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Effect of activation cross section uncertainties in transmutation analysis of realistic low-activation steels for IFMIF

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Abstract. We address uncertainty analysis to draw conclusions on the reliability the activation calculation in the *International Fusion Materials Irradiation Facility* (IFMIF) under the potential impact of activation cross section uncertainties. The Monte Carlo methodology implemented in ACAB code gives the uncertainty estimates due to the synergetic/global effect of the complete set of cross section uncertainties. An element-by-element analysis has been demonstrated as a helpful tool to easily analyse the transmutation performance of irradiated materials.

1 Introduction

The subject of transmutation calculations in IFMIF facility using the Intermediate Energy Activation File (IEAF) 2001 [1] or the European Activation File (EAF) 2005 [2] has been covered extensively. At this respect, the IFMIF community has made a lot of work on integral experimental activation benchmarks used to validate several inventory codes [3]: FISPACT, ALARA, ANITA... The calculated results with our ACAB [4] code are in a quantitative agreement with the experimental data similar to that obtained with other computational approaches already validated for IFMIF applications.

However, very few works have addressed uncertainty analysis to draw conclusions on the reliability of those acceptable results under the potential impact of activation cross section uncertainties. To address the problem in a comprehensive way we have applied a Monte Carlo method (implemented in our inventory ACAB code) based on a simultaneous random sampling of all the cross section probability density functions. We will make use of the recent EAF2005 uncertainty library to perform this job.

The element-by-element analysis has been demonstrated as a helpful tool to easily analyse the transmutation performance of irradiated materials. The contribution of each source-element to the generation of any transmutant product is obtained in a straightforward way. We calculate the effect of cross section uncertainties in the IFMIF activation of all different elements. We have found that the induced uncertainty in the activation performance of most of the elements is not relevant, but there are a few, but very important ones, that exhibit uncertainties in the activation response with a relevant practical significance in order to assess the acceptability of some intended structural materials for MFE/IFE irradiated in IFMIF.

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2 Computational methodology and validation process

In a previous work [5], transmutation calculations for IFMIF were conducted with an updated version of ACAB radionuclide generation/depletion code that could handle the numerous reaction channels for neutron energies over 20 MeV. The activation cross section library processed for IFMIF was the IEAF2001. This library contains the neutron activation cross section files for 679 nuclides, including stable and isomeric states up to 150 MeV. We used the group-wise IEAF2001 library in GENDF format with 256 neutron energy structure. IEAF2001 requires only a list of resultant isotopes and cross sections for the production of each one.

In this work, the nuclear data used for activation calculation are those from EAF2005 (62,637 reactions involving 775 different targets from H-1 to Fm-257). EAF2005 relies on a table of fixed reaction types (250) up to 60 MeV with a 211 neutron energy structure.

We have taken XS uncertainty data from the EAF2005/UN library [2]. The uncertainties provided by EAF2005/UN are the most complete uncertainty library in regards to the number of nuclides considered for inventory uncertainty prediction. The information included in this uncertainty file reefers to the relative error in the XS, denoted hereafter as Δ_{EAF} (in fact, the information included in these files is $\Delta^2_{j,EAF}$, where j is the energy group). Uncertainties $\Delta_{j,EAF}$ are provided in a four-energy group structure (up to 60 MeV) for non-threshold reactions and in one/two energy group for threshold reactions. It is assumed that errors in XS included in an energy group are 100% correlated, and that the errors in the different energy groups are uncorrelated. We have taken into account the uncertainties values, $\Delta_{j,EAF}$, as three times the experimental standard deviation of XS, that is $\Delta_{j,EAF} = 3 * \Delta_{j,EXP}$, in order to represent a 99.73% confidence limit.

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2.1 Monte Carlo methodology

To assess the impact of cross section uncertainties on transmutation/evolution of irradiated materials, we present the formulation of the Monte Carlo uncertainty analysis implemented into the inventory code ACAB.

The Monte Carlo procedure is based on simultaneous random sampling of all the cross sections involved in the problem, taken from EAF2005/UN. Authors of the EAF library have noted that when evaluating cross sections, the quantity $\log(\sigma_{\mathrm{expt}}/\sigma_{\mathrm{calc}})$ was approximately normally distributed. Consequently, it can be said that for any given cross section σ_{j} we can define the random variable $\log(\sigma_{\mathrm{j}}/\sigma_{\mathrm{j0}})$ that follows a normal distribution with mean zero and variance $\Delta^2_{\mathrm{j,EXP}}$. The value σ_{j0} is the best-estimate XS from the standard XS file (i.e.: EAF2005/A), and $\Delta^2_{\mathrm{j,EXP}} = \Delta^2_{\mathrm{j,EAF}}/9$ ($\Delta^2_{\mathrm{j,EAF}}$ is given in the uncertainty file, i.e., EAF2005/UN). The probability distributions of isotopic inventory are obtained with this method. Results are obtained for a 1000 history-sampling.

