Chapter 3

THE JEF-2.2 FISSION YIELD LIBRARIES

Introduction

This chapter summarises the methodology underlying the JEF-2.2 fission product yield evaluation, which was adopted from the UK evaluation UKFY2.

In the UK the evaluation of fission product yields for use in computer libraries was pioneered by E.A.C. Crouch at Harwell [1]. The libraries he produced were named Crouch 1, 2, and 3. After his retirement, the work was continued at Winfrith, first on an interim library, Crouch 4 [2], and then on UKFY1, produced by Banai, *et al*. [3], which was adopted by the first stage, JEF-1, of the Joint Evaluated File. A detailed comparison between different libraries was made in an earlier paper, presented at a meeting on decay heat at Studsvik by James [4].

The latest complete UK library, UKFY2, which has been adopted for JEF2, is a considerable advance on all of the earlier UK libraries (although, of course, it builds on them). Many more fissioning systems were included, the database of measurements was brought up to date, a new analysis of fractional independent yields had been made, and the method of fitting the yields to constraints arising from conservation laws was improved. The library produced from this evaluation is in the ENDF/B-VI format. Both independent (pre-delayed neutron emission) and cumulative (post-delayed neutron emission) yields are available, together with their standard deviations. For a given fission reaction, the yields are correlated by the fitting process; a prescription is available for the production of their covariance matrices. This work was funded jointly by the Central Electricity Generating Board, British Nuclear Fuels plc, and the United Kingdom Atomic Energy Authority; the UKAEA's contribution was mostly through its Underlying Research Programme. The work was carried out jointly by the University of Birmingham and the UKAEA at the Winfrith Atomic Energy Establishment.

The UKFY2 evaluation was described in full in three reports by James, *et al*. [5,6,7]. The methodology of the evaluation is described in full in the first of these reports [5]. We have produced tables of evaluated, unadjusted chain and independent yields, which are given in the second report [6]. In the third report, a detailed description of the remaining discrepancies is given [7]. The complete library in ENDF/B-VI format is available from the NEA Data Bank, along with the FITFYS subroutine and some of the input data files. Several remaining problems were identified or emphasised by this work. A few are listed below.

- There were considerable gaps in the data, especially in charge distributions, but also even in chain yields for the more important fission reactions, and obviously for nearly all fission products from the higher actinides. There also remained some significant discrepancies between measurements, including some for chain yields from the thermal neutron induced fission of ^{235}U. More measurements are needed, but in the meantime improved extrapolation

techniques, preferably based on sound theory, were needed. We noted that it is necessary to use extrapolation both for unmeasured yields for fairly well investigated fission reactions, and for most yields for some reactions which are almost entirely unstudied.

- More measurements were needed to test and improve the existing semi-empirical formulae.

- It was still not clear how yields vary with incident neutron energy. This was particularly uncertain for independent yields and for ternary fission products.

These problems were felt to require further study. British Nuclear Fuels plc has since funded a continuation of this work leading toward a new evaluation, UKFY3.

UKFY2

Many of the problems encountered in this work are found to a greater or lesser extent in any evaluation, and so some of the techniques developed may be of wider interest. To be generally useful, any data library must be as accurate and as complete as possible. Accuracy requires an up to date and complete compilation of experimental results, as well as a statistically sound method of treating the measurements and of considering the inevitable discrepancies between some of them. Completeness demands considerable care in interpolation and extrapolation to fill the equally inevitable gaps where there are no measured data at all. Since a user needs to know the accuracy of the data, it is also necessary to estimate as carefully as possible the standard deviations of the evaluated data and the correlations between them. This last task is sometimes the longest and hardest. The database, evaluation methods and the interpolation of data and parameters are considered below.

Fission product yield nuclear data should satisfy some simple conditions arising from physical conservation laws of nucleon number and of charge. Different evaluating teams use these conditions differently: either to adjust the data, or, if they have not been used for adjustment, as tests subsequent to the evaluation process. There are essentially four such conditions:

1) The yields, apart from those of the relatively rare light products from ternary fission, should sum to 2.

2) There should be conservation of nucleon number.

