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A new UK fission yield evaluation UKFY3.7

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Abstract. The JEFF neutron induced and spontaneous fission product yield evaluation is currently unchanged from JEFF-3.1.1, also known by its UK designation UKFY3.6A. It is based upon experimental data combined with empirically fitted mass, charge and isomeric state models which are then adjusted within the experimental and model uncertainties to conform to the physical constraints of the fission process. A new evaluation has been prepared for JEFF, called UKFY3.7, that incorporates new experimental data and replaces the current empirical models (multi-Gaussian fits of mass distribution and Wahl Zp model for charge distribution combined with parameter extrapolation), with predictions from GEF. The GEF model has the advantage that one set of parameters allows the prediction of many different fissioning nuclides at different excitation energies unlike previous models where each fissioning nuclide at a specific excitation energy had to be fitted individually to the relevant experimental data. The new UKFY3.7 evaluation, submitted for testing as part of JEFF-3.3, is described alongside initial results of testing. In addition, initial ideas for future developments allowing inclusion of new measurements types and changing from any neutron spectrum type to true neutron energy dependence are discussed. Also, a method is proposed to propagate uncertainties of fission product yields based upon the experimental data that underlies the fission yield evaluation. The covariance terms being determined from the evaluated cumulative and independent yields combined with the experimental uncertainties on the cumulative yield measurements.

1. Introduction

Reliable and complete libraries of fission product yields with specified accuracies are needed for many different nuclear reactor calculations, including those on decay heat, dosimetry, burn-up, fuel handling, nuclide inventory and safety.

This paper describes the latest such UK evaluation of fission yields. In the UK the evaluation of yields for use in computer libraries was pioneered by Crouch at Harwell [1]. The work was then continued at Winfrith, producing C4U and C4A known as UKFY1 [2], which were submitted to the first stage, JEF1, of the Joint Evaluated File. UKFY2 [3] and UKFY3.6A [4,5] followed resulting in the JEF-2.2 and JEFF-3.1.1 fission yield libraries.

The new library, UKFY3.7, which has been submitted to the JEFF project for testing, builds upon the earlier libraries. Improvements include bringing the database of fission yield measurements up to date by including 11 newly published measurements and using the GEF model [6] to predict unmeasured mass and charge yield distributions for all fissioning systems rather than fitting the experimental data to a combination of semi-empirical models for each system (multi-Gaussian fits of mass distribution and Wahl Zp model for charge distribution). The evaluation procedure is described and the effects of the changes from JEFF-3.1.1 studied.

Initial testing of the UKFY3.7 library, using the JEFF-3.1.1 decay data is described for calculation of delayed neutron emission per fission, fission product decay heat pulse benchmarks and spent fuel decay heat.

The possible future developments of the fission yield libraries are then discussed. These include; (i) production of covariance terms so that useful uncertainties can be determined on fission product inventories, (ii) including non-traditional fission product yield measurements in evaluations and (iii) changing the fission product yield evaluations from a typical standard neutron spectra to an energy dependent description.

2. The UKFY3.7 evaluation

The production of the UKFY3.7 library is based upon 6 steps described previously [4];

- Statistical analysis of all available experimental data producing a recommended value and uncertainty for all measured yields.
- For all important fissioning system, see Table 1, fill all missing mass distributions and independent yields (including the ternary yields) using an appropriate model that estimates both the value and it uncertainty.
- Adjust the independent yields for each fissioning system to minimise the differences for each physical constraint such as conservation of mass and charge, and ensuring that complement element yields are equal.
- Split the independent yields using the isomeric splitting ratios based upon the Madland and England model.
- Calculate cumulative yields using the independent yields and JEFF-3.1.1 decay data. Then using the

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Table 1. Fissioning systems in the UKFY3.7 that were deemed important in previous work based upon the maximum fraction of fissions in UOX, MOX and thorium fuels in fast and thermal reactors [4] and, following a user request, U236 thermal fission.