2.2 Validation

Our ACAB code has tested with a set of FZK integral activation experiments [6] having a neutron spectrum very close to the IFMIF. Four materials were irradiated: SS316, F82H, V and V-4Ti-4Cr alloy. The neutron flux intensity is about 4.10×10^{11} n/cm^{2}s, assuming a continuous irradiation of 7,525 s. We have adopted the average neutron flux in a 45group energy structure at the centre position of the irradiated steel sample reported in ref. [6], the average neutron energy is 11.2 MeV.

In table 1, we present the comparison of activation prediction for a sample of SS316. The calculation-to-experiment ratios (C/E) obtained by ACAB/G-IEAF-2001 and ACAB/EAF-2005 averaged over the measured decay times are shown in table 1. Results in column 4 of table 1 (Δ%) refers to the relative standard error obtained by Monte Carlo method. For the most important radionuclides to the total activity and contact dose rate (^{56}Mn, ^{54}Mn, ^{57}Ni, ^{58}Co and ^{60}Co) the predictions have demonstrated a reasonable agreement, C/E ratios are between 1.02/1.23. For these isotopes, the relative error is less than 10%, therefore, the effect of XS uncertainties on the activation results is insignificant. For the rest of isotopes, larger deviations of C/E from unity were found; C/E ratios are between 0.03/3.73 and 0.02/4.34 for IEAF2001 and EAF2005, respectively. Larger discrepancies between IEAF2001 and EAF2005 are found: ^{46}Sc, ^{48}V, ^{48}Cr, ^{52}Mn, ^{52}Fe, ^{56}Co, ^{56}Ni, ^{88}Zr and ^{90}Nb.

The isotopes with the maximum values of uncertainty are ^{48}Cr (82.9%), ^{87m}Y (77.3%) and ^{90}Mo (71.5%), their main build-up sequences for isotope generation are: i) ^{48}Cr is mainly due to the reactions ^{50}Cr(n,3n)^{48}Cr, ii) ^{87m}Y the critical reaction is ^{92}Mo(n,dα)^{87m}Y, and iii) ^{90}Mo the critical one is ^{92}Mo(n,3n)^{90}Mo. The effective 1-group cross section uncertainties (in %) processed by EAF2005/UN for these reactions are: 67%, 70% and 67%, respectively.

Table 1. Calculation-to-experiment average ratios for the activity inventories induced in the SS316 intermediate energy activation experiment [6].

	IEAF2001	EAF2005	
Isotope	C/E	C/E	Δ%
Sc 46	1.66	2.46	10.8
Sc 48	1.28	1.74	15.3
V 48	2.72	1.28	29.6
Cr 48	3.73	1.54	82.9
Cr 49	0.82	0.71	3.8
Cr 51	1.00	1.09	3.3
Mn 52	3.13	1.31	26.8
Mn 54	*1.02*	*1.16*	*9.4*
Mn 56	*1.23*	*1.22*	*0.6*
Fe 52	1.44	4.34	19.9
Fe 59	1.07	1.18	17.8
Co 55	2.12	1.45	64.1
Co 56	2.98	1.31	27.7
Co 57	1.02	1.12	0.9
Co 58	*1.20*	*1.19*	*3.0*
Co 60	*1.12*	*1.03*	*3.3*
Co 61	2.26	2.66	17.5
Ni 56	1.57	0.37	45.2
Ni 57	*1.19*	*1.22*	*0.5*
Y 87m	0.07	0.15	77.3
Y 87	0.46	0.82	63.3
Y 88	1.00	0.61	25.4
Zr 86	0.03	0.03	73.7
Zr 88	0.99	0.45	9.2
Zr 89	1.20	1.48	5.4
Zr 97	0.03	0.02	3.0
Nb 90	0.58	1.80	34.2
Nb 92m	1.51	1.46	4.1
Nb 95	1.53	1.65	6.1
Nb 95m	1.18	0.84	9.4
Nb 96	1.65	1.88	8.5
Mo 90	1.64	1.97	71.5
Mo 93m	2.50	1.81	44.2
Mo 99	1.18	1.29	1.7
Tc 99m	1.19	1.30	1.4

3 Uncertainty analysis for element-by-element transmutation

We have considered the IFMIF scenario (7.30×10^{14} n/cm^2 s, $\langle E \rangle$ ~5.64 MeV) to perform an uncertainty analysis for element-by-element transmutation under 1 year of irradiation time. Firstly, in table 2 we present the H and He gas production and the evolution of solid transmutants for the major and minor steel constituents. Secondly, we predict the relative error or coefficient of variation (ratio between standard deviation and the mean) of the final concentration of each element.