3) There should be overall conservation of charge.

4) There should be detailed conservation of charge giving equal yields of complementary elements. (This condition is weakened slightly by the occurrence of ternary fission.)

UK evaluations have applied successively more constraints. For example, the library Crouch published in 1977 used the first two conditions as constraints and the others as tests, while the present evaluation, like its immediate predecessor UKFY1 [3], used all four as constraints. Further, as the yields are constrained using a least-squares method, it is a straightforward matter to obtain a covariance matrix.

Up to this stage in our evaluation process, little account has been taken of the occurrence of isomers among the fission products, since all the techniques (with a slight exception in the initial treatment of measured chain yields) apply to the total independent yield of a nuclide, including all

isomers. The experimental values of the ratios of independent yields of isomeric to ground states was reviewed. The method of Madland and England [8] was used to calculate ratios for which there were no measurements.

The calculation of cumulative from independent yields is then described. This requires data on branching ratios of radioactive decays, including P_n, values for delayed neutron precursors, and these were all obtained from the preliminary JEF-2 decay data library, supplemented where necessary by the theoretical values of Klapdor [9].

The need to complete the UKFY2 evaluation within a fairly short period had meant that several quite important topics have had to be glossed over. Equally, other matters requiring further investigation have arisen in the course of the work. These were later investigated as part of the UKFY3 evaluation.

Fissioning systems

It was felt desirable to base the selection of fission reactions in the UK libraries on objective criteria. Consequently a series of calculations were made with the inventory code FISPIN, described by Burstall [10], and its 1988 libraries for both thermal and fast reactors. For the former, initial fuelling by enriched uranium, recycled uranium, mixed plutonium/uranium and thorium/uranium, were individually considered. The ratings and irradiations applied to the calculations were greater than actually achieved in practice at present, but were values regarded as feasible within the foreseeable future. Reactions were regarded as important if they contributed more than 0.1% of the fission rate at any time. Thus, it is thought that the derived list is more than adequate for some time to come. It does, of course, depend on the initial fuel compositions and on the assumed capture and fission cross-sections for the higher actinides; it is acknowledged that some of the latter may be considerably in error.

In addition, the library includes fission of ^{232}Th, ^{233}U, ^{235}U , and ^{238}U by “high energy” (about 14 MeV) neutrons; these reactions were in the earlier UK libraries. We have also considered the yields from the spontaneous fission of ^{242}Cm and ^{244}Cm which are important as sources of neutrons in reactors and in fuel handling, and of ^{252}Cf, which is important as a standard.

The complete set is given in Table 3.1. The reactions considered by the burn-up calculations are given in three sub-sets, in the three left-hand columns. These are distinguished by the value of the maximum fission rate percentage due to the nuclide in question at any time during the irradiation. (The range in which the percentage falls is indicated in the column heading). Clearly, the required accuracy of yields is greater if the percentage fission rate is greater; hence we consider that nuclides in the first column need the most careful treatment, followed by those in the second column and then by those in the third column.

Definitions and notation

The atomic number and mass number of the fissioning nucleus are denoted by Z_f and A_f respectively. For the neutron-induced fission of a nuclide of mass number A_{target}, $A_f = A_{target} + 1$, while for spontaneous fission, A_f is the mass number of the fissioning nuclide.

Table 3.1. The 39 fissioning systems in UKFY2

Maximum 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}Cf Sp
^{235}U* TFH	^{245}Cm TF	^{234}U F	^{242}Cm Sp
^{238}U* FH		^{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 [5,7].
T Thermal fission.
F Fast fission.
H 14 MeV fission.
Sp Spontaneous fission.

A fission product nuclide is specified symbolically by the triplet (*A*,*Z*,*I*), where *A* and *Z* are respectively the mass number and atomic number, and *I* indicates the isomeric state (*I* = 0 for the ground state, *I* = 1,2 for the first and second excited states). If a fission product has no isomers, or if we are referring to the sum of yields for all its isomers, we use the doublet (*A*,*Z*).

