Agenzia nazionale per le nuove tecnologie,
l'energia e lo sviluppo economico sostenibile

MINISTERO DELLO SVILUPPO ECONOMICO

Ricerca di Sistema elettrico

Updating of the Libraries Included in the ANITA-2000 Code Package on the Basis of the JEFF-3.1.1 Radioactive Decay Data Library

Manuela Frisoni

Report RdS/PAR2013/078

Updating of the Libraries Included in the ANITA-2000 Code Package on the Basis of the JEFF-3.1.1 Radioactive Decay Data Library

Manuela Frisoni - ENEA

Settembre 2014

Report Ricerca di Sistema Elettrico

Accordo di Programma Ministero dello Sviluppo Economico - ENEA
Piano Annuale di Realizzazione 2013
Area: Produzione di energia elettrica e protezione dell'ambiente
Progetto: Sviluppo competenze scientifiche nel campo della sicurezza nucleare e collaborazione ai programmi internazionali per il nucleare di IV Generazione
Obiettivo: Sviluppo competenze scientifiche nel campo della sicurezza nucleare
Responsabile del Progetto: Felice De Rosa, ENEA

Titolo

Updating of the Libraries Included in the ANITA-2000 Code Package on the Basis of the JEFF-3.1.1 Radioactive Decay Data Library

Descrittori

Tipologia del documento: Rapporto tecnico

Collocazione contrattuale: Accordo di programma ENEA-MSE su sicurezza nucleare e reattori di IV generazione

Argomenti trattati: Fisica nucleare, dati nucleari, librerie di dati di decadimento

Sommario

ANITA-2000 is a code package for the activation characterization of materials exposed to neutron irradiation released by ENEA at OECD-NEADB (NEA-1638). The package contains: a) the activation code ANITA-4M, based on the original code developed at CEC JRC Ispra, able to compute the radioactive inventory of a material exposed to neutron irradiation, continuous or stepwise, b) two activation cross section libraries, c) the decay data library (file "fl1") containing the quantities describing the decay properties of unstable nuclides and d) the library (file "fl2") containing the gamma ray spectra emitted by the radioactive nuclei in the ORNL-SCALE 18-γ energy group structure. The data contained in the "fl1" and "fl2" libraries of the ANITA-2000 code package are based on the evaluated data library FENDL/D-2.0. Taking into account a specific interest of ENEA and Ansaldo Nucleare, the ANITA-2000 "fl1" and "fl2" libraries were updated on the basis of the JEFF-3.1.1 Radioactive Decay Data Library. This work required the setting up of a series of proper interface codes in order to process and convert the JEFF-3.1.1 evaluated decay data (in ENDF-6 standard format) into the format required by ANITA-4M code. A preliminary validation of the new libraries has been performed through the comparison of the ANITA-4M calculations against measurements of electron-photon decay heat and activity of neutron activated materials from FNG (Frascati Neutron Generator) experiment.

Note

Author: Manuela Frisoni

Copia n. **In carico a:**

REV.	DESCRIZIONE	DATA		REDAZIONE	CONVALIDA	APPROVAZIONE
2			NOME			
			FIRMA			
1			NOME			
			FIRMA			
0	EMISSIONE	02/09/2014	NOME	M. Frisoni	F. Padoani	F. De Rosa
			FIRMA	Manuela Frisoni	F. Padoani	

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September 2014

1 INTRODUCTION

ANITA-2000 is a code package for the activation characterization of materials exposed to neutron irradiation developed by ENEA and freely distributed at OECD-NEADB [1] and ORNL-RSICC [2]. It has been widely used, improved and validated in the past by ENEA [3][4][5][6][7][8][9][10][11]. ANITA-2000 has been also utilized in M*ANCINTA*P, a computational "4D rigorous-2-step" tool, developed at Ansaldo Nucleare, that automatically combines neutron transport calculations (via MCNP5) with activation calculations (via ANITA-2000) in order to evaluate decay gamma dose rates due to activated materials (the name of the tool mixes the acronyms of the transport and activation computer programs). *MANCINTAP* has been successfully applied for the activation analysis of the lower reactor cavity of AP1000 reactor and in nozzle gallery regions of a 2-loop PWR reactor [12][13].

The main component of the ANITA-2000 package is the activation code ANITA-4M that computes the radioactive inventory of a material exposed to neutron irradiation, continuous or stepwise. It traces back to the ANITA code (Analysis of Neutron Induced Transmutation and Activation) [14]. The ANITA-4M code provides activity, atomic density, decay heat, biological hazard, clearance index and decay gamma-ray sources versus cooling time. Results are given as for each nuclide as for the material.

The ANITA-2000 code package is provided with a complete data base allowing to perform calculations for all the elements with the atomic number up to 94. The libraries contained in the code package are:

1) Neutron activation data libraries
2) Decay, Hazard and Clearance data library ("fl1" file)
3) Gamma library ("fl2" file)

Two neutron activation cross section data libraries are contained in the ANITA-2000 code package based on the European Activation File EAF-99 [15] and on the Fusion Evaluated Nuclear

Activation Data Library FENDL/A-2.0 [16], respectively. The libraries “fl1” and “fl2” contained in the package are based on the Fusion Evaluated Nuclear Decay Data Library FENDL/D-2.0 [17].

Actually, new activation and decay data libraries are available and therefore the updating of the ANITA-2000 libraries is now feasible. On the basis of a common interest of ENEA and Ansaldo Nucleare, as users of ANITA-2000, the Decay, Hazard and Clearance data library and the Gamma library have been updated using the JEFF-3.1.1 Radioactive Decay Data Library [18]. The ANITA-4M code actually uses the neutron cross section European Activation File EAF-2010 [19] contained in the EASY-2010 code package [20].

A preliminary validation of the new data libraries has been performed, following the work already made in the past [6][11], through the comparison of ANITA-4M results against measurements of electron-photon decay heat and activity of neutron activated materials from FNG (Frascati Neutron Generator) experiment.

2 ANITA-4M ACTIVATION CODE

2.1 Main features of the activation code

The package ANITA-2000 includes the activation code ANITA-4M that computes the radioactive inventory of a material exposed to neutron irradiation, continuous or stepwise. The ANITA-4M code provides activity, atomic density, decay heat, biological hazard, clearance index and decay gamma-ray source spectra at shutdown and at different cooling times. It treats all the elements with the atomic number up to 94.

The analytical computational method used by ANITA-4M is highly performing as far as the computer time is concerned.

2.2 Analytical Method

The calculation method [21] used by the code is summarized in the following.

The neutron irradiation of an atomic species A(N,Z) gives rise to several possible nuclear reactions whose number increases with increasing the energy of the incident particles. The new atomic species produced by the neutron-induced reactions may be stable or unstable or may be produced in the ground or a metastable state. Unstable nuclei will sooner or later decay into a new state or into a new species of nuclei, which in turn could be stable or decay again. These processes give rise to a decay chain that will end when a stable state is reached.

The time dependence of the concentration of a given nuclide N_i obeys the following balance equation:

$$\frac{dN_i}{dt} = \text{Formation Rate} - \text{Destruction Rate} - \text{Decay Rate} \qquad (1)$$

ANITA-4M code considers radioactive disintegration and neutron induced reactions as the processes appearing on the right-hand side of the Eq. (1). The time rate of change of the concentration for a particular nuclide N_i , in terms of these phenomena, can be written as:

$$\frac{dN_i}{dt} = \sigma_{r,i-1} N_{i-1} \phi + \lambda_i' N_i' - \sigma_{r,i} N_i \phi - \lambda_i N_i \qquad (2)$$

where (i= 1....I), and

- $\sigma_{r,i-1}\ N_{i-1}\ \phi$ is the transmutation rate into N_i due to the neutron induced reaction r on the nuclide N_{i-1},

- $\lambda'_i N'_i$ is the rate of formation of N_i due to the radioactive decay of nuclides N'_i,
- $\sigma_{r,i} N_i \phi$ is the destruction rate of N_i due to all possible neutron induced reactions (n,γ ; n,α ; n,p ;n,2n ; n,np ; etc.), and
- $\lambda_i N_i$ is the radioactive decay rate of N_i

Considering all the I nuclides of the chain, the Eq. (2) represents a coupled set of homogenous first order linear differential equations with constant coefficients. The ANITA-4M code solves this set of equations by the analytical matrix exponential method.

The Eq. (2) can be written in matrix notation as

$$\frac{d\tilde{N}}{dt} = \tilde{\tilde{A}}\,\tilde{N} \tag{3}$$

where $\tilde{N}$ is the vector of nuclide concentrations and $\tilde{\tilde{A}}$ is the transition matrix containing the rate coefficients for radioactive decay and neutron absorption. Eq. (3) has the known solution

$$\tilde{N}(t) = \tilde{N}(0)e^{\tilde{\tilde{A}}\,t} \tag{4}$$

where $\tilde{N}(0)$ is the vector of initial nuclide concentrations. The Eq. (4) can be expanded as

$$\tilde{N}(t) = \tilde{N}(0)\sum_{m=0}^{\infty}\frac{(\tilde{\tilde{A}}\,t)^m}{m!} \tag{5}$$

The Eq. (5) yields a complete solution to the problem. The irradiation is assumed to start at time zero when $N_1(0)$ is known and N_i (0) = 0 for i > 1. By defining these initial conditions the solutions of the system of Eq. (2) can be calculated by recurrence relations quite suitable for computer programming.

The particular cases when the decay time of an unstable nucleus of the chain is much longer or shorter than the irradiation time interval are taken into account and treated separately. The Eq. (2) holds during the irradiation time. At the end of this time the Bateman equations are solved describing the naturally occurring radioactive decay chains with the densities, solutions of the system (Eq. 2) at the end of irradiation, as initial conditions. Continuous or multi-steps (up to 2000 burn-dwell intervals) can be considered for the operational scenario. A different level of the irradiation flux can be used for each one of the exposure time steps.

3 DATA LIBRARIES

The ANITA-2000 code package is provided with a complete data base allowing to perform calculations for all the elements with the atomic number up to 94.

The ANITA-4M activation code requires the following data libraries:

- Decay, Hazard and Clearance data library (file "**fl1**")
- Gamma library (file "**fl2**")
- Neutron activation data library (file "**lib175**")

The schematic block diagram of the data/libraries required by the ANITA-4M code is shown in Figure 1.