Normally, for gas production, the largest uncertainties are in He production. In the case of Fe, uncertainties for H and He transmutants are 7.6% and 5.3%, respectively. For Ni, 7.0% and 6.7%, for H and He transmutants, respectively.

Table 2. Transmutants (appm) and relative error (%) of typical intended and impurities elements in reduced activation steels under 1 year of irradiation time in HFTM/IFMIF. Calculations performed with ACAB/EAF2005.

		H		He		Z-2		Z-1		Z		Z+1		Z+2	
Z	Element	appm	%	appm	%	appm	%	appm	%	appm	%	appm	%	appm	%
5	B	809	8.7	3473	8.4	2461	10.8	352	8.6	−3360	8.1	0	16.1	0	38.0
6	C	425	17.8	3425	56.9	477	7.0	358	20.6	−1847	35.3	0	30.0	0	78.3
7	N	2712	15.7	2464	16.1	1831	5.4	2699	15.8	−4847	9.9	0	59.7	0	103.6
8	O	359	10.6	1393	10.1	1359	10.2	216	15.9	−1606	9.0	0	49.5	0	51.8
13	Al	1084	9.3	677	10.0	230	6.4	1097	10.7	−1355	8.9	13	12.1	0	41.0
14	Si	2304	4.2	1199	5.3	1248	5.9	926	5.8	−2195	4.1	1	14.9	0	33.1
15	P	3929	20.5	883	21.8	257	73.9	3608	22.4	−3907	21.3	23	30.3	0	95.3
16	S	4294	11.2	2677	14.5	2852	14.2	1512	27.2	−4397	13.0	1	13.7	0	27.2
22	Ti	988	9.7	406	34.9	382	37.3	317	11.7	−701	21.0	1	14.6	0	18.9
23	V	658	9.8	81	6.9	5	35.2	666	12.6	−724	12.3	54	11.3	0	38.7
24	Cr	1106	6.5	265	8.4	304	7.9	1906	3.8	−2212	3.5	0	19.0	0	21.5
25	Mn	845	22.2	200	40.4	124	64.7	1563	12.1	−1775	11.6	87	10.1	0	34.0
26	Fe	1440	7.6	288	5.3	392	8.9	1074	7.5	−1502	7.3	0	12.5	0	19.1
27	Co	1235	20.2	260	38.6	150	66.3	2960	9.2	−3132	9.3	14	14.7	0	44.3
28	Ni	5808	7.0	1148	6.7	4112	5.8	2364	3.2	−6629	4.5	1	10.2	0	12.7
29	Cu	2009	19.0	317	5.1	259	4.9	4146	9.2	−4906	7.8	483	3.2	0	32.8
39	Y	789	22.5	53	10.0	8	11.5	3101	6.5	−3226	6.3	111	15.3	0	39.2
41	Nb	735	15.3	119	14.4	59	12.3	2268	5.6	−2349	5.4	2	15.5	0	55.0
42	Mo	1119	16.2	104	10.0	231	14.9	1035	17.0	−1934	9.6	607	7.4	30	15.8
73	Ta	191	22.5	19	26.7	9	46.9	4698	10.4	−7052	8.1	2345	10.6	0	135.7
74	W	204	12.0	26	11.8	102	25.9	1677	12.7	−3443	6.8	1660	4.5	3	11.2

Regarding major steel constituents, the transmutation of C, P and Ti elements have the largest uncertainties, 35.3%, 21.3% and 21% respectively. For Fe, uncertainty is 7.3%.

4 Uncertainty analysis for steels: EUROFER

Firstly, to assess the effect of the uncertainties we have calculated the contact γ-dose rate for EUROFER under 1 fpy of irradiation time in HFTM/IFMIF [7]. The uncertainty analysis has been performed using ACAB code with EAF2005/UN library.