The independent yield *y*(*A*,*Z*,*I*) is the number of atoms of (*A*,*Z*,*I*) produced directly from one fission, after the emission of prompt neutrons (but before the emission of delayed neutrons). It can be written as the product of three factors:

$$y(A,Z,I) = Y(A)\, f(A,Z)\, R(A,Z,I)$$

where the sum yield *Y*(*A*) is the total independent yield (before delayed neutron emission) of all fission products of mass number *A*; *f*(*A*,*Z*) is the fractional independent yield of all isomers of (*A*,*Z*); and *R*(*A*,*Z*,*I*), the isomeric yield ratio, is the fraction of (*A*,*Z*) produced directly as isomer *I*.

From the definition, it follows that:

$$\sum_{Z} f(A,Z) = 1 \qquad \text{for all } A$$

$$\sum_{I} R(A,Z,I) = 1 \qquad \text{for all } (A,Z)$$

so that:

$$Y(A) = \sum_{Z,I} y(A,Z,I) \qquad \text{for all A}$$

The usefulness of these formulae derives from the fact that, with the exception of delayed neutron (β^-,*n*) emission and the few very long-lived α decays, all the radioactive decays of fission products are β^- or β^+, or isomeric transitions, and in none of these is *A* altered. Thus, to a very good approximation, the fission products can be considered as belonging to distinct mass chains. It should be noted that in the UKFY2 evaluation corrections were applied for these small effects.

The cumulative yield *c*(*A*,*Z*,*I*) of (*A*,*Z*,*I*) is the total number of atoms of that nuclide produced over all time after one fission. If the nuclide is stable and at the end of a mass chain, the cumulative yield is the total number of atoms remaining per fission, and is termed the chain yield *Ch*(*A*). Similarly, for a nuclide with a much longer half-life than any of its precursors, *c*(*A*,*Z*,*I*) is very nearly equal to the amount of it produced at a time short compared to its half-life but long compared to those of its precursors. However, for a radioactive nuclide for which this is not the case, some atoms will have decayed before all have been produced, so that at no time will there actually be *c*(*A*,*Z*,*I*) atoms per fission present.

An equivalent definition that is more useful is the following: immediately at the end of an "infinite" irradiation at the rate of 1 fission per second, *c*(*A*,*Z*,*I*) is the rate of decay of (*A*,*Z*,*I*) if that nuclide is radioactive, or its rate of production if it is stable. Consequently cumulative yields are useful in computing total fission product decay energies and delayed neutron emission rates.

The sum yield *Y*(*A*) and the chain yield *Ch*(*A*) for a mass chain *A* may differ by a few per cent, because the former applies before, and the latter after, delayed neutron emission. Tables of the calculated differences for each chain of some fissioning systems are given in Ref. [5]. It is sometimes difficult to decide which of these two quantities has been measured; this is an area to which more study should be devoted in future evaluations. Further discussion of cumulative yields can be found below.

Databases and data collection

The database used for the UKFY2 evaluation consisted of three files, containing data measured absolutely, relatively, and by "ratio of ratio" methods.

The most straightforward of these are the absolute measurements, in which the yield of a nuclide per fission is measured. However, this method requires knowledge of the number of fissions, which can be difficult to determine practically.

In the second type, a nuclide with a yield that is assumed to be accurately known is used to estimate the number of fissions. Thus, the unknown yield is determined relative to the standard yield.

The third type of measurement uses the "ratio of ratio" or "*R*-value" method. This assumes that the yields of both the fission product of interest (*x*) and a monitor fission product (*r*) are known from a reference fission reaction (indicated by the subscript 2). Then, if the yield of the monitor *r* is also known from the fission reaction of interest (subscript 1), the yield of *x* from reaction 1 can be found from:

$$y_1^x = y_2^x \left[\frac{A_1^x A_2^r}{A_2^x A_1^r} \right] \frac{y_1^r}{y_2^r}$$

where *y* is a yield and *A* an activity, which is the quantity actually measured.

The term in brackets in the above equation is the "*R*-value" and is made up of the measured activities determined in a simultaneous standard reaction irradiation. The other components of the right hand side must be determined absolutely or assumed. In this evaluation measured yields only, and not predictions of unmeasured yields, are used to convert *R*-value or relative measurements to absolute values. Thus much of such data could not be converted into a useable form.