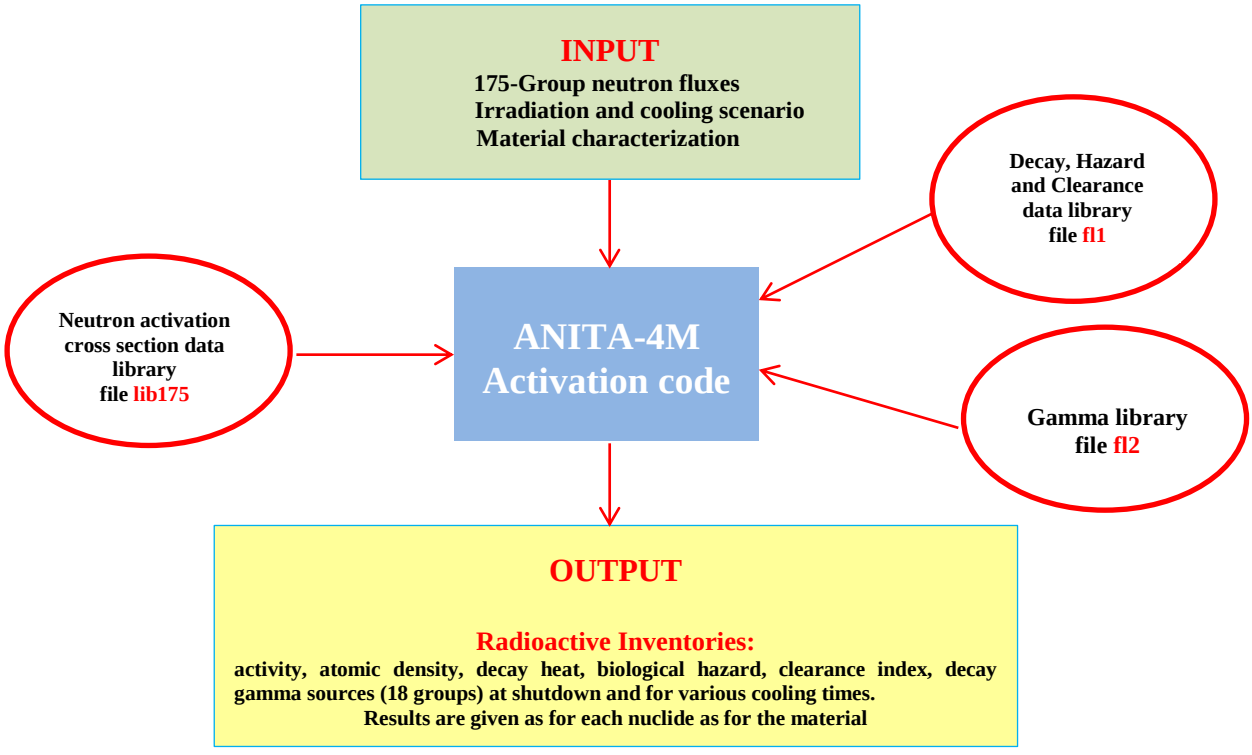


Figure 1 – Anita-4M activation code block diagram

3.1 Decay, Hazard and Clearance Data library (file "fl1")

This library contains the information describing the decay properties of unstable nuclides useful for the calculations performed by ANITA-4M.

For each nuclide, the decay data, as the decay mode, the decay constant (s^{-1}), the total energy (MeV) released in the decay and the energy (MeV) released in the form of gamma or X-rays are provided. Different competitive decay modes are taken into account when contemporary.

The file contains also the hazard data (ALI) for each radionuclide describing its potential biological impact on human beings. The ALI quantities are defined as the Annual Limit of Intake (Bq) by ingestion or inhalation for the public or workers.

The library contains also the clearance level for each radionuclide.

The **fl1** file has been completely updated and actually contains data for 3433 nuclides. The description of the data contained in the file and their sources are described in the following.

3.1.1 Decay data

The decay data have been taken from the JEFF-3.1.1 Radioactive Decay Data library [18]. The standard library JEFF-3.1.1 is in ENDF-6 [22] format. The radioactive decay data are given in the section identified by MF=8, MT=457 (in ENDF-6 standard format notation). This section is restricted to single nuclides in their ground state or an isomeric state (a "long lived" excited state of the nucleus). The main purpose of MT=457 is to describe the energy spectra resulting from radioactive decay and give average parameters useful for applications such as decay heat and waste disposal studies, shielding, etc. For each isotope the following decay data are given: nuclide identification, half-life, number of decay modes, fractions of decay in each decay mode (branching ratio), energy released by the decay, gamma-ray intensity and energy spectrum in each decay mode. The standard library contains data for 3853 nuclei, ranging from the neutron (0-nn-1) to roentgenium 272 (111-Rg-272).

In the **fl1** file used by ANITA-4M code the following basic decay data are included for each unstable nuclide:

- nuclide identification
- decay mode
- decay constant
- total energy released in the decay (MeV) used to calculate decay heat
- energy released in the form of gamma or X-rays (MeV)

For the stable nuclides the isotopic abundances are given taken from Ref. [23].
The new **fl1** file contains data for the nuclei ranging from the 1-H-1 to 94-Pu-247.

3.1.2 Hazard data

The ALI quantities were obtained from the "eaf_haz_20100" file contained in the EASY-2010 code package [24]. In the **fl1** file used by the ANITA- 4M code, the ALI values by ingestion for the public are given. A conversion factor of 0.001 (Sv/y) has been adopted to convert the dose coefficients from Ref. 24 to the ALI quantities. The ALI quantity is provided only for the 2006 nuclides contained in the "eaf_haz_20100" file.

3.1.3 Clearance level data

The **fl1** file provides also for each radionuclide the clearance level C_L (Bq/g). This value allows to establish if a radioactive material can be potentially moved out of the originating facility and recycled.

The safe handling of radioactive waste is recognized as crucial to ensure protection of human health and the environment. IAEA publish regulations on these issues and reference [25] gives information on suggested clearance level values for a set of important radionuclides.

The clearance level data contained in the new **fl1** file have been produced by including the information contained in [25].

The clearance levels for the 242 nuclides up to Pu-244 contained in Table 2 of Ref. [25] were included in the file **fl1**. The clearance level C_L=10 has been attributed to ^{40}K as suggested in Table 1 of Ref. [25].

Following the suggestion of Table 1 of Ref. [25], moreover, the clearance level C_L=1 has been attributed to radionuclides of natural origin. The list of the "Radioactive Nuclides in Nature" has been taken from Ref. [23].

For any other nuclide the clearance level was calculated by using the following Eq. (6) taken from Ref. [26]:

$$C_L=\min \{1/(E_\gamma+ 0.1 \times E_\beta) ; ALI_{inhaled}/10^3 ; ALI_{ingested}/10^5\} \quad (6)$$

The values of E_γ and E_β in Eq. (6) have been taken from the JEFF-3.1.1 library [18].

The ALI quantities in Eq. (6) have been obtained from the "eaf_haz_20100" file of EASY-2010 [24]. The conversion factor of 0.020 (Sv/y) has been adopted to convert the dose coefficients from Ref. [24] to the ALI quantities.

3.1.4 Nuclide and Material Clearance Indexes

The Isotope Clearance Index (**ICI**) of a single nuclide is calculated in ANITA-4M as:

$$Isotope \quad Clearance \quad Index = \frac{C_i}{C_{Li}} \quad (7)$$

where C_i is the specific activity of the radionuclide "i" in the material and C_{Li} is the clearance level for that radionuclide.

In Eq. (7) activities and clearance levels have units of Bq g^{-1}.

When a material contains several nuclides, the equation given below, and suggested in [26], is used to evaluate in ANITA-4M the Material Clearance Index (**MCI**) :

$$Material \quad Clearance \quad Index = \sum_{i=1}^{n} \frac{C_i}{C_{Li}} \tag{8}$$

If **MCI** ≤ 1 then it is possible to clear the material.

3.1.5 Structure of the "fl1" file

The structure of the **fl1** file used by ANITA-4M is described in the following:

Card 1 NUCLIB,TITLIB
(I10**,**15A4)
where: NUCLIB: number of nuclides (stable or unstable) contained in the file
TITLIB : alphanumeric title

For each nuclide two cards are given:

Card 2a IDNUC, IDEC, λ_1, Q_1,G_1, λ_2, Q_2, G_2
(I7,1X,I2,E10.4,2F10.7,E10.4,2F10.7)
Card 2b IDNUC, IDEC, Q_T,ALI,CLEAR, SYMB
(I7,1X,I2,F10.7,2E10.2,1X,A11)

where:

IDNUC identification of the nuclide= Z*10000 + A*10 + M
Z= atomic number
A= mass number
M= 0,1,2 for the ground state, the first and the second metastable state, respectively

IDEC identification of the decay type (see Table 1)
0< IDEC < 10 single decay
10≤ IDEC double decay
"blank" indicates stable isotopes; in this case "Q_1" is the isotopic abundance and λ, Q, G are zeroes;

=0	indicates naturally occurring very long-lived radioactive nuclei. Q_1 in this case is their isotopic abundance and the decay parameters are given as λ_2, Q_2, G_2.

λ_1	decay constant (s^{-1})
Q_1	total energy (MeV) released in the decay (used to calculate the decay heat)
G_1	energy released (MeV) in the form of X or γ rays

When a nuclide has two decay modes a second set of values λ_2, Q_2, G_2 is given. In this case the decay constants λ_1 e λ_2 were obtained by multiplying the decay constant λ for the branching-ratio of each decay mode while Q_2 e G_2 are equal to Q_1 e G_1 .

When one of the two decay modes has a negligible probability only the dominant mode has been given with branching ratio, BR= 1. When more than two decay modes are present only the two most important are considered in the library, with the BR normalised in order to have a total BR=1. These particular cases are outlined by a comment.