Max. Fraction of Fission Rate			
>10%	**1–10%**	**0.1%–1%**	**Spont. fission**
nuclides: 5	**2**	**12**	**3**
^{*233}*U TFH*	^{*240}*Pu F*	^{*232}*Th FH*	^{252}*Ct Sp*
^{*235}*U TFH*	^{245}*Cm TF*	^{234}*U F*	^{242}*Cm SP*
^{*238}*U TFH*		^{236}*U F*	^{244}*Cm SP*
^{*239}*Pu TF*		^{237}*Np TF*	
^{*241}*Pu TF*		^{238}*Np TF*	
		^{238}*Pu TF*	
		^{242}*Pu F*	
		^{241}*Am TF*	
		^{242m}*Am TF*	
		^{243}*Am TF*	
		^{243}*Cm TF*	
		^{244}*Cm TF*	

∗ Nuclides in UKFY1 and previous UK libraries.
T Thermal fission.
F Fast fission.
H 14Mev Fission.
Sp Spontaneous fission.

experimental cumulative yields and their uncertainties, produce uncertainties for all the cumulative yields.

– Produce an ENDF formatted file containing the data.

2.1. Changes in the UKFY3.7 evaluation

2.1.1. New data

The previous UK evaluation included a literature search complete up to 2000. A review was carried out in 2013 and ten important new references identified. In addition, a further reference was identified in 2016 for fast fission yields of neodymium isotopes that was also included. The totals of absolute, relative and "ratio of ratio" measurements in the old and new databases are shown in Table 2. The split of the new data between different fissioning systems are shown in Table 3. For the fast neutron spectra cases the new data refers to neodymium cumulative yields and the results of the statistical analysis for the affected Nd148 cumulative yields are shown in Table 4 with their uncertainties.

The improvements to the mass distributions are of two classes; firstly, where previously unmeasured yields are now available, and secondly, where new data of has altered the best estimate of a yield. The first class includes; thermal fission of Np238 where new data is now available between masses 74 and 85, Pu239 where data for masses 80, 82 and 130 have now been measured, and Cf249 where data is now available for masses 69 to 82. For the second class, Fig. 1 shows the relative changes in the mass yields for the other thermal fission yields including new data. It should be noted that the new data significantly alters many of the values, especially in the valley and wings of the mass distribution.

Table 2. Data items in the previous and current database.

Dataset	**Absolute**	**Relative**	**"ratio of ratio"**	**Total**
UKFY3.6A	11887	1352	1471	14710
UKFY3.7	12924	1442	1471	15837

Table 3. Number of measured data items for fissioning systems with new data.

Neutron spectra	**Fissioning nuclide**	**UKFY3.6**	**New data**	**UKFY3.7**
Thermal	Th229	337	72	409
Thermal	U233	757	188	945
Thermal	U235	2390	151	2541
Thermal	Np238	115	63	178
Thermal	Pu239	861	225	1086
Thermal	Pu241	334	63	397
Thermal	Cm245	161	219	380
Thermal	Cf249	305	239	544
Fast	U235	724	5	729
Fast	Pu239	390	5	395
Fast	Pu241	111	5	116

Table 4. The fast neutron spectra ^{148}Nd cumulative yields determined from measurements.

Fissioning nuclide	**UKFY3.7**	**UKFY3.6A**
U235	1.677 ± 0.020	1.696 ± 0.019
Pu239	1.700 ± 0.029	1.699 ± 0.025
Pu241	1.943 ± 0.041	1.946 ± 0.045

2.1.2. New modelling

In the JEFF-3.1.1 (UKFY3.6A) evaluation the chain yields were modelled using the 5-Gaussian approximation with the parameters fitted for each fissioning system where possible and the parameters were extrapolated for fissioning system with too little data to be fitted. Similarly, the Wahl Zp model [4] was used to fit systems with enough data and the model parameters were extrapolated for other systems.

Recently, a new fission model code, GEF ("GEneral description of Fission observables") has shown good agreement for mass and charge distributions against experiment [6]. A great advantage of the model is that it uses a standard set of selected and fitted parameters for predicting yields from the fission of isotopes of elements from thorium to californium, and at neutron energies from thermal up to and including second chance fission.

Following some initial comparisons between the UKFY3.6A database and the GEF predictions in the JEFF community it was decided to use the GEF model predictions for mass and charge distributions to replace the 5-Gaussian and Zp models.

The GEF model can also estimate isomeric splitting of independent yields but due to the lack of experimental data and the lack of an updated JEFF-3.3 draft decay data file (from which the models get the spins of the ground and isomeric states) it was decided to use the existing isomeric splitting in this evaluation. In addition, the JEFF-3.1.1 decay data library is used throughout the evaluation and testing reported in this paper.