The evaluation proceeded in two iterative stages. In the first, only absolute measurements (i.e. of the first type described above) were used. In the second, the two types of relative measurements were included as well, using for the standard yields values obtained in the first stage. Because these standards are, by definition, known accurately, their values will hardly be changed in the second stage and so further iterations were assumed not to be required.

Experimental fission yield data were collected from three computer readable sources:

1) Crouch's fission yield database, which was used in the Crouch [1] and the Banai, *et al*. [3] evaluations.

2) The international database EXFOR described by Calamand, *et al*. [11]; the last update for UKFY2 was received in November 1989.

3) A database of recent references, produced after a thorough search of recent literature.

We believe the combined UKFY2 database to be complete up to 1988, and to contain some results published in 1989. It has 39% more items of data than that used by Crouch [1] (12 137 compared with 7 448), including 60% more chain yield measurements.

The measurements were examined to remove duplications and to ensure consistency of isomeric states. In the evaluation, discrepant data were extensively examined to remove entry errors and to increase some unacceptably low estimates of error. The experimentalists uncertainties were adjusted in the previous UK evaluations to be always greater than 5% [1], unless significant justification was present in the reference. Considering the more accurate measurements now possible with mass separators this limit has been reduced to 1% for this type of measurement. However, if significantly different from other measurements a discrepant data point was down-weighted, and the discrepancy could not be resolved by deeper study of the references (see below). Only in extreme cases were discrepant measurements entirely deleted from the UKFY2 database, and this was recorded in the reference database.

Evaluation method

General treatment of measurements

We have previously mentioned a change in the treatment of reported uncertainties for mass-spectrometric measurements. For convenience, the revised rules used in attributing input uncertainties are stated here. Throughout this work all uncertainties are quoted at the 1 standard deviation level.

- For recent mass-spectrometric measurements, the quoted uncertainty was used provided it was not less than 1%. Otherwise, 1% was used, unless there was good justification for the published value in the reference.

- For other types of measurement, the quoted uncertainty was used provided it was it was not less than 5%. Otherwise, 5% was used, unless there was good justification for the published value in the reference.

- Mass-spectrometric results quoted without any estimate of uncertainty were given a standard deviation of 10%.

- Other results quoted without any estimate of uncertainty were given a standard deviation of 15%.

These standard deviations were then used to obtain weighted means in the following way. For n measurements $y_i \pm \sigma_i$, $1 \le i \le n$, the mean is:

$$Y = \sum w_i y_i / W$$

where:

$$W = \sum w_i$$

and the i^{th} weight is:

$$w_i = 1/\sigma_i^2$$

The internal and external standard deviations of the mean are respectively:

$$\sigma_I = 1/\sqrt{W}$$

and:

$$\sigma_E = \sqrt{\sum_{i=1}^{i=n} w_i (y_i - \bar{y})^2 / W(n-1)}$$

The value of χ^2 is:

$$\chi^2 = \sum_{i=1}^{i=n} w_i (y_i - \bar{y})^2$$

with $n - 1$ degrees of freedom if there are no constraints between the y_i. A useful quantity for indicating the consistency of the data is the "Birge factor":

$$R_B = \sqrt{\frac{\chi^2}{n-1}}$$

It will be seen that:

$$\sigma_E = R_B \sigma_I$$

If R_B ~1, then the data are consistent and $\sigma_E \sim \sigma_I$. If $R_B > 1$, then the data are inconsistent (though not necessarily significantly so) and $\sigma_E > \sigma_I$.