Q_{TOT}	= Q_1 (MeV)
ALI	is the Annual Limit of Intake (Bq) by ingestion, for the public
CLEAR	clearance level (Bq/g)
SYMB	alphanumeric symbol

IDEC	Type of decay	"Parent nucleus"	"Daughter nuclei"		
1	β^-	A Z m	A	Z+1	0
2	β^+/EC		A	Z-1	0
3	IT_1		A	Z	0
4	α		A-4	Z-2	0
5	IT_2		A	Z	m-1
10	β^-		A	Z+1	0
			A	Z+1	1
12	β^- and β^+		A	Z+1	0
			A	Z-1	0
13	β^- and IT		A	Z+1	0
			A	Z	0
20	β^+/EC		A	Z-1	0
			A	Z-1	1
23	β^+ and IT		A	Z-1	0
			A	Z	0

Table 1 – Decay processes

An example of the **fl1** file (related to some Co isotopes) is given in the following.

```
 *JEFF-3.1.1 Decay&Hazard&Clearance Data                                          |Card 1
.....................................................................................................................
 270540  2 3.587E+00 4.4213428 1.0210000                                         |Card 2a
 270540  2 4.4213428  6.67E+07  7.35E-01 27-CO- 54                               |Card 2b
 270541  2 7.806E-03 5.9777899 3.9305599                                         |Card 2a
 270541  2 5.9777899  1.09E+05  2.42E-01 27-CO- 54M                              |Card 2b
 270550  2 1.098E-05 2.4436109 2.0070300                                         |Card 2a
 270550  2 2.4436109  1.00E+06  1.00E+01 27-CO- 55                               |Card 2b
 270560  2 1.038E-07 3.7138441 3.5916100                                         |Card 2a
 270560  2 3.7138441  4.00E+05  1.00E-01 27-CO- 56                               |Card 2b
 270570  2 2.952E-08 0.1435085 0.1252160                                         |Card 2a
 270570  2 0.1435085  4.76E+06  1.00E+00 27-CO- 57                               |Card 2b
 270580  2 1.132E-07 1.0105141 0.9762030                                         |Card 2a
 270580  2 1.0105141  1.35E+06  1.00E+00 27-CO- 58                               |Card 2b
 270581  3 2.163E-05 0.0240866 0.0018165                                         |Card 2a
 270581  3 0.0240866  4.17E+07  1.00E+04 27-CO- 58M                              |Card 2b
 270590                    1.                                                    |Card 2a
 270590                                   27-CO- 59                              |Card 2b
 270600  1 4.167E-09 2.6006136 2.5038400                                         |Card 2a
 270600  1 2.6006136  2.94E+05  1.00E-01 27-CO- 60                               |Card 2b
 270601 13 2.758E-06 0.0624753 0.0067864 1.101E-03 0.0624753 0.0067864          |Card 2a
 270601 13 0.0624753  5.88E+08  1.00E+03 27-CO- 60M                              |Card 2b
 270610  1 1.167E-04 0.5633246 0.0969656                                         |Card 2a
 270610  1 0.5633246  1.35E+07  1.00E+02 27-CO- 61                               |Card 2b
 270620  1 7.702E-03 3.2399399 1.6002600                                         |Card 2a
 270620  1 3.2399399  1.96E+05  5.67E-01 27-CO- 62                               |Card 2b
 270621 13 8.222E-04 3.5220399 1.7611300 8.305E-06 3.5220399 1.7611300          |Card 2a
 270621 13 3.5220399  2.13E+07  1.00E+01 27-CO- 62M                              |Card 2b
 270630  1 2.530E-02 1.7124330 0.1440830                                         |Card 2a
 270630  1 1.7124330  1.23E+06  3.32E+00 27-CO- 63                               |Card 2b
 270640  1 2.310E+00 3.4698150 0.1811650                                         |Card 2a
 270640  1 3.4698150  5.56E+07  1.96E+00 27-CO- 64                               |Card 2b
 270650  1 5.776E-01 2.7796230 0.1147330                                         |Card 2a
 270650  1 2.7796230  1.22E+07  2.62E+00 27-CO- 65                               |Card 2b
 270660  1 2.975E+00 6.1114502 2.7542801                                         |Card 2a
 270660  1 6.1114502  3.57E+07  3.24E-01 27-CO- 66                               |Card 2b
 270670  1 1.631E+00 3.4482501 0.6941000                                         |Card 2a
 270670  1 3.4482501  2.70E+07  1.03E+00 27-CO- 67                               |Card 2b
 270680  1 3.483E+00 7.2848501 3.4444201                                         |Card 2a
 270680  1 7.2848501  2.56E+07  2.61E-01 27-CO- 68                               |Card 2b
 270681 13 2.166E-01 4.1629400 2.1189699 2.166E-01 4.1629400 2.1189699          |Card 2a
 270681 13 4.1629400  3.03E+06  4.30E-01 27-CO- 68M                              |Card 2b
 270690  1 3.053E+00 6.6265812 3.3065500                                         |Card 2a
 270690  1 6.6265812  2.08E+07  2.75E-01 27-CO- 69  *only decay type 1 considered*  |Card 2b
.....................................................................................
```

3.2 Gamma Library (file "fl2")

This data base contains the gamma ray spectra emitted by the radioactive nuclei in the ORNL-SCALE 18-γ energy group structure given in Table 2.

Group	Energy	Group	Energy
1	10-100 KeV	10	1.66-2.0 MeV
2	.1-.2 MeV	11	2.0-2.5 MeV
3	.2-.4 MeV	12	2.5-3.0 MeV
4	.4-.6 MeV	13	3.0-4.0 MeV
5	.6-.8 MeV	14	4.0-5.0 MeV
6	.8-1. MeV	15	5.0-6.5 MeV
7	1.0-1.22 MeV	16	6.5-8.0 MeV
8	1.22-1.44 MeV	17	8.0-10.0 MeV
9	1.44-1.66 MeV	18	10.-20. MeV

Table 2 – ORNL-SCALE 18-γ energy group structure

The data contained in the library are based on the JEFF-3.1.1 evaluated decay data file (gamma radiation spectra). In the gamma library of ANITA-4M in each group the contribution in MeV of the total γ energy emitted is given. The gamma spectra include both the γ-rays spectra and the x-rays and annihilation radiation spectra (photons not arising as transitions between nuclear states) (STYP=0 and STYP=9 in the ENDF-6 standard format). In the library, four cards are given for each nuclide: the first one contains the identification number IDNUC (Z*10000+A*10+M), the alphanumeric symbol and the total Eγ energy calculated as the sum over the 18-group values. Then three cards follow for the 18-group values.

As an example of the structure of the file, the data related to the isotopes from 4-Be-7 to 7-N-13, are given in the following.

```
40070      4-Be-  7             4.98619E-02                                    5
0.00000E+00 0.00000E+00 0.00000E+00 4.98619E-02 0.00000E+00 0.00000E+00       6
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00       7
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00       8
40110      4-Be- 11             1.39541E+00                                    9
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      10
0.00000E+00 0.00000E+00 0.00000E+00 4.96216E-03 7.01184E-01 2.69058E-03      11
0.00000E+00 9.33261E-02 1.48234E-01 4.45012E-01 0.00000E+00 0.00000E+00      12
50120      5-B - 12             5.68179E-02                                   13
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      14
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      15
0.00000E+00 5.68179E-02 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      16
50130      5-B - 13             2.79976E-01                                   17
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      18
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      19
2.79976E-01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      20
50140      5-B - 14             5.93628E+00                                   21
```

```
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 1.36771E-02 0.00000E+00      22
0.00000E+00 3.49440E-02 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      23
0.00000E+00 0.00000E+00 5.23946E+00 6.48200E-01 0.00000E+00 0.00000E+00      24
60100      6-C - 10             1.74429E+00                                  25
5.68297E-11 0.00000E+00 0.00000E+00 1.02162E+00 7.07702E-01 0.00000E+00      26
1.49682E-02 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      27
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      28
60110      6-C - 11             1.01944E+00                                  29
4.19710E-10 0.00000E+00 0.00000E+00 1.01944E+00 0.00000E+00 0.00000E+00      30
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      31
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      32
60150      6-C - 15             3.60900E+00                                  33
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      34
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      35
0.00000E+00 0.00000E+00 3.60255E+00 5.40143E-04 5.91552E-03 0.00000E+00      36
70120      7-N - 12             1.19062E+00                                  37
4.19727E-14 0.00000E+00 0.00000E+00 1.02121E+00 0.00000E+00 0.00000E+00      38
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      39
4.82295E-02 1.21182E-01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      40
70130      7-N - 13             1.02014E+00                                  41
9.29712E-10 0.00000E+00 0.00000E+00 1.02014E+00 0.00000E+00 0.00000E+00      42
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      43
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00      44
```

The data given in the gamma library are used in ANITA-4M to compute the intensity and the energy distribution of the gamma-rays emitted by the irradiated composition. This gamma-ray source (Photons/cm^3 s) in the ORNL-SCALE 18-γ energy group structure (see Table 2) may be given as input to a radiation transport code to compute the space and energy distribution of the decay gamma-rays and the relative dose equivalent rate.

The production of the new **fl1** and **fl2** files required the development of a series of proper interface codes in order to process the JEFF-3.1.1 evaluated decay data (in ENDF-6 standard format), to calculate the ALI and clearance level data and to convert these data into the format required by ANITA-4M.

The flexibility of the procedures developed makes it possible to produce any other similar library in the ANITA-4M format based on whatever nuclear evaluated decay data file. It is also possible to define otherwise, if required, the ALI data and clearance levels.

3.3 Neutron activation cross section data library (file "lib175")

As shown in Figure 1 the ANITA-4M code requires a neutron activation cross section data library, defined as **lib175** in binary format, in order to perform the activation calculations.

In the ANITA-2000 code package in free distribution at NEADB and RSICC two different libraries are included:

- The activation library "eaf99_lib", based on the EAF-99 neutron activation cross section data library [15]. It contains 12,039 activation reactions, up to Pu-247, in the 175- group VITAMIN-J neutron energy structure.
- The activation library "fendl2a_lib", based on the Fusion Evaluated Nuclear Data File FENDL/A-2.0 [16]. It contains 12,392 activation reactions, up to Pu-247, in the 175- group VITAMIN-J neutron energy structure.

The format of these multi-group libraries (VITAMIN-J 175 neutron groups structure [27]) is the LIBOUT format of the code FOUR ACES (ENEA Bologna) with two additional comment lines for each reaction. For the reaction numbers the ENDF-6 reaction number MT multiplied by 10 has been adopted, with the convention that for the excitation of each isomeric state the reaction number is increased by one. The material numbers consist of Z,A and an identifier, LIS, to indicate ground or isomeric target (MAT=Z*10000+A*10+LIS). The order of the cross sections is in accordance with increasing Z,A,LIS and MT. The cross section values of each reaction MT are in accordance with decreasing energy of the 175 VITAMIN-J group structure.