3. Initial testing of UKFY3.7

Fission product yields are important in many different types of calculations, but for the initial testing it was

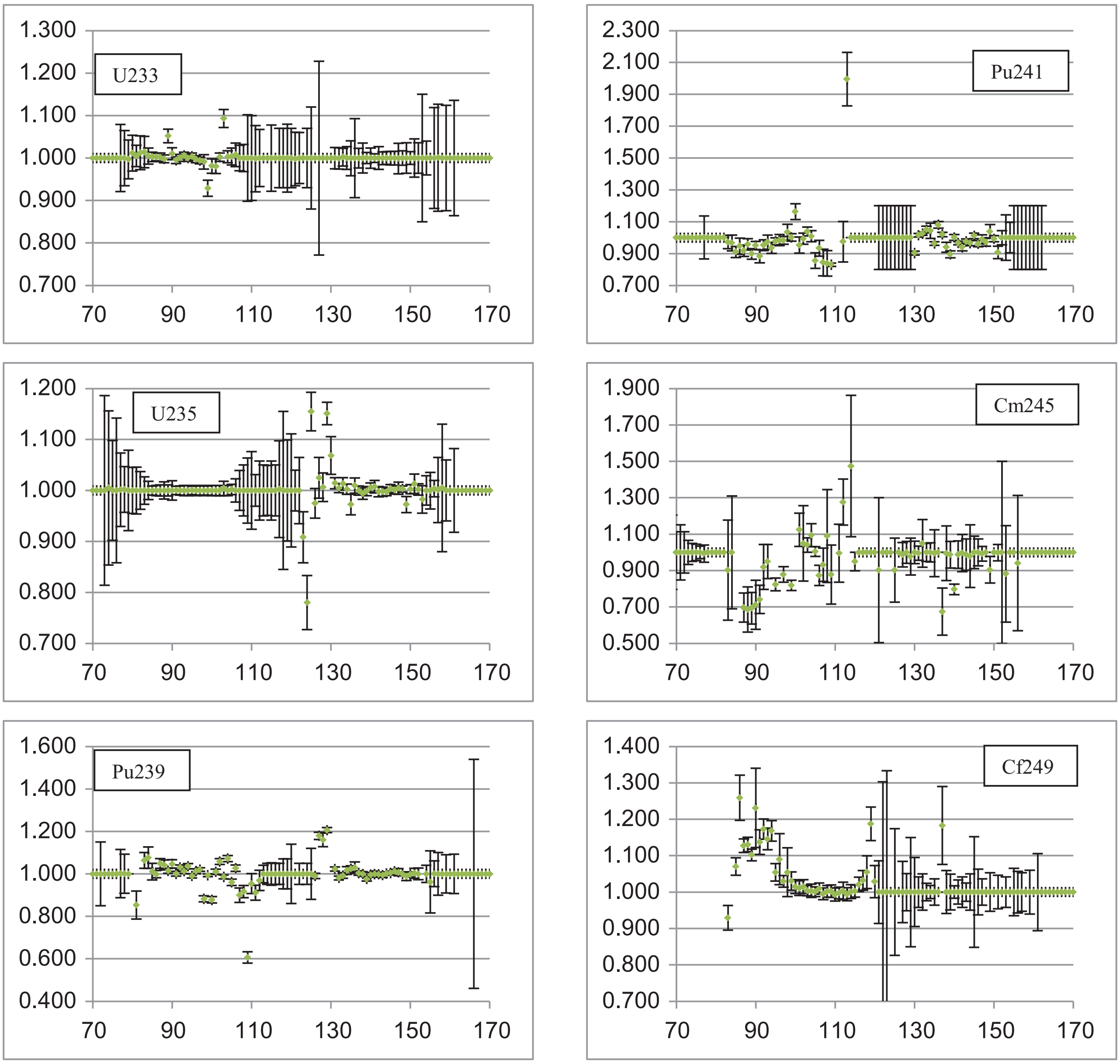

Figure 1. For nuclides with significant new data, the plots show changes to the mass yields determined from the UKFY3.7 database as a ratio to those determined previously in UKFY3.6A against the yield mass. The new uncertainties are shown to illustrate the accuracy.

decided to use three types of calculation; (i) the average number of delayed neutrons per fission, (ii) the decay heat following a single fission pulse and (iii) the decay heat measured from spent PWR fuel assemblies.