From χ^2 and the number of degrees of freedom, the probability of the data being consistent can be calculated. Those with a probability of less than 10% were listed in a set of discrepancy tables, values less than 1% and 0.01% being flagged for special consideration. In these cases, the data were checked for transcription errors between the quoted values in the references and the values in the database. Next, the relevant papers were studied to see if there were reasons for re-normalising or down-weighting the measurements. Usually, obvious corrections such as these could not be found; after all, any published results are subject to much checking and review. The amount of detailed study was in any case limited by the quantity of data. Consequently, after references had been checked, an automatic down-weighting procedure was applied to the data to reduce major discrepancies. This technique was based upon the normalised residual:

$$R_i = \sqrt{w_i W/(W - w_i)}(y_i - \bar{y})$$

which should be normally distributed with a mean of zero and a standard deviation of unity. R_i^2 is equal to the decrease in χ^2 that would occur if the i^{th} measurement were removed. The $|R_i|$ were constrained to be less than 2.5, for all yields with more than two measurements, by down-weighting the measurement with the largest value. If the maximum $|R_i|$ was greater than 2.5 the w_i was adjusted to give R_i equal to 2.5, and then the averaging process was repeated. This procedure reduces the weight of points far from the mean, thus reducing the effect of discrepant data on the weighted mean. The theoretical justification for these definitions and statements is given in James, *et al*. [12]; see also the appendix of an earlier report by the same author [5].

The tables of evaluated yields in James, *et al*. [6] clearly indicate where down-weighting has been employed. Both internal and external standard deviations of the mean are quoted and the larger of the two recommended.

Automatic down-weighting by the above method is not advised if there are only two measurements, which are mutually discrepant but of similar precision. Indeed, it is of doubtful use in considering any clearly bi-modal distribution of data, which indicates systematic differences probably due to different experimental techniques that should be investigated in depth.

We would like to emphasise that the automatic down-weighting described here (or any alternative method) should not be used in preference to a detailed analysis of the original measurements. It is only when the latter is fruitless, or, as in the present case, time prevents more than a partial study of the literature, that an automatic procedure should be considered in an evaluation, and then its use should be clearly indicated.

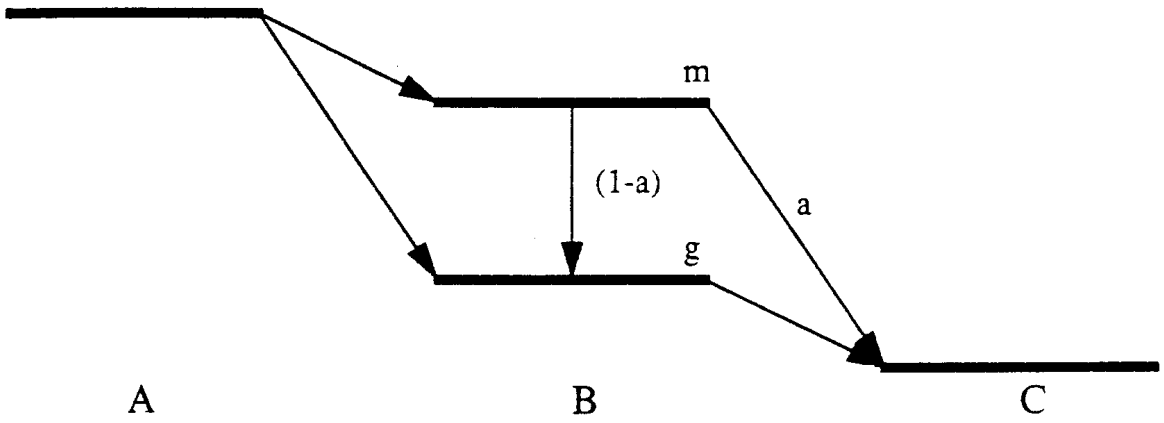
Separate unadjusted evaluations were made for chain, fractional independent and fractional cumulative yields. From these evaluations, sets of mean chain yields, fractional independent and cumulative yields with standard deviations were produced that could be used as input in the fitting of semi-empirical models as described below.

Chain yields

Measurements were included both of a chain yield itself and of cumulative yields of nuclides close enough to the end of the decay chain and with sufficiently small independent yields for their

cumulative yields to be good approximations to the chain yield. As several chains have nuclides with isomers near the stable end, a typical decay scheme of the form shown in Figure 3.1 was considered.

Figure 3.1. Typical decay chain including isomeric states



Nuclide *C* is either stable, or its cumulative yield can be assumed to be equal to the chain yield *Y*. Nuclide *B* has two isomers: a ground state, *g*, with cumulative yield *G* and an excited state, *m*, with a significant half-life (> 0.1 sec usually) with cumulative yield *M*. A fraction *a* of the excited state decays are by β^- emission to *C*, the remainder are by internal transition to the ground state.