These libraries are given in card-image format. The MODBIN module, provided in the package, makes the conversion to **lib175** in binary format as required by ANITA-4M code

The updating of the **fl1** file, that now contains data for more nuclides than the original one, allows ANITA-4M code to perform activation calculations by using the neutron-induced cross section library EAF-2010 [19] contained in the package EASY-2010 [20], named "eaf-ngxs_175_fus_20100". This cross section library contains 66,256 excitation functions involving 816 different targets from ^{1}H to ^{257}Fm, atomic numbers 1 to 100, in the energy range 10^{-5} eV to 20 MeV. It was obtained at Culham by processing the point-wise file with a micro-flux weighting spectrum combining a thermal Maxwellian at low energies, a 1/E function at intermediate energies, and a velocity exponential fusion peak spectrum with a peak at 14.07 MeV, in the 175-group VITAMIN-J 175 neutron energy structure.

The card image library "eaf2010_lib" for ANITA-4M has been derived from the file "eaf-ngxs_175_fus_20100" of EASY-2010 package. It contains 63,512 activation reactions, up to Pu-247, in the 175- group VITAMIN-J neutron energy structure. The MODBIN module must be used for the conversion of the card image file to **lib175** in binary format as required by ANITA-4M code.

4 ANITA-4M VALIDATION AGAINST ELECTRON-PHOTON DECAY HEAT AND ACTIVITY MEASUREMENTS AT FNG ENEA-FRASCATI

The aim of this assessment is the validation of the ANITA-4M activation code using the new data libraries based on the JEFF-3.1.1 Decay Data Library and the EAF-2010 neutron activation cross section library.

A preliminary validation has been performed through the comparison of the material decay heats and activities measured in experiments performed at the Frascati Neutron Generator (FNG) with those calculated by the ANITA-4M activation code.

The total activity of a neutron irradiated material is directly proportional to the activation reaction cross section and the electron and photon decay heats are proportional to the product of the of the cross section and the mean decay beta and gamma energies. Through the comparison with the FNG experimental results it is possible to validate both the cross sections library and the decay database used by ANITA-4M.

4.1 The FNG experimental configuration

The experiments were carried out at the ENEA Research Centre of Frascati at the 14-MeV Frascati Neutron Generator (FNG) based on the T(d,n)α fusion reaction. FNG produces up to 10^{11} neutrons/s in steady state or pulse mode. FNG can also produce 2.5-MeV neutrons via the D(d,n)^{3}He fusion reaction [28].

The FNG group used a neutron reflector that forms an irradiation cavity where the neutron spectrum simulates that existing in the first wall of a typical fusion device.

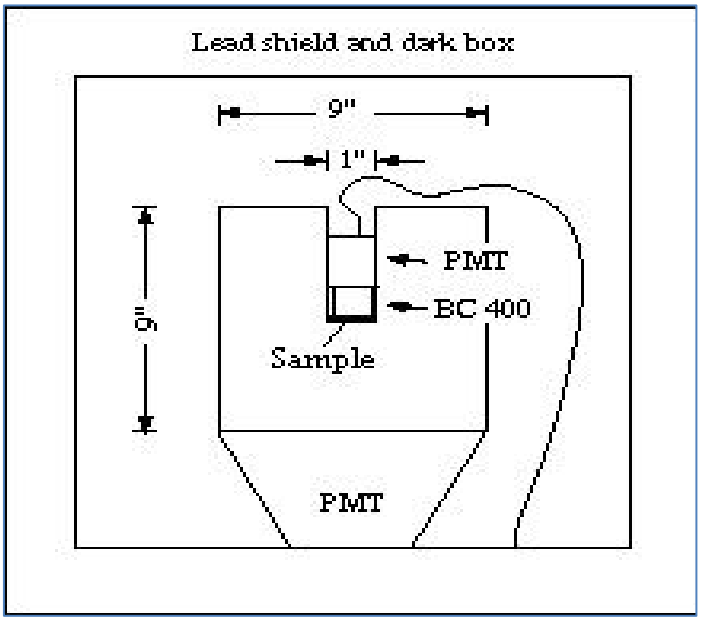
Samples could be irradiated at several distances from the 14 MeV neutron source of FNG, enclosed in the cavity. Twelve high purity samples of different materials (i.e. Mo, Cu, Hf, Mg, Ni, Cd, Sn, Re, Ti, W, Ag, Al) were irradiated at a fixed position close to the FNG neutron target.

The details of the experimental setup, taken from Ref. [28], are briefly described in the following.

The neutron yield was monitored by the associated particle method [29] while the neutron spectrum was measured with several activation foils and unfolded using suitable computer codes[30] [31].The irradiation time and the neutron yield were adjusted in order to have similar decay heat rates in the spectrometer. The irradiation time ranged between 160 and 1600 s and the typical total neutron flux was in the range from 1×10^8 to 1×10^9 n cm^{-2} s^{-1}. After the irradiation the samples were manually transported and inserted in the spectrometer. This procedure required about 120 s; then the counting was started. Each sample was measured about 4-6 times, for 30 s.

The spectrometer consists of a large cylindrical (22.8 x 22.8 cm) well-type CsI(Tl) scintillator and a small (1.9 cm diameter, 2.6 cm high) plastic BC400 scintillator inserted in the well (see

Figure 2). The CsI(Tl) crystal have larger density and atomic number compared to more common NaI(Tl) scintillators. The dimensions chosen permit to detect with high efficiency (≈100%) almost only photon radiation while electrons are adsorbed and eventually converted into x-rays in the entrance window. The BC400 scintillator is window-less; it has low density and atomic number. Its dimensions where chosen to detect virtually only β radiation and conversion electrons with about 50% efficiency (2π geometry). Time response of this detector is very fast, a 0.5 μs shaping constant was used to reduce any coincidence effect.



(BC 400 is a plastic scintillator; PMT is a CsI(Tl) scintillator)

Figure 2 – Sketch of the spectrometer assembly

Both detectors have been energy calibrated using standard radiation sources, while accurate detection efficiency is calculated by modelling the spectrometer and the material sample under study using the MCNP-4C radiation transport code [32]. Thin material samples (disc-shaped, ≤ 25 μm thick, 1.8 cm diameter) are used to reduce radiation self-adsorption. The very different sensitivity to photons and electrons of the two scintillators permits, after a software correction that takes into account the small sensitivity of one detector to the unwanted radiation, a determination of the absolute activity and the total photon and electron heats. Both scintillators are thermally stabilised using a suitable unit to avoid a temperature dependent light response. The decay heat (in units of μW/g) is deduced from the two pulse-height spectra (PHS) recorded by multi-channel analysers according to the following formula (9) given in Ref. [28]:

$$\text{Decay heat} = 1.6\times10^{-19}\times f_i \times \sum_i (C_i \times E_i)/(T_c \times m) \qquad (9)$$

Each count (C_i) of the PHS in the channel-i is multiplied by the corresponding energy (E_i) and summed to obtain the total deposited energy. The total energy is divided by the counting time T_c and the sample mass m; f_i is the correction factor for the efficiency calculated by MCNP-4C and corresponds to the fraction of the energy lost.

Typical backgrounds in the spectrometer are about 0.3 Bq for activity detection and 1.4×10^{-5}, 2.5×10^{-8} μW for photon and electron heat measurements respectively.

The experimental errors involved in the measurements are summarized in the following Table 3 (from [28]).

Source	Activity uncertainty (%)	Heat uncertainty (%)
Sample weight	< 0.5	< 0.5
Energy calibration	1	3
Background subtraction	0.5 ÷ 1.5	1 ÷ 2.5
Dead time correction	1	5
Detection efficiency	5 ÷ 60	2 ÷ 20
Neutron flux	10	10

Table 3 – Uncertainty sources in the measurements

The main contribution comes from the correction factors for the detection efficiency.

4.2 Calculation approach

Sample decay heat (and activity) at various times after the end of the irradiation have been evaluated using the ANITA-4M activation code. The new Decay, Hazard and Clearance Data library (file **fl1**) based on JEFF-3.1.1 data and the neutron activation file based on EAF-2010 were used in the calculations. The assessment refers to Mo, Cu, Hf, Mg, Ni, Cd, Sn, Re, Ti, W, Ag, and Al samples.

The details of the experimental set-up (material composition, irradiation time, flux, etc.) used in the activation input files in order to model each experiment are summarized in Table 4.

The unfolded neutron flux spectrum in the 175 VITAMIN-J energy group structure has been provided by FNG team (see Figure 3). It has been used as input for the ANITA calculations for each material sample under analysis.

For sake of comparison the EASY-2010 code package (FISPACT-2010 code + EAF-2010 libraries) [20] has been also used for decay heat an activity calculations.

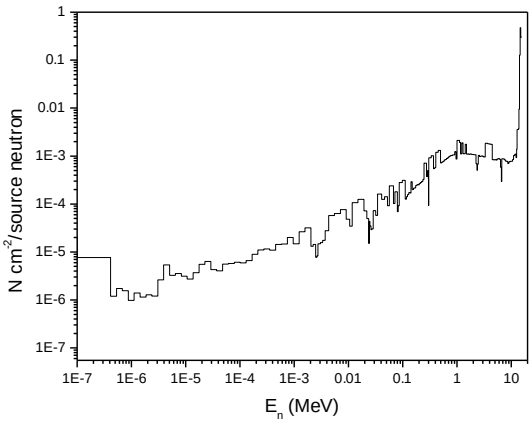


Figure 3 – 175 group VITAMIN-J unfolded neutron flux spectrum

Material : Molybdenum (Mo)

Sample weight : 6.8560 x 10^{-5} kg
Sample composition (wt%):
Mo 100
Total neutron irradiation flux 3.131 x 10^{8} n/cm^2 s
Sample irradiation time 330 s

Material : Copper (Cu)

Sample weight : 5.1460 x 10^{-5} kg
Sample composition (wt%):
Cu 100
Total neutron irradiation flux 2.462 x 10^{8} n/cm^2 s
Sample irradiation time 161 s

Material : Hafnium (Hf)

Sample weight : 7.9200 x 10^{-5} kg
Sample composition (wt%):
Hf 100
Total neutron irradiation flux 4.710 x 10^{8} n/cm^2 s
Sample irradiation time 300 s

Material : Magnesium (Mg)