Figure 1 shows that from the moment of shutdown up to ~10 h, the relative error is less than 10%. Nevertheless, the uncertainty analysis results show that for times over ~24 h the relative error in the contact dose rate can be as large as 23% (see fig. 1). Therefore, the effect of XS uncertainties on the activation results during times relevant for maintenance activities and from waste management point of view could be important.

However, in this work we have focused on the uncertainty analysis for transmutation. The element-by-element transmutation presented in table 2 leads to predict the transmutation performance of any material irradiated in IFMIF.

Table 3 shows the main transmutants for EUROFER under 1 fpy in HFTM/IFMIF using IEAF2001 and EAF2005. H and He transmutants are larger with IEAF2001 (iron produces the most important levels of H and He, ~90% and ~80% respectively). After one year of irradiation, these gaseous transmutant concentrations can be comparable to some initial steel constituents.

In column 5 table 3, we predict the relative error of each element. The transmutant uncertainty analysis for H and He IFMIF.

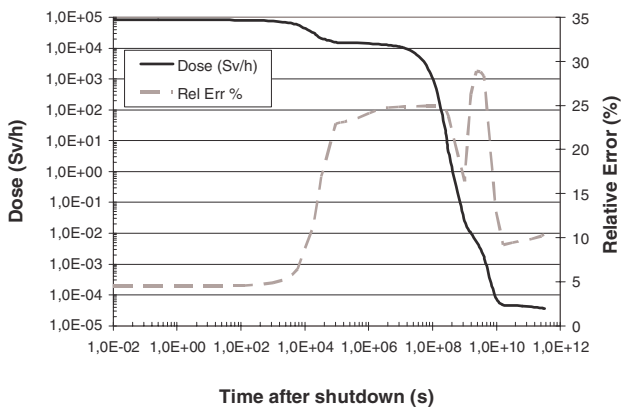

Fig. 1. Contact dose rate (Sv/h) and the relative error (%) for EUROFER under 1 year of irradiation time in HFTM/IFMIF.

shows a relative error of 7.3% for H, and 5.6% for He. For C (74.3%), P (41%) and Nb (34.8%) we have predicted the largest transmutant uncertainties.

5 Conclusions

The ACAB code is able to deal with transmutation calculations in IFMIF facility using IEAF2001 and EAF2005. A more complete benchmark of ACAB against the already validated computational methodologies used for activation and transmutation calculations has been performed.

In addition, the impact of potential activation cross section uncertainties on the transmutation calculations is assessed.

Table 3. Transmutation (appm) of EUROFER constituents under 1 year of irradiation time in the HFTM/IFMIF. Calculations performed with ACAB/IEAF-2001 and EAF2005.

	INITIAL	IEAF2001	EAF2005	Rel Err
Element	appm	appm	appm	%
H	0	1450	1397	7.3
He	0	307	304	5.6
Li	0	0.3	0.1	2.6
Be	0	2	2	6.9
B	51	4	4	10.4
C	4860	−6	−5	74.3
N	1191	−4	−6	10.4
O	347	−1	−1	9,2
Mg	0	2	1	5,4
Al	206	1	1	9,3
Si	990	−2	−2	7,6
P	90	0.04	−0.2	41,0
S	87	−0.4	−0.4	14,0
Ti	116	29	31	7,9
V	2183	211	182	3,4
Cr	96233	164	141	25.0
Mn	4048	970	944	7.8
Fe	885882	−1377	−1330	7.6
Co	47	0.1	−0.02	15.0
Ni	47	−0.1	−0.1	16.6
Cu	44	−0.2	−0.2	8.0
Nb	6	0.01	0.02	34.8
Mo	29	−0.1	−0.1	10.1
Hf	0	1	1	11.0
Ta	215	4	4	19.1
W	3327	−10	−11	7.4
Re	0	5	6	4.5
Os	0	0.01	0.01	0.0

The implemented Monte Carlo method in ACAB is applied to transmutation uncertainty analysis, showing its capability to deal with comprehensive cross section uncertainty data.

We have assessed the effect of the uncertainties in the contact γ-dose rate for EUROFER under 1 fpy of irradiation time in HFTM/IFMIF. The uncertainty analysis results showed that for times over ~24 h the relative error in the contact dose rate can be as large as 23%.

We have calculated the effect of cross section uncertainties in the IFMIF activation of all different elements. For EUROFER, uncertainties in H and He transmutants are 7.3% and 5.6%, respectively. We have found significant uncertainties in the transmutation response for C, P and Nb.

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