Measurements of *M*, *G* and *Y* were first considered separately, and then their means adjusted by least-squares to fit the condition:

$$Y = G + a\,M$$

which holds if the independent yield of *C* is negligible.

If the unadjusted means and standard deviations are indicated by bars, then the adjusted chain yield is given by:

$$Y = \overline{Y} - \left(\overline{Y} - \overline{G} - a\overline{M}\right)\overline{\sigma}_{\overline{Y}}^2 \big/ D$$

with standard deviation σ_Y given by:

$$\sigma_Y^2 = \overline{\sigma}_{\overline{Y}}^2 \left(\overline{\sigma}_{\overline{G}}^2 + a^2\overline{\sigma}_{\overline{M}}^2\right)\big/ D$$

where:

$$D = \overline{\sigma}_{\overline{Y}}^2 + \overline{\sigma}_{\overline{G}}^2 + a^2\overline{\sigma}_{\overline{M}}^2$$

and where $\overline{\sigma}_Y$, etc. are the unadjusted standard deviations of *Y*, etc. determined by the methods of the previous sub-section. (Any uncertainty in the branching fraction a is ignored, in order to ensure consistency with the decay data.)

The value of χ^2 for the fit is:

$$\chi^2 = \left(\overline{Y} - \overline{G} - a\overline{M}\right)^2 \Big/ D$$

with 1 degree of freedom. If $\chi^2 > 1$, then the standard deviation σ_Y was multiplied by the Birge factor $R_B = \sqrt{(\chi^2)}$.

Fractional independent and cumulative yields

For nuclides away from the stable ends of mass chains, measurements may be of either fractional or of absolute yields: the former being obtained if the same experiment also determines the chain yield. For the present purpose, fractional yields were required, so absolute values in the database were converted by dividing by the evaluated (unadjusted) mass yield. The latter was either the experimental mass yield average (see above) or obtained from a fit to the mass yield distribution (see below).

Interpolation and extrapolation to fill gaps

General

To produce independent and cumulative yield libraries for reactor and decay heat calculations, all significant chain yields and fractional independent yields need to be known.

About 120 chain yields are required (mass 60 to 180) for these purposes. As even the system with the best coverage of measurements, ^{235}U thermal, has only 111 measured chains and some systems (for example ^{243}Am) have none, a model or method of prediction is required for chain yields. Similarly, if fractional independent yields greater than 10^{-8} are considered to be important, approximately 900 are required, whereas even for ^{235}U less than 250 have been measured.

There are several semi-empirical models and methods of interpolation or extrapolation for fractional independent and chain yields which can be used.

Chain yields

Three techniques were tried for filling gaps in chain yields:

- *Method 1*
  For a given fissioning system, interpolation of log (chain yield) as a function of chain mass, i.e. the standard mass-yield curve. This technique was the simplest, but could only be used effectively for a small gap of one or two missing yields, as the function is rapidly varying and has a varying slope, and clearly could not be used for systems with no experimental data.

- *Method 2*
  For a given mass chain, interpolation of log (chain yield) as a function of the effective fissioning mass, i.e. the mass of the fissioning system minus the mean number of prompt neutrons $\overline{\nu}_p$. Some of these graphs show slowly varying trends, which could be used to produce estimates of unmeasured chain yields. However for most chain masses the data are sparse or have large uncertainties, which makes interpolation difficult.

- *Method 3*
  The fitting to the mass-yield curve by a set of Gaussians, as proposed by Musgrove, *et al*. [13] and used more recently by Dickens [14]. This technique is based upon the apparent similarity of the chain yield distributions to Gaussian distributions. This method is the most versatile of the three, as it can be readily used to predict yields from systems on which few or even no measurements have been made. Details of it and of its present application are given in the next sub-section.