Sample weight : 1.3205 x 10^{-5} kg
Sample composition (wt%):
Mg 100
Total neutron irradiation flux 4.642 x 10^{8} n/cm^2 s
Sample irradiation time 300 s

Material : Nickel (Ni)

Sample weight : 6.1598 x 10^{-5} kg
Sample composition (wt%):
Ni 99.9998, C 0.0001, Fe 0.0001
Total neutron irradiation flux 5.723 x 10^{8} n/cm^2 s
Sample irradiation time 600 s

Material : Cadmium (Cd)

Sample weight : 5.8490 x 10^{-5} kg
Sample composition (wt%):
Cd 100
Total neutron irradiation flux 4.229 x 10^{8} n/cm^2 s
Sample irradiation time 300 s

Table 4 – Material samples characteristics and irradiation condition

Material : Tin (Sn)

Sample weight : 4.7297 x 10^{-5} kg
Sample composition (wt%):
Sn 99.99523, Cu 0.001, In 0.0001, Fe 0.00005, Pb 0.002, Mg 0.00002, Ag 0.0001, Sb 0.0015
Total neutron irradiation flux 3.704 x 10^{8} n/cm^2 s
Sample irradiation time 300 s

Material : Rhenium (Re)

Sample weight : 1.4710 x 10^{-4} kg
Sample composition (wt%):
Re 100
Total neutron irradiation flux 5.558 x 10^{8} n/cm^2 s
Sample irradiation time 1500 s

Material : Titanium (Ti)

Sample weight : 2.8070 x 10^{-5} kg
Sample composition (wt%):
Ti 99.99932, Fe 0.00055, V 0.00013
Total neutron irradiation flux 4.966 x 10^{8} n/cm^2 s
Sample irradiation time 600 s

Material : Tungsten (W)

Sample weight : 1.3100 x 10^{-4} kg
Sample composition (wt%):
W 100
Total neutron irradiation flux 5.630 x 10^{8} n/cm^2 s
Sample irradiation time 1500 s

Material : Silver (Ag)

Sample weight : 6.8900 x 10^{-5} kg
Sample composition (wt%):
Ag 99.9979, Cu 0.0005, Cd 0.0005, Fe 0.0002, Mg 0.0002, Ca 0.0002, Si 0.0005
Total neutron irradiation flux 2.419 x 10^{8} n/cm^2 s
Sample irradiation time 300 s

Material : Aluminum (Al)

Sample weight : 1.5700 x 10^{-5} kg
Sample composition (wt%):
Al 100
Total neutron irradiation flux (Test-1) 4.734 x 10^{8} n/cm^2 s
Total neutron irradiation flux (Test-2) 3.243 x 108 n/cm^2 s
Sample irradiation time (Test-1) 600 s
Sample irradiation time (Test-2) 901 s

Table **4** – Material samples characteristics and irradiation condition *(continued)*

4.3 Calculation results and comparison with the experimental values

The experimental values and the corresponding ANITA-4M and FISPACT-2010 calculated results are shown in Table 5 for the material samples electron decay heat and in Table 6 for the photon decay heat, at different cooling times for each sample.

In those tables, the C/E ratios between the calculated and the experimental results (both for ANITA-4M and FISPACT-2010 codes) are also shown. In Table 5 and Table 6 the calculation uncertainties are those provided by EASY-2010 system. They are obtained taking into account both the cross section and half-life uncertainties. It is assumed that the same uncertainties can be attributed also to the ANITA-M results due to the fact that in the calculations the same EAF-2010 neutron activation cross section library has been used.

Material sample activities have been also measured by FNG group at different times after irradiation. Calculations have been performed both using ANITA-4M and FISPACT-2010. The corresponding results are shown in Table 7.

In Figure 4 to Figure 6 the C/E values (with the error bars) for material samples electron, photon decay heat and activity are shown. The calculated values C are those obtained by using ANITA-4M. For each nuclide the C/E values have been calculated as a mean over the cooling times. The error bars are a proper combination of the experimental error and the error calculated by FISPACT code and attributed to ANITA code (the relative error on C/E has been calculated as the sum of the relative errors of both the C and E values).

FNG experiment : electron decay heat								
Material	**Cooling time**	**Measurements**	**Calculation**				**Uncertainties**	
			ANITA-4M (EAF-2010)	**C/E**	**FISPACT-2010 (EAF-2010)**	**C/E**	**Exp.**	**Calc.**
	[s]	[kW]	[kW]		[kW]			
Mo	148	2.21E-13	2.80E-13	1.27	2.86E-13	1.29	± 2.1%	± 26.6%
	320	1.95E-13	2.38E-13	1.22	2.43E-13	1.25	± 2.2%	± 27.7%
	625	1.53E-13	1.88E-13	1.23	1.92E-13	1.25	± 2.3%	± 27.9%
	926	1.24E-13	1.51E-13	1.22	1.54E-13	1.24	± 2.4%	± 27.8%
Cu	172	1.18E-12	1.27E-12	1.08	1.27E-12	1.08	± 10.2%	± 9.8%
	348	9.64E-13	1.03E-12	1.07	1.02E-12	1.06	± 10.2%	± 9.9%
	880	5.10E-13	5.47E-13	1.07	5.45E-13	1.07	± 10.2%	± 9.9%
	1443	2.63E-13	2.82E-13	1.07	2.81E-13	1.07	± 10.2%	± 9.8%
Hf	136	1.36E-14	8.16E-15	0.60	8.58E-15	0.63	± 6.9%	± 16.5%
	318	6.84E-15	3.70E-15	0.54	4.10E-15	0.60	± 7.9%	± 22.6%
	638	4.72E-15	2.73E-15	0.58	3.10E-15	0.66	± 6.6%	± 19.7%
	963	3.51E-15	2.15E-15	0.61	2.48E-15	0.71	± 5.5%	± 18.6%
Mg	136	9.08E-14	7.30E-14	0.80	7.30E-14	0.80	± 2.5%	± 14.0%
	316	1.76E-14	1.32E-14	0.75	1.32E-14	0.75	± 3.8%	± 25.8%
	616	8.46E-15	7.06E-15	0.83	7.07E-15	0.84	± 5.1%	± 45.4%
	958	8.49E-15	6.83E-15	0.80	6.84E-15	0.81	± 5.1%	± 46.7%
Ni	139	5.10E-14	7.44E-14	1.46	6.47E-14	1.27	± 3.3%	± 13.4%
	318	2.91E-14	4.95E-14	1.70	4.12E-14	1.42	± 4.3%	± 14.9%
	617	1.88E-14	3.41E-14	1.81	2.77E-14	1.47	± 5.4%	± 15.9%
	918	1.43E-14	2.60E-14	1.82	2.11E-14	1.48	± 6.0%	± 15.3%
Cd	136	5.10E-14	4.51E-14	0.88	3.96E-14	0.78	± 4.1%	± 11.7%
	317	4.60E-14	3.67E-14	0.80	3.14E-14	0.68	± 4.3%	± 13.4%
	618	4.12E-14	3.21E-14	0.78	2.72E-14	0.66	± 4.5%	± 14.2%
	917	3.69E-14	2.96E-14	0.80	2.49E-14	0.67	± 4.8%	± 14.4%
Sn	137	3.76E-14	4.03E-14	1.07	3.27E-14	0.87	± 3.3%	± 11.0%
	316	2.97E-14	3.24E-14	1.09	2.50E-14	0.84	± 3.6%	± 12.7%
	616	2.39E-14	2.72E-14	1.14	2.03E-14	0.85	± 4.0%	± 13.7%
	917	2.09E-14	2.39E-14	1.14	1.76E-14	0.84	± 4.3%	± 14.4%
Re	136	7.99E-14	5.60E-14	0.70	5.76E-14	0.72	± 5.8%	± 15.6%
	318	7.93E-14	5.39E-14	0.68	5.53E-14	0.70	± 5.7%	± 16.2%
	619	7.75E-14	5.32E-14	0.69	5.44E-14	0.70	± 5.8%	± 16.5%
	919	7.65E-14	5.31E-14	0.69	5.40E-14	0.71	± 6.0%	± 16.5%
	1141	7.65E-14	5.31E-14	0.69	5.38E-14	0.70	± 5.5%	± 16.6%
Ti	137	2.17E-14	2.00E-14	0.92	2.00E-14	0.92	± 3.6%	± 34.5%
	317	1.28E-14	1.10E-14	0.86	1.10E-14	0.86	± 4.5%	±19.4%
	617	8.54E-15	7.37E-15	0.86	7.38E-15	0.86	± 5.4%	± 8.7%
	918	7.93E-15	6.60E-15	0.83	6.61E-15	0.83	± 5. 6%	± 8.4%
W	139	3.55E-13	4.89E-13	1.38	4.88E-13	1.37	± 16.3%	± 19.1%
	320	1.11E-13	1.54E-13	1.39	1.52E-13	1.37	± 10.2%	± 17.6%
	619	2.56E-14	3.30E-14	1.29	3.15E-14	1.23	± 7.2%	± 12.8%
	923	1.31E-14	1.46E-14	1.11	1.32E-14	1.01	± 7.6%	± 12.5%
	1085	1.07E-14	1.17E-14	1.09	1.04E-14	0.97	± 4.6%	± 13.1%
Ag	138	2.16E-12	1.59E-12	0.74	1.59E-12	0.74	± 2.6%	± 23.0%
	319	1.12E-12	8.10E-13	0.72	8.10E-13	0.72	± 2.2%	± 21.2%
	621	5.30E-13	3.76E-13	0.71	3.76E-13	0.71	± 1.9%	± 22.1%
	923	3.53E-13	2.48E-13	0.70	2.48E-13	0.70	± 1.9%	± 26.5%
Al (Test-1)	138	6.04E-13	5.29E-13	0.88	5.29E-13	0.88	± 1.6%	± 9.7%
	323	4.90E-13	4.20E-13	0.86	4.20E-13	0.86	± 1.6%	± 9.7%
	621	3.46E-13	2.93E-13	0.85	2.93E-13	0.85	± 1.7%	± 9.7%
	922	2.44E-13	2.06E-13	0.84	2.06E-13	0.84	± 1.8%	± 9.8%
Al (Test-2)	4547	1.66E-14	1.34E-14	0.81	1.34E-14	0.81	± 2.0%	± 39.0%
	6324	1.42E-14	1.13E-14	0.80	1.13E-14	0.80	± 2.1%	± 45.1%