3.1. Delayed neutron summation calculation

The average number of delayed neutrons per fission ($\overline{\nu}_d$) can be calculated using the cumulative yields of a fissioning system (C_i) and the number of delayed neutrons emitted per decay of a nuclide i (P_n^i)using

$$\overline{\nu}_d = \sum_{i=0}^{n} C_i P_n^i \tag{1}$$

The calculation results for UKFY3.7 and JEFF-3.1.1 fission product yields using the JEFF-3.1.1 decay data are shown in Table 5.

The variance of the $\overline{\nu}_d$ culations can be determined given the values and variances of the cumulative yields and the P_n^i values using

$$\sigma^2_{\overline{\nu}_d} = \sum_{i=0}^{n} \sigma^2_{C_i} P_n^{i^2} + \sum_{i=0}^{n} C_i^2 \sigma p_n^{i^2} \tag{2}$$

The delayed neutron emission is strongly dependent upon the yield distribution away from stability where delayed neutron emission is possible. In previous work [4] it was noted that the ratio of the calculation to experiment showed a trend with the mass of the fissioning nucleus. Although there are large uncertainties on the summation calculations it is noted that the UKFY3.7 calculations, given in Fig. 2, shows a scatter around about a ratio of 0.95 but showed no significant trend in nucleus mass. It is too early to decide if this slight improvement results from switching the previous JEFF-3.1.1 extrapolation of Zp model parameters to the more self-consistent GEF model, but at the very least the UKFY3.7 results are no worse than the previous JEFF-3.1.1 results.

Table 5. Calculation of $\bar{\nu}_d$ using UKFY3.7 and JEFF-3.1.1.

System	Neutron energy	UKFY3.7	JEFF-3.1.1	$\bar{\nu}_d$ from experiment [4]
Th232	Fast	4.081 ± 0.184	5.384 ± 0.237	5.47 ± 0.12
Th232	14 MeV	2.907 ± 0.165	3.056 ± 0.211	2.85 ± 0.13
U233	Thermal	0.738 ± 0.062	0.724 ± 0.056	0.664 ± 0.018
U233	Fast	0.757 ± 0.063	1.042 ± 0.079	0.729 ± 0.019
U233	14 MeV	0.411 ± 0.040	0.559 ± 0.060	0.422 ± 0.025
U234	Fast	1.079 ± 0.082	1.342 ± 0.169	1.06 ± 0.12
U235	Thermal	1.471 ± 0.083	1.477 ± 0.079	1.654 ± 0.042
U235	Fast	1.444 ± 0.080	1.698 ± 0.087	1.714 ± 0.022
U235	14 MeV	0.800 ± 0.064	0.934 ± 0.071	0.927 ± 0.029
U236	Thermal	2.487 ± 0.118		
U236	Fast	1.933 ± 0.111	2.386 ± 0.152	2.31 ± 0.26
U238	Fast	3.535 ± 0.131	4.037 ± 0.129	4.51 ± 0.061
U238	14 MeV	2.295 ± 0.093	2.369 ± 0.098	2.73 ± 0.08
Np237	Thermal	1.303 ± 0.083	1.130 ± 0.076	1.07 ± 0.10
Np237	Fast	1.141 ± 0.064	1.169 ± 0.064	1.22 ± 0.03
Np238	Thermal	1.658 ± 0.202	1.419 ± 0.135	
Np238	Fast	1.783 ± 0.188	1.635 ± 0.202	
Pu238	Thermal	0.376 ± 0.035	0.319 ± 0.038	0.456 ± 0.051
Pu238	Fast	0.455 ± 0.043	0.483 ± 0.067	0.456 ± 0.051
Pu239	Thermal	0.628 ± 0.043	0.605 ± 0.043	0.624 ± 0.024
Pu239	Fast	0.605 ± 0.044	0.675 ± 0.046	0.664 ± 0.013
Pu240	Fast	0.809 ± 0.054	0.920 ± 0.058	0.96 ± 0.11
Pu241	Thermal	1.306 ± 0.059	1.232 ± 0.058	1.56 ± 0.16
Pu241	Fast	1.270 ± 0.062	1.290 ± 0.067	1.63 ± 0.16
Pu242	Fast	1.679 ± 0.081	1.684 ± 0.078	2.28 ± 0.25
Am241	Thermal	0.488 ± 0.043	0.378 ± 0.047	0.44 ± 0.05
Am241	Fast	0.486 ± 0.059	0.414 ± 0.055	0.394 ± 0.024
Am242	Thermal	0.712 ± 0.111	0.582 ± 0.106	0.69 ± 0.05
Am242	Fast	0.714 ± 0.048	0.567 ± 0.075	
Am243	Thermal	1.038 ± 0.063	0.842 ± 0.113	
Am243	Fast	1.034 ± 0.060	0.816 ± 0.099	
Cm242	Spont.	0.115 ± 0.026	0.120 ± 0.022	
Cm243	Thermal	0.275 ± 0.029	0.221 ± 0.043	
Cm243	Fast	0.284 ± 0.028	0.212 ± 0.030	
Cm244	Spont.	0.331 ± 0.044	0.317 ± 0.041	
Cm244	Thermal	0.416 ± 0.037	0.326 ± 0.055	
Cm244	Fast	0.376 ± 0.032	0.334 ± 0.042	
Cm245	Thermal	0.570 ± 0.044	0.526 ± 0.071	0.59 ± 0.04
Cm245	Fast	0.591 ± 0.042	0.466 ± 0.065	
Cf252	Spont.	0.668 ± 0.039	0.585 ± 0.030	0.86 ± 0.10

