contribution from the nuclide is important

Using the sensitivity coefficients and suitable values for the errors in the cross-sections an estimate of the error in the production of a nuclide can be calculated from standard error theory. The fractional errors shown above were estimated from the values at 14.5 MeV either from experimental values or from systematics[4]. These values indicate that the fractional errors in the production of the nuclides are for ^{42}Ar ±0.95 and for ^{39}Ar ±1.46.

Some calculations of impurities in iron are shown in Table 1. 1 ppm of the element is placed in a matrix of ^{51}Fe. This nuclide is a 'pseudo-nuclide' - it is stable and has no neutron induced reactions, thus the matrix does not change in any way. However, it has the correct material properties so that absorption of gamma radiation and the bremsstrahlung correction are correct. These results are similar in most cases to earlier calculations published by Giancarli[13] using UKCTRIIIA/ORIGEN, but some differences are discussed below.

The surface gamma-dose rate from Se, Br, Kr, Rb, Sr and Y is substantially increased by the inclusion of the bremsstrahlung contribution from ^{85}Kr (for Sr at 100 y this is 32% of the total). In the case of Y and Zr the contribution from ^{90}Y is in fact dominant (a factor of about 30 at 100 y for Y). ^{90}Y has a half life of only 64.1 h, but is produced in the decay of ^{90}Sr and so can be important at long cooling times. A criterion for deciding on the amount of impurity that would be acceptable in a material is defined as 'the total surface gamma-dose rate at 100 y cooling must be less than 25 $\mu Sv h^{-1}$'. Using this criterion the present calculations predict that only about 3.8% of Y is possible in an iron based material, in comparison to the status of 'no restriction' given by Giancarli and Ponti[14].

It is worth noting that the present version of FISPACT does not include the tritium produced in the (n,t) and (n,n't) reactions as part of the inventory of materials of reaction products. In some impurities, e.g. V, Cr, Mn, this tritium is stated by Giancarli as giving the major activity. It is planned to include this within FISPACT in a future version, although for practical handling of materials in fusion reactors the presence of so much tritium from the breeding blankets would mean that routine detritification would be necessary before recycling or disposal of materials.

Conclusions

The inventory code FISPACT and its associated data libraries are described. This is designed for calculating amounts of nuclides, activities, dose rates and biological hazards due to irradiation of materials in a neutron flux from a fusion reactor. Improvements to the capture data in the library UKACT1 are in hand. These will improve predictions for designs with considerable moderating material in the blankets and also make the library and code more applicable to non-fusion applications.

Some calculations of major pathways for production of activity in the irradiation of Ti are described and results of calculations of some elements as impurities in an iron matrix given.

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