Table 5 – FNG experiment: electron decay heat – Experimental and calculated results

FNG experiment : photon decay heat								
Material	Cooling time	Measurements	Calculation				Uncertainties	
			ANITA-4M (EAF-2010)	C/E	FISPACT-2010 (EAF-2010)	C/E	Exp.	Calc.
	[s]	[kW]	[kW]		[kW]			
Mo	148	2.32E-13	2.25E-13	0.97	2.29E-13	0.99	± 2.1%	± 22.4%
	320	1.84E-13	1.73E-13	0.94	1.76E-13	0.96	± 2.3%	± 25.7%
	625	1.44E-13	1.33E-13	0.92	1.36E-13	0.94	± 2.3%	± 26.5%
	926	1.19E-13	1.07E-13	0.90	1.09E-13	0.92	± 2.8%	± 26.5%
Cu	172	1.38E-12	1.01E-12	0.73	1.01E-12	0.73	± 10.2%	± 9.7%
	348	1.09E-12	8.12E-13	0.74	8.16E-13	0.75	± 10.2%	± 9.8%
	880	5.63E-13	4.33E-13	0.77	4.36E-13	0.77	± 10.2%	± 9.8%
	1443	2.88E-13	2.24E-13	0.78	2.26E-13	0.78	± 10.2%	± 9.7%
Hf	136	4.29E-14	1.62E-14	0.38	1.81E-14	0.42	± 5.4%	± 19.6%
	318	2.53E-14	7.78E-15	0.31	9.59E-15	0.38	± 6.4%	± 27.2%
	638	1.38E-14	5.67E-15	0.41	7.33E-15	0.53	± 7.4%	± 26.4%
	963	8.87E-15	4.48E-15	0.51	6.00E-15	0.68	± 7.1%	± 27.1%
Mg	136	8.14E-14	6.59E-14	0.81	6.59E-14	0.81	± 2.8%	± 36.6%
	316	6.35E-14	5.25E-14	0.83	5.25E-14	0.83	± 3.0%	± 45.6%
	616	5.94E-14	5.06E-14	0.85	5.06E-14	0.85	± 2.8%	± 47.1%
	958	6.03E-14	5.03E-14	0.83	5.03E-14	0.83	± 2.6%	± 47.2%
Ni	139	9.17E-14	5.93E-14	0.65	7.11E-14	0.78	± 2.9%	± 11.5%
	318	6.25E-14	3.84E-14	0.61	4.86E-14	0.78	± 3.2%	± 12.3%
	617	4.78E-14	2.79E-14	0.58	3.58E-14	0.75	± 3.6%	± 12.8%
	918	4.06E-14	2.32E-14	0.57	2.94E-14	0.72	± 4.7%	± 12.2%
Cd	136	1.12E-13	7.97E-14	0.71	8.16E-14	0.73	± 3.1%	± 14.4%
	317	1.01E-13	7.29E-14	0.72	7.47E-14	0.74	± 3.1%	± 14.9%
	618	8.85E-14	6.64E-14	0.75	6.81E-14	0.77	± 2.7%	± 15.2%
	917	8.44E-14	6.16E-14	0.73	6.32E-14	0.75	± 3.3%	± 15.2%
Sn	137	7.43E-14	5.41E-14	0.73	5.37E-14	0.72	± 3.1%	± 13.6%
	316	4.91E-14	3.62E-14	0.74	3.47E-14	0.71	± 3.7%	± 13.3%
	616	3.34E-14	2.53E-14	0.76	2.30E-14	0.69	± 5.1%	± 10.3%
	917	2.88E-14	1.98E-14	0.69	1.74E-14	0.60	± 6.9%	± 8.3%
Re	136	3.41E-14	1.50E-14	0.44	1.36E-14	0.40	± 10.9%	± 8.3%
	318	3.16E-14	1.42E-14	0.45	1.31E-14	0.41	± 11.9%	± 8.3%
	619	3.13E-14	1.36E-14	0.43	1.28E-14	0.41	± 13.3%	± 8.1%
	919	3.10E-14	1.31E-14	0.42	1.26E-14	0.41	± 14.4%	± 7.9%
	1141	2.46E-14	1.28E-14	0.52	1.24E-14	0.50	± 8.4%	± 7.8%
Ti	137	5.84E-14	3.91E-14	0.67	3.91E-14	0.67	± 3.0%	± 34.8%
	317	3.60E-14	2.18E-14	0.61	2.18E-14	0.61	± 3.3%	± 19.3%
	617	2.65E-14	1.54E-14	0.58	1.54E-14	0.58	± 4.7%	± 9.0%
	918	2.65E-14	1.45E-14	0.55	1.45E-14	0.55	± 5.8%	± 8.8%
W	139	1.55E-13	9.91E-14	0.64	9.70E-14	0.63	± 17.2%	± 15.1%
	320	6.96E-14	4.45E-14	0.64	4.32E-14	0.62	± 12.6%	± 12.4%
	619	3.45E-14	2.11E-14	0.61	2.07E-14	0.60	± 8.6%	± 12.9%
	923	2.91E-14	1.45E-14	0.50	1.46E-14	0.50	± 12.1%	± 13.0%
	1085	2.10E-14	1.26E-14	0.60	1.28E-14	0.61	± 5.5%	± 12.6%
Ag	138	7.66E-13	5.04E-13	0.66	5.04E-13	0.66	± 2.6%	± 26.6%
	319	6.65E-13	4.34E-13	0.65	4.34E-13	0.65	± 2.3%	± 28.2%
	621	5.56E-13	3.63E-13	0.65	3.63E-13	0.65	± 1.9%	± 29.2%
	923	4.79E-13	3.11E-13	0.65	3.11E-13	0.65	± 1.8%	± 29.4%
Al (Test-1)	138	8.77E-13	7.50E-13	0.86	7.50E-13	0.86	± 1.6%	± 10.2%
	323	7.12E-13	6.09E-13	0.86	6.09E-13	0.86	± 1.6%	± 10.7%
	621	5.19E-13	4.47E-13	0.86	4.47E-13	0.86	± 1.7%	± 12.0%
	922	3.88E-13	3.35E-13	0.86	3.35E-13	0.86	± 1.8%	± 13.9%
Al (Test-2)	4547	1.01E-13	8.66E-14	0.86	8.66E-14	0.86	± 1.6%	± 44.7%
	6324	9.59E-14	8.24E-14	0.86	8.24E-14	0.86	± 1.6%	± 45.9%

Table 6 – FNG experiment: photon decay heat – Experimental and calculated results

FNG experiment : material samples activity								
Material	Cooling time	Measurements	Calculation				Uncertainties	
			ANITA-4M (EAF-2010)	C/E	FISPACT-2010 (EAF-2010)	C/E	Exp.	Calc.
	[s]	[Bq]	[Bq]		[Bq]			
Mo	148	1.321E+03	1.56E+03	1.18	1.59E+03	1.20	± 4.2%	± 20.9%
	320	1.106E+03	1.23E+03	1.11	1.25E+03	1.13	± 4.5%	± 23.3%
	625	8.510E+02	9.30E+02	1.09	9.47E+02	1.11	± 4.7%	± 24.4%
	926	7.080E+02	7.29E+02	1.03	7.42E+02	1.05	± 5.9%	± 24.8%
Cu	172	8.114E+03	6.35E+03	0.78	6.35E+03	0.78	± 10.4%	± 9.6%
	348	6.489E+03	5.15E+03	0.79	5.15E+03	0.79	± 10.4%	± 9.6%
	880	3.443E+03	2.78E+03	0.81	2.78E+03	0.81	± 10.5%	± 9.5%
	1443	1.833E+03	1.47E+03	0.80	1.47E+03	0.80	± 10.8%	± 9.2%
Hf	136	4.900E+02	2.30E+02	0.47	2.39E+02	0.49	± 13.5%	± 14.6%
	318	1.500E+02	5.28E+01	0.35	6.12E+01	0.41	± 14.4%	± 21.3%
	638	9.300E+01	4.20E+01	0.45	4.99E+01	0.54	± 16.1%	± 20.7%
	963	6.500E+01	3.56E+01	0.55	4.29E+01	0.66	± 18.0%	± 21.0%
Mg	136	3.810E+02	3.35E+02	0.88	3.35E+02	0.88	± 6.5%	± 15.9%
	316	1.120E+02	1.03E+02	0.92	1.03E+02	0.92	± 11.5%	± 35.3%
	616	7.200E+01	7.80E+01	1.08	7.81E+01	1.08	± 14.3%	± 46.2%
	958	7.600E+01	7.67E+01	1.01	7.67E+01	1.01	± 13.0%	± 46.8%
Ni	139	1.913E+03	3.22E+03	1.68	3.22E+03	1.68	± 21.5%	± 24.0%
	318	1.593E+03	2.68E+03	1.68	2.68E+03	1.68	± 26.0%	± 23.8%
	617	1.100E+03	2.05E+03	1.86	2.05E+03	1.86	± 26.1%	± 22.8%
	918	8.230E+02	1.60E+03	1.94	1.60E+03	1.94	± 30.0%	± 21.6%
Cd	136	2.523E+03	1.76E+03	0.70	1.75E+03	0.69	± 9.4%	± 15.4%
	317	2.346E+03	1.53E+03	0.65	1.51E+03	0.64	± 9.4%	± 16.4%
	618	2.261E+03	1.39E+03	0.61	1.36E+03	0.60	± 8.1%	± 16.6%
	917	2.020E+03	1.29E+03	0.64	1.26E+03	0.62	± 9.4%	± 16.6%
Sn	137	6.080E+02	4.95E+02	0.81	5.06E+02	0.83	± 8.6%	± 11.6%
	316	5.180E+02	4.24E+02	0.82	4.32E+02	0.83	± 9.3%	± 12.4%
	616	4.280E+02	3.61E+02	0.84	3.66E+02	0.86	± 11.4%	± 12.8%
	917	3.840E+02	3.18E+02	0.83	3.21E+02	0.84	± 14.1%	± 12.9%
Re	136	1.865E+03	1.33E+03	0.71	1.33E+03	0.71	± 25.7%	± 13.2%
	318	1.772E+03	1.24E+03	0.70	1.24E+03	0.70	± 23.8%	± 13.8%
	619	1.692E+03	1.19E+03	0.70	1.20E+03	0.71	± 24.7%	± 14.1%
	919	1.725E+03	1.17E+03	0.68	1.18E+03	0.68	± 29.1%	± 14.2%
	1141	1.683E+03	1.16E+03	0.69	1.16E+03	0.69	± 23.2%	± 14.3%
Ti	137	1.770E+02	1.44E+02	0.81	1.44E+02	0.81	± 10.0%	± 19.1%
	317	1.310E+02	1.04E+02	0.79	1.04E+02	0.79	± 9.9%	± 10.4%
	617	1.060E+02	8.79E+01	0.83	8.79E+01	0.83	± 13.6%	± 8.3%
	918	1.020E+02	8.33E+01	0.82	8.34E+01	0.82	± 17.2%	± 8.4%
W	139	2.443E+04	1.73E+04	0.71	1.73E+04	0.71	± 63.6%	± 19.6%
	320	7.006E+03	5.18E+03	0.74	5.19E+03	0.74	± 57.7%	± 18.6%
	619	1.170E+03	9.22E+02	0.79	9.27E+02	0.79	± 37.6%	± 13.5%
	923	4.020E+02	3.45E+02	0.86	3.48E+02	0.87	± 38.7%	± 8.6%
	1085	3.060E+02	2.76E+02	0.90	2.79E+02	0.91	± 23.9%	± 8.9%
Ag	138	2.452E+04	1.99E+04	0.81	1.99E+04	0.81	± 6.4%	± 19.6%
	319	1.139E+04	9.17E+03	0.81	9.17E+03	0.81	± 4.8%	± 20.4%
	621	5.392E+03	4.44E+03	0.82	4.44E+03	0.82	± 4.2%	± 22.5%
	923	3.679E+03	3.04E+03	0.83	3.04E+03	0.83	± 4.1%	± 26.7%
Al (Test-1)	138	4.648E+03	4.71E+03	1.01	4.71E+03	1.01	± 3.5%	± 9.7%
	323	3.658E+03	3.76E+03	1.03	3.76E+03	1.03	± 3.7%	± 9.7%
	621	2.572E+03	2.64E+03	1.03	2.64E+03	1.03	± 4.0%	± 9.8%
	922	1.813E+03	1.87E+03	1.03	1.87E+03	1.03	± 4.2%	± 9.8%
Al (Test-2)	4547	1.530E+02	1.45E+02	0.95	1.45E+02	0.95	± 9.0%	± 40.3%
	6324	1.340E+02	1.26E+02	0.94	1.26E+02	0.94	± 9.6%	± 45.3%