3.2. Single fission pulse decay heat

There exists many measurements of fission product decay heat from different nuclides following a short fission pulse. In this work, the standard benchmark for thermal fission of U235 and Pu239 [7], which were derived from the analysis of many experiments, were compare with summation calculations. The FISPIN inventory code [8] was used with the UKFY3.7 and JEFF-3.1.1 fission yield files and the JEFF-3.1.1 decay data to compare with these benchmarks. These results are shown in Figs. 3 and 4.

There is a small difference between these two sets of results, although only just outside the one standard deviation range. Below 10 seconds there is a small improvement, between 10 and 1000 seconds there is a slight worsening and at longer times there is little difference. These results suggest that the change between the previous Wahl Zp model and the new GEF model for these fissioning systems has little effect on the important nuclides for decay heat for these actinides. However, given that these systems have the most complete sets of measured yields this is not too surprising.

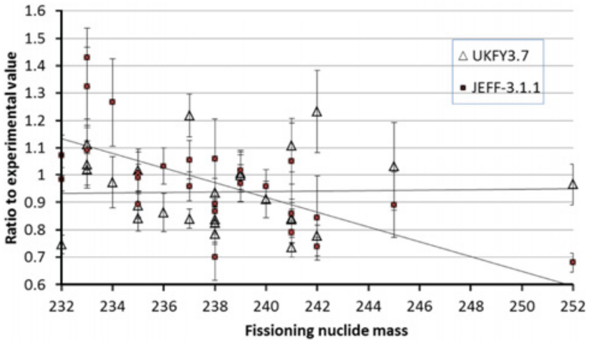

Figure 2. Plot of $\bar{\nu}_d$ calculation over experiment ratio using UKFY3.7 and JEFF-3.1.1 yields with JEFF-3.1.1 decay data shown against the fissioning nucleus mass. The lines are fitted to the two sets of results using y = ax +b.

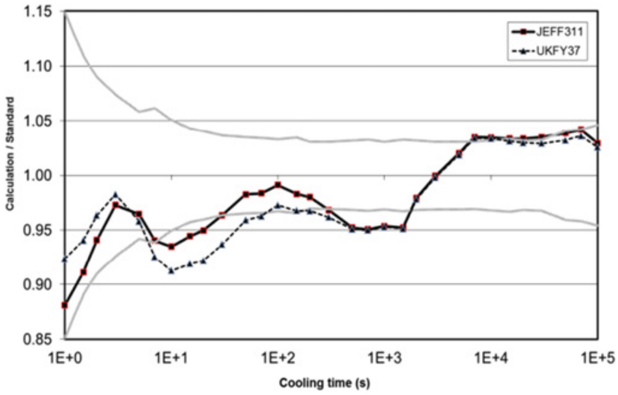

Figure 3. Plot of U235 decay heat against time following a single thermal neutron induced fission pulse using UKFY3.7 and JEFF-3.1.1 yields compared against the Tobias benchmark shown with a one standard deviation range [7].