Five Gaussian fit to chain yields

We have followed Musgrove, *et al*. [13] in using five Gaussians (viz. two for each peak of the mass distribution, and one for near-symmetric fission). More recently theoretical justification for such a multiple Gaussian fit has been attempted, see for example Brosa, *et al*. [15]. The 15 parameters (strength, mean and width of each Gaussian) were reduced to 8 by assuming symmetry and requiring a total yield of 2. This model gives the chain yield $Y(A)$ as:

$$\begin{aligned} Y(A) = & \frac{N_1}{\sigma_1\sqrt{2\pi}}\left[e^{-\left(A-\overline{A}-D_1\right)^2/2\sigma_1^2} + e^{-\left(A-\overline{A}+D_1\right)^2/2\sigma_1^2}\right] \\ & + \frac{N_2}{\sigma_2\sqrt{2\pi}}\left[e^{-\left(A-\overline{A}-D_2\right)^2/2\sigma_2^2} + e^{-\left(A-\overline{A}+D_2\right)^2/2\sigma_2^2}\right] \\ & + \frac{N_3}{\sigma_3\sqrt{2\pi}}e^{-\left(A-\overline{A}\right)^2/2\sigma_3^2} \end{aligned}$$

where N_i is the coefficient of the i^{th} Gaussian and σ_i its width parameter, $\overline{A}$ is the mean mass of the distribution and D_i is the separation of the i^{th} Gaussian peak from $\overline{A}$.

Because the chain yields sum to 2:

$$N_3 = 2(1-N_1-N_2)$$

The evaluated chain yields were fitted to this model, and Table 3.2 gives the values of the parameters for systems for which there were sufficient data for satisfactory fits to be obtained. The fits for ^{235}U thermal and fast, ^{233}U thermal, and ^{239}Pu thermal are shown in James, *et al*. [5], Figures 2-5. Such a representation by only five Gaussians, of course, smooths the distribution, removing the small fluctuations that are observed experimentally.

To extend the 5-Gaussian representation to systems with sparse data, the parameters already obtained in Table 3.2, were plotted against fissioning mass and charge, and fitted by linear or quadratic functions of A_f. (No systematic trend with Z_f could be detected.) Then new 5-Gaussian fits were made to the chain yield data, allowing only one of the parameters to vary in turn. Linear or quadratic fits were then made to each of the varied parameters, with the functions of A_f. After all parameters had been fitted in this manner, the whole process was repeated. After two iterations the refitting procedure failed to produce any improvement in χ^2. The functions thus obtained are found in Table 3.3.

Table 3.2. Fitted parameters for the 5-Gaussian model

Actinide	$\overline{A}$	N_1	σ_1	D_1	N_1	σ_2	D_2	σ_3
^{233}U Thermal	115.86	0.7116	4.230	24.63	0.2855	3.048	17.11	13.79
^{235}U Thermal	116.90	0.7158	4.298	24.02	0.2823	2.423	16.63	9.250
^{239}Pu Thermal	118.50	0.7100	5.587	21.34	0.2887	2.630	15.27	2.237
^{229}Th Thermal	114.03	0.7146	3.081	27.80	0.2832	2.335	21.73	11.22
^{232}Th Fast	115.49	0.7079	3.522	26.45	0.2823	2.472	19.10	11.80
^{235}U Fast	116.79	0.7081	4.516	23.76	0.2868	2.503	16.42	13.09
^{238}U Fast	118.02	0.7102	5.031	22.85	0.2852	2.131	15.85	9.525
^{232}Th High	114.65	0.6989	4.451	24.88	0.1164	4.264	18.78	11.17
^{233}U High	115.12	0.5586	5.959	23.12	0.2190	5.243	19.27	11.78
^{235}U High	116.01	0.6241	5.535	23.26	0.1824	3.208	16.00	11.99
^{238}U High	117.42	0.6605	5.962	22.32	0.1921	2.938	15.81	11.80