Table 7 – FNG experiment : material samples activity – Experimental and calculated results

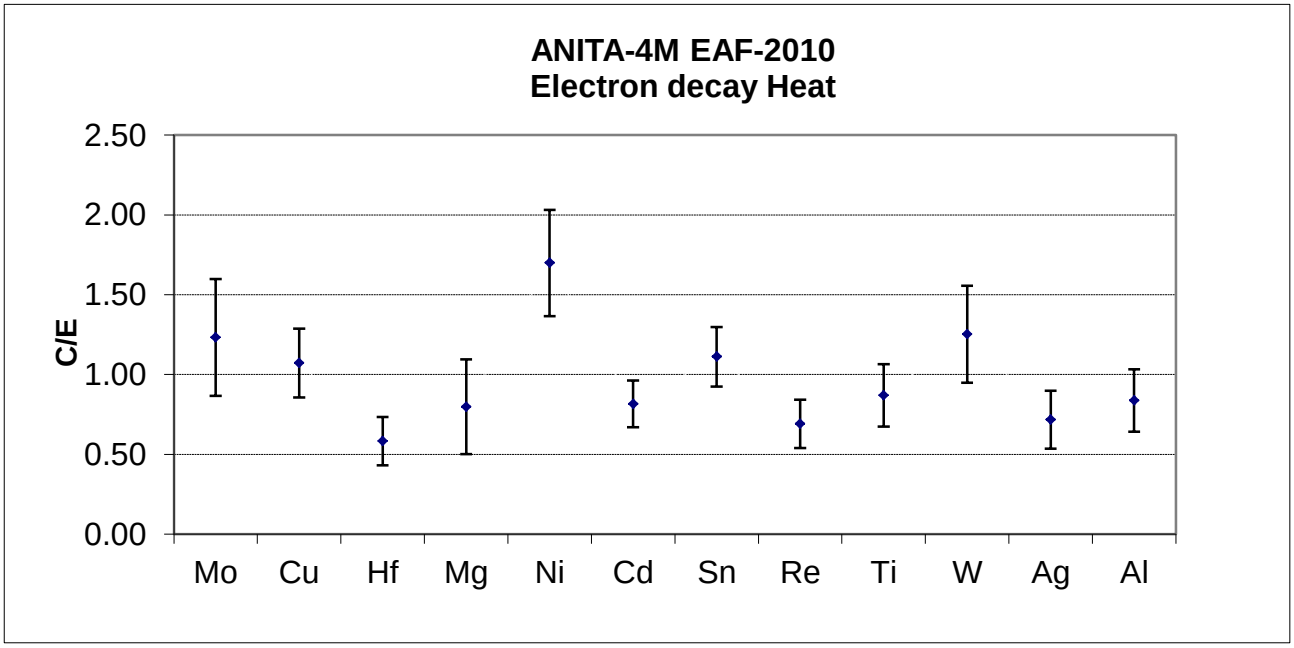


Figure 4 – Material electron-decay heat: Calculated (C) (ANITA-4M, EAF-2010 library) and Experimental (E) comparison

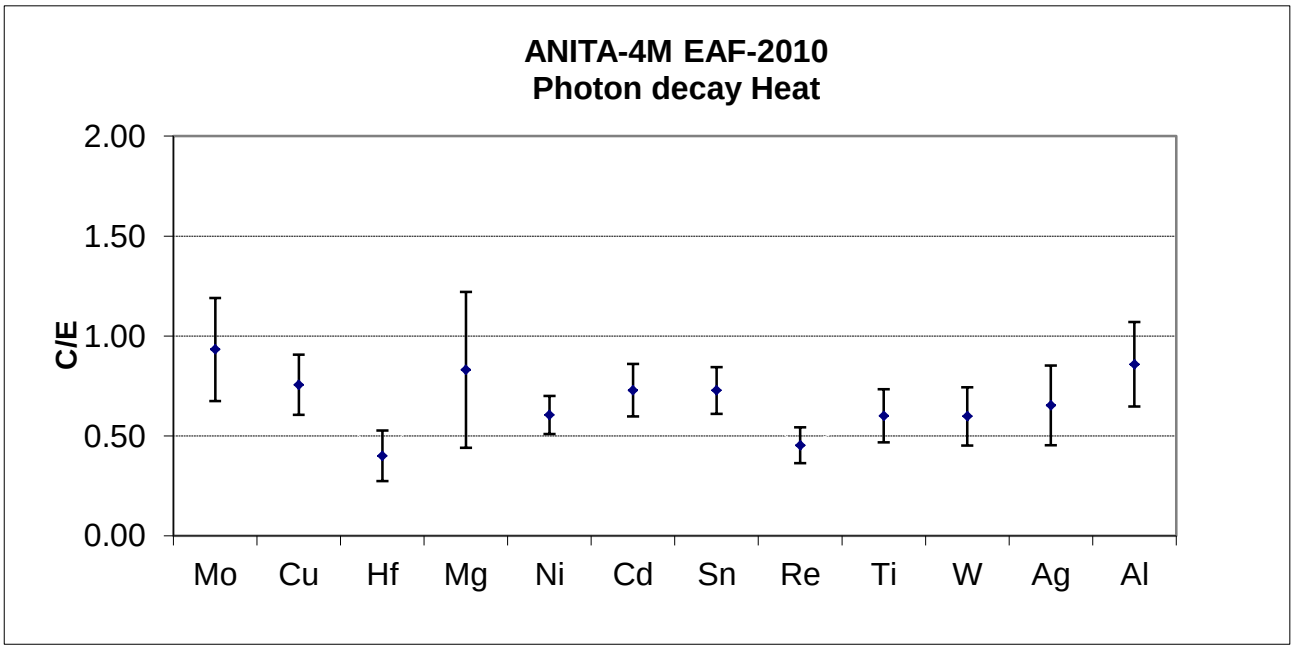


Figure 5 – Material photon-decay heat: Calculated (C) (ANITA-4M, EAF-2010 library) and Experimental (E) comparison

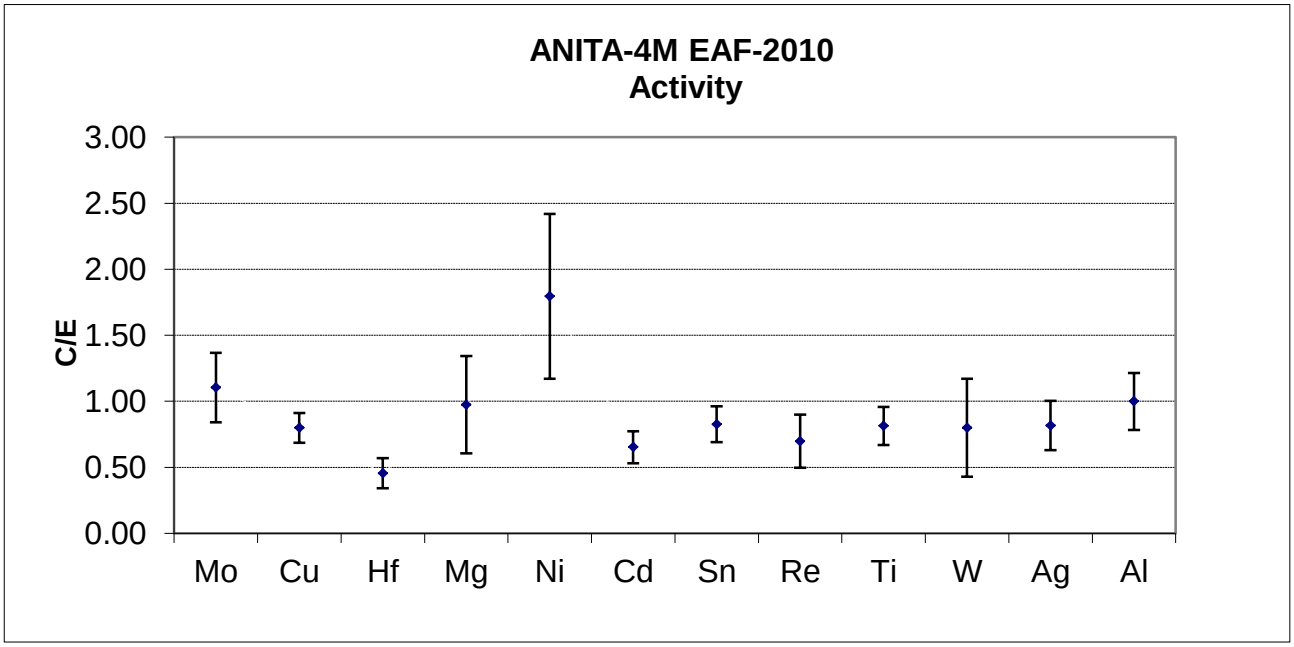


Figure 6 – Material sample activity: Calculated (C) (ANITA-4M,EAF-2010 library) and Experimental (E) comparison

4.4 Results analysis

From the validation work the following remarks can be drawn.