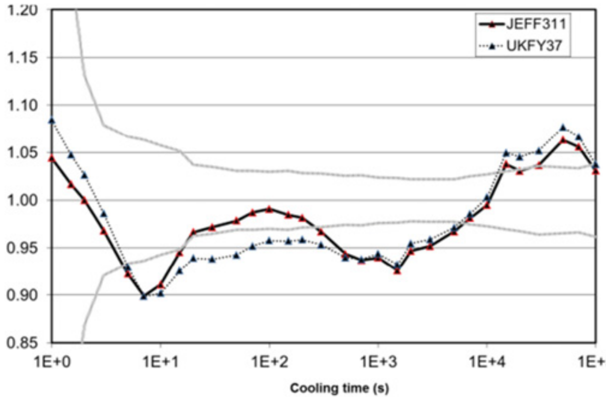

Figure 4. Plot of Pu239 decay heat following a single thermal neutron induced fission pulse using UKFY3.7 and JEFF-3.1.1 yields compared against the Tobias benchmark shown with a one standard deviation range [7].

3.3. PWR spent fuel assembly decay heat

In previous work the agreement between measured decay heats from PWR assemblies at the CLAB facility [9] were compared to a series of inventory calculations using JEF-2.2 and JEFF-3.1.1 [10]. The modelling used in this

Table 6. Description of the PWR assemblies measured at CLAB [9] and the calculation over experiment (C/E) ratio using simple inventory calculations using JEF-2.2, JEFF-3.1.1 and UKFY3.7. JEF-2.2 and JEFF-3.1.1 from [10].

Assembly	Reactor	U235 Wt%	U236 ppm	Final Irradition MWd/t	Cooling (days)	Cooling (years)	Irradiation step 1 MWd/t	Irradiation step 2 MWd/t	Irradiation step 3 MWd/t	Irradiation step 4 MWd/t	Irradiation step 5 MWd/t	Irradiation step 6 MWd/t	Measured heat (W)	JEF-2.2 C/E	JEFF-3.1.1 C/E	UKFY37 C/E
0C9	Ringhals 3	3.101	150	38442	6551	17.94	9884	8192	10350	10016			491.2	1.000	0.991	0.993
0E2		3.103	150	41628	5823	15.94	7496	13034	11308	9790			587.9	0.974	0.967	0.970
0E6		3.103	150	35993	5829	15.96	12490	13031	10472				487.7	0.986	0.975	0.977
1C2		3.101	150	33318	6559	17.96	6249	5019	11509	10541			417.7	0.999	0.988	0.990
1C5		3.101	150	38484	6593	18.05	9884	8102	10411	10087			499.2	0.983	0.974	0.977
1E5		3.103	150	34638	5818	15.93	10556	13134	10948				468.8	0.986	0.975	0.978
2A5		2.1	150	20107	7297	19.98	12228	7879					233.7	1.015	1.000	1.002
2C2		3.101	150	36577	6550	17.93	7783	8345	9932	10517			466.5	0.998	0.988	0.990
3C1		3.101	150	36572	6545	17.92	7783	8341	9931	10517			470.2	0.988	0.978	0.980
3C4		3.101	150	38447	6544	17.92	9884	8192	10354	10017			497.3	0.984	0.976	0.978
3C5		3.101	150	38373	6543	17.91	9884	8113	10343	10033			501.4	0.980	0.971	0.974
3C9		3.101	150	36560	6552	17.94	7783	8377	9876	10524			468.4	0.992	0.982	0.985
4C4		3.101	150	33333	6572	17.99	6249	4991	11030	11063			422	0.989	0.978	0.980
4C7		3.101	150	38370	6549	17.93	9884	8101	10347	10038			498.7	0.983	0.975	0.977
5A3		2.1	150	19699	6972	19.09	11696	8003					237.7	0.991	0.976	0.978
					6975	19.10							236.6	0.996	0.981	0.982
					6977	19.10							243.4	0.968	0.953	0.955
					7291	19.96							230.9	1.005	0.990	0.991
					7304	20.00							230.2	1.007	0.992	0.994
5F2		3.404	150	47308	4724	12.93	13475	6922	10337	8930	7644		714	0.976	0.971	0.974
C01	Ringhals 2	3.095	150	36688	8468	23.18	11247	9403	7569	8469			415.7	1.006	0.998	0.999
C12		3.095	150	36385	8403	23.01	11247	9318	7390	8430			410.3	1.009	1.000	1.001
C20		3.095	150	35720	6950	19.03	11247	9377	7454	7642			415.8	1.034	1.026	1.028
					6951	19.03							426.1	1.009	1.001	1.003
					6952	19.03							428.9	1.003	0.994	0.996
					6959	19.05							435.6	0.987	0.979	0.981
C42		3.095	150	35639	5803	15.89	16565	7619	8126	3329			442.3	0.991	0.983	0.985
					5804	15.89							448.4	0.978	0.970	0.972
D27		3.252	150	39676	7669	21.00	9510	12889	9267	8010			456	0.991	0.983	0.985
D38		3.252	150	39403	8005	21.92	6367	9331	7358	8701	7646		442.4	1.001	0.992	0.994
E38		3.199	150	33973	7999	21.90	7568	8458	9879	8068			376.3	0.995	0.984	0.986
					8000	21.90							374.3	1.000	0.989	0.991
E40		3.199	150	34339	8075	22.11	7705	7249	10655	8730			381.2	0.992	0.982	0.983
F14		3.197	150	34009	7722	21.14	5069	10755	9898	8287			381.8	1.003	0.992	0.994
F21		3.197	150	36273	7376	20.19	4767	6317	10046	8255	6888		420.9	0.992	0.982	0.984
F25		3.197	150	35352	7725	21.15	8307	10749	8316	7980			396.7	1.011	1.000	1.002
F32		3.197	150	50962	5860	16.04	10553	10609	8391	7761	6629	7019	692	0.994	0.990	0.994
G11		3.188	150	35463	6990	19.14	6890	10422	7868	6943	3340		416.3	0.992	0.982	0.984
G23		3.206	150	35633	6984	19.12	10268	10035	7618	7712			420.7	0.996	0.986	0.988
I09		3.203	150	40188	5849	16.01	6727	8950	9065	7568	7878		507.9	1.011	1.003	1.006
I20		3.203	150	34313	6588	18.04	8300	9010	9108	7895			403.5	0.987	0.976	0.978
I24		3.203	150	34294	6601	18.07	8245	8967	9144	7938			410	0.983	0.972	0.974
I25		3.203	150	36859	6198	16.97	5207	4991	9803	8998	7860		445.8	1.000	1.000	1.003
Mean and Standard Deviation of C/E values										Ringhals 3				0.990 ± 0.012	0.979 ± 0.010	0.981 ± 0.010
										Ringhals 2				0.999 ± 0.012	0.990 ± 0.012	0.992 ± 0.012
										Combined				0.995 ± 0.013	0.985 ± 0.012	0.987 ± 0.012

work was rudimentary but it was felt adequate as a sanity check prior to JEFF-3.3 decay data becoming available and JEFF-3.3 libraries becoming available for reactor modelling codes.

The results in Table 6 show an agreement with experiment that is comparable to previous libraries and within the 2% uncertainty estimate on the measured decay heat.

3.4. Conclusions

The results from these three initial tests show either a slight improvement or no significant changes. Further testing needs to be done and the improvements when combined with the new JEFF-3.3 decay data, when ready, will need to be assessed but the current study shows no initial concerns precluding further testing.

4. Future developments

4.1. Uncertainties on engineering quantities

It is an important requirement for future development of nuclear technology that rigorous uncertainties on important engineering quantities need to be calculable. As fission yields are highly correlated it is necessary to provide the methods and covariance information to handle uncertainties for fission product related inventories and aggregate properties such as decay heat and radiative emissions.

There are several possible approaches to generate covariance data being considered based upon; (i) minimisation of physical constraints, (ii) perturbation of the model parameters underlying the yield distributions, (iii) LSQ or maximum likelihood methods using both an underlying model of fission and experimental data, examples can be found in the [6,11–14] and the references therein. However, as the cumulative yields can be directly calculated from the independent yields using decay data, it is also possible to determine the covariance terms iteratively from the experimental data in this evaluation [15]. Now that the new evaluation is complete it is intended to test this iterative data driven method and collaborate with colleagues in the ENDF and JEFF communities to study the effectiveness of the other techniques.

4.2. New measurement types

The current evaluation process only considers measurements of specific mass, charge, and where relevant isomeric state, yields. Measurements that have a resolution of more than one mass or charge unit have been ignored, but these contain much useful information. In future evaluations it is hoped to generalize the analysis method so that these data can be included.

4.3. Yields against neutron energy

The current evaluations are based upon representative neutron spectra; “thermal”, “fast” and “14 MeV”. The new GEF model allows the easy production of many specific energy yield sets for a nuclide. It is hoped that future evaluations will be able to use the GEF method with experimental data to generate energy dependent yield sets with sufficient resolution to be useful in calculation, although a computation infrastructure, such as that used for neutron cross-sections, would need to be developed to use such data.

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