Comparison between experimental results and ANITA-4M (new fl1 file and EAF-2010 neutron cross section activation library)

1. *Electron decay heat (see Figure 4):*
   - The discrepancies between the calculated mean electron decay heat C and the experimental E values are inside 20% for Cu, Mg, Cd, Sn, Ti, Al and up to 30% for Mo, W and Ag. Materials with discrepancies greater than 30% are: Hf (42%), Ni (70%) and Re (31%);
   - The mean electron decay heat C/E values show agreement within error bars for Mo, Cu, Mg, Sn, Ti, W and Al.

2. *Photon decay heat (see Figure 5):*
   - The calculated photon decay heat values are lower than the corresponding experimental values for all the material samples;
   - The discrepancies between the calculated mean photon decay heat C and the experimental E values are inside 20% for Mo, Mg , Al and up to 30% for Cu, Cd and Sn. The materials with discrepancies greater than 30% are: Hf (60%), Ni (40%) , Re (55%); Ti (40%), W (40%) and Ag (35%);
   - The photon decay heat C/E values show agreement within the error bars only for Mo, Mg and Al.

3. *Activity (see Figure 6):*
   - The calculated activity values are in general lower than the corresponding experimental values except for Mo and Ni;
   - The mean activity values for Mo, Mg and Al show a good agreement between the experimental and calculated results (discrepancies $\leq$ 10%). The discrepancies are inside 20% for Cu, Sn, Ti, W and Ag. The largest discrepancies are for Hf (55%), Ni (79%) , Cd (35%) and Re (30%).

Comparison between ANITA-4M and EASY-2010 (FISPACT-2010 code+ EAF-2010 libraries)

For the electron decay heats, the ANITA-4M and FISPACT-2010 calculated results differ by less than 5% for all the materials except for Hf , Ni, Cd and Sn. For Sn, ANITA-4M

overestimates the experimental values whereas, on the contrary, FISPACT-2010 gives an underestimation. For the photon decay heats, the ANITA-4M and FISPACT-2010 calculated results differ by less than 5% for all the materials, except for Hf, Ni and Sn.

For the activity, the ANITA-4M and FISPACT-2010 calculated results differ by less than 2% for all the materials, except for Hf.

It has to be underlined that the present calculations have been performed, both for ANITA-4M and FISPACT-2010 activation codes, by using the same EAF-2010 neutron activation cross section library. Some differences in the decay data involved in the calculations (i.e, life-times, beta and gamma energies, etc.) and/or a different numerical treatment of the nuclear chains are responsible of the observed discrepancies.

The electron and photon decay heats are calculated by using the values contained in the decay data files. ANITA-4M uses the decay data contained in the **fl1** file based on the JEFF-3.1.1 evaluated data, whereas FISPACT-2010 uses the data contained in the decay data library of the EASY-2010 package, based on different evaluations [33].

As an example, let's consider the case of Ni for which ANITA-4M give different predictions for both electron and photon decay heats with respect to FISPACT code.

In Table 8 and in Table 9 the dominant nuclides contributing to the total electron decay heat for Nickel sample at 139 s of cooling time calculated by ANITA and FISPACT are reported. In Table 10 and in Table 11 the dominant nuclides contributing to the total photon decay heat for Nickel sample at 139 s of cooling time calculated by ANITA and FISPACT are reported.

	Electron decay heat	Percent
	(kW)	%
Co 62	2.31E-14	3.11E+01
Co 60m	2.29E-14	3.08E+01
Co 62m	2.19E-14	2.95E+01
Co 61	2.18E-15	2.93E+00
--	--	--
Total	7.44E-14	

Table 8 – Nickel sample. Cooling time 139 s. Dominant nuclides contributing to electron decay heat in ANITA-4M calculations

Nuclide	Electron decay heat	Percent
	(kW)	%
Co 62	2.31E-14	3.58E+01
Co 60m	2.29E-14	3.54E+01
Co 62m	1.26E-14	1.95E+01
Co 61	2.18E-15	3.37E+00
--	--	--
Total	6.47E-14	

Table 9 – Nickel sample. Cooling time 139 s. Dominant nuclides contributing to electron decay heat in FISPACT-2010 calculations

The total electron decay heat is 7.44E-14 kW for ANITA and 6.47E-14 kW for FISPACT, as already reported in Table 5. In both the calculations the most important nuclides are: Co 62, Co 60m and Co 62m. The electron decay heats for Co 62 and Co 60m are the same in both

the calculations. On the contrary, the electron decay heat of Co 62m is 2.19E-14 kW in ANITA whereas is 1.24E-14 kW in FISPACT calculations, giving a total value less than ANITA code.

Nuclide	Photon decay heat	Percent
	(kW)	%
Co 62	2.26E-14	3.80E+01
Co 62m	2.19E-14	3.70E+01
Ni 57	8.94E-15	2.95E+01
--	--	--
Total	5.93E-14	

Table 10 – Nickel sample.Cooling time 139 s. Dominant nuclides contributing to photon decay heat in ANITA-4M calculations

Nuclide	Photon decay heat	Percent
	(kW)	%
Co 62m	3.36E-14	4.73E+01
Co 62	2.26E-14	3.17E+01
Ni 57	8.95E-15	1.26E+01
--	--	--
Total	7.11E-14	

Table 11 – Nickel sample.Cooling time 139 s. Dominant nuclides contributing to photon decay heat in FISPACT-2010 calculations

The total photon decay heat is 5.93E-14 kW for ANITA and 7.11E-14 kW for FISPACT, as reported in Table 6. In both the calculations the most important nuclides are: Co 62 , Co 62m (in a different order) and Ni 57. The photon decay heats for Co 62 and Ni 57 are nearly the same in both the calculations. On the contrary, the photon decay heat of Co 62m is 2.19E-14 kW in ANITA whereas is 3.36E-14 kW in FISPACT calculations, giving a total value greater than ANITA code.

These differences can be explained by comparing the decay data for Co 62m used in the two calculations. In the **fl1** file used by ANITA the evaluated data are based on JEFF-3.1.1. In this library the mean energies E_β and $E\gamma$ released in the β^-,IT decay are 1.76 MeV and 1.76 MeV, respectively.

In the decay data library of EAF-2010 used by FISPACT the evaluation for Co 62m in based on JEFF-2.2 evaluated data. In this library the mean energies E_β and $E\gamma$ released in the decay are 1.01 MeV and the 2.70 MeV, respectively. These different values explain the discrepancies found between ANITA and FISPACT calculations.

The same analysis can be performed in order to explain the other discrepancies between the results of the two codes.

The FISPACT calculations have been repeated with the inclusion of the effects of the sequential charged particle reactions (SCPR) in the inventory (SEQUENTIAL card in the input file) that by default are not considered. The importance of the “sequential (x,n) reactions” on element activation in fusion reactors had been pointed out in the past [34]. The introduction of the SCPR treatment has given quite negligible changes on the FISPACT results.

5 CONCLUSION

ANITA-2000 is a code package for the activation characterization of materials exposed to neutron irradiation developed by ENEA and freely distributed at OECD-NEADB and ORNL-RSICC. The main component of the ANITA-2000 package is the activation code ANITA-4M that computes the radioactive inventory of a material exposed to neutron irradiation,

The data libraries required by the activation code ANITA-4M, the Decay, Hazard and Clearance data library (file "fl1") and the Gamma library (file "fl2"), have been updated on the basis of the JEFF-3.1.1 Radioactive Decay Data Library.

In order to test the new libraries, a preliminary validation has been performed through the comparison of the material decay heats and activities measured in experiments performed at the Frascati Neutron Generator (FNG) with those calculated by the ANITA-4M activation code. The EAF-2010 neutron activation cross section library has been used in the ANITA-4M calculations.

The discrepancies between the calculated mean electron decay heat C and the experimental E values are inside 20% for Cu, Mg, Cd, Sn, Ti, Al and up to 30% for Mo, W and Ag. Materials with discrepancies greater than 30% are: Hf (42%), Ni (70%) and Re (31%). The mean electron decay heat C/E values show agreement within error bars for Mo, Cu, Mg, Sn, Ti, W and Al.

The calculated photon decay heat values are lower than the corresponding experimental values for all the material samples. The discrepancies between the calculated mean photon decay heat C and the experimental E values are inside 20% for Mo, Mg , Al and up to 30% for Cu, Cd and Sn. The materials with discrepancies greater than 30% are: Hf (60%), Ni (40%) , Re (55%); Ti (40%), W (40%) and Ag (35%).The photon decay heat C/E values show agreement within the error bars only for Mo, Mg and Al.

The calculated activity values are in general lower than the corresponding experimental values except for Mo and Ni. The mean activity values for Mo, Mg and Al show a good agreement between the experimental and calculated results (discrepancies $\leq$ 10%). The discrepancies are inside 20% for Cu, Sn, Ti, W and Ag. The largest discrepancies are for Hf (55%), Ni (79%) , Cd (35%) and Re (30%).

For sake of comparison FISPACT-2010 code has been also used for decay heat an activity calculations using the same neutron activation cross section library (EAF-2010). The differences between the ANITA and FISPACT results can be explained as due to differences in the decay data (e.g. life-times, electron energies, gamma energies, etc.) and/or a different numerical treatment of the nuclear chains.

The discrepancies found in Table 5, Table 6 and Table 7 between the experimental results and the ANITA/FISPACT evaluations show that the decay data and the neutron activation cross sections also of the most recent evaluations need a further improvement.

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