Table 3.3

$$\overline{A} = \frac{A_f - \overline{\nu}_p}{2} \qquad \text{[fixed by nucleon conservation]}$$

$$N_1 = 0.0003846A_f + 0.6215 \qquad \text{[fast]}$$

$$N_1 = 0.0010563A_f + 0.4579 \qquad \text{[thermal]}$$

$$\sigma_1 = 0.2017A_f - 42.906$$

$$D_1 = 27.1 - 0.67832\left(A_f - 230\right) + 0.013664\left(A_f - 230\right)^2$$

$$N_2 = 0.286$$

$$\sigma_2 = 0.1125A_f - 24.375$$

$$D_2 = 19.9 - 0.595\left(A_f - 230\right) + 0.00125\left(A_f - 230\right)^2$$

$$\sigma_3 = 12.0$$

Although this is a simple model and the goodness of fit to the parameters only moderate, reasonable results were obtained when chain yields were calculated for the systems in Table 3.2 using the predicted (instead of the fitted) Gaussian parameters and compared with experimental data. In James, *et al*. [5] figures show "predicted" and evaluated measured chain yields for ^{235}U thermal and fast chain yield distributions. Quite good agreement was also obtained with evaluated measured chain yields for other systems which had not been included in Table 3.2; James, *et al*. [5] show the comparisons for ^{236}U fast, ^{238}U fast, and ^{237}Np thermal and fast.

The yields calculated from the formulae were then plotted with measured yields against ($A_f - \overline{\nu}_p$) as in the interpolation method described in Method 2 above. The present method gave good

agreement in some cases but many comparisons were inconclusive; either the uncertainties were too large or there were too few points to test the prediction. However, a definite trend away from the prediction occurs in the region of masses 89-100 for ($A_f - \bar{\nu}_p$) < 232. There, a straight line fitted experimental data better than the curve from the derived 5 Gaussians.

Therefore chain yields for UKFY3 were first taken from the experimental averages. Then short gaps were filled by interpolation as noted in the description for Method 1 (above). Larger gaps were filled using the 5-Gaussian model with parameters from Table 3.2 if appropriate, or obtained from the above equations if not. The predictions from this model were modified before being used to produce complete data sets. First, the central Gaussian was not allowed to contribute outside the two main peaks (to avoid unrealistic flaring of the distribution at very low yields). Secondly the predictions were re-normalised with the experimental data. This re-normalisation considered the two cases of: (a) the wings of the distribution, and (b) gaps in the experimental data. The predictions in the wings, up to the first experimental point, were re-normalised by a constant factor so that for this point the predicted yield equalled the measured value. In gaps, predicted yields at each end were fitted to measured values by making the logarithm of the normalisation factor vary linearly with mass across the gap. Finally, for ($A_f - \bar{\nu}_p$) < 232and for $89 \le A \le 100$, straight line fits of log Y against ($A_f - \bar{\nu}_p$) were used in preference to the other methods of interpolation.

This procedure gave a complete set of chain yields for each fissioning system based as firmly as possible on experimental data. Graphs of these chain yields are given in James, *et al*. [5] for some of the 39 fissioning systems considered.

Fractional independent yields

The fractional independent yields can be fitted by either the A_p', or the Z_p models, developed and described by Wahl [16,17] and the references therein; these represent the fractional independent yields as Gaussian distributions in mass and charge respectively, modified by an odd-even effect. We concentrated on the Z_p model and have used the same parametrisation as Wahl. An earlier attempt to fit each chain by distributions with individual parameters failed, because many of the chains had such sparse or inaccurate data that the resulting parameters were clearly unphysical. Consequently, it was necessary to restrict the number of fitted quantities by requiring, like Wahl, that the Gaussian parameters for the different mass chains be relatively simple functions of mass number.

The fractional independent yields $f(A,Z)$, (summing over isomers), are modelled by:

$$f(A,Z) = 1/2\, F(A,Z) N(A) \left\{ erf\left[\frac{Z - Z_p(A) + 1/2}{\sigma_Z \sqrt{2}} \right] - erf\left[\frac{Z - Z_p(A) - 1/2}{\sigma_Z \sqrt{2}} \right] \right\}$$

where $F(A,Z)$ gives the odd-even effect, $N(A)$ is a normalisation constant to ensure summation to 1 for each mass, and Z_p, and σ_z are the mean and width of the Gaussian distribution without the odd-even effect.

Z_p is equal to the unchanged charge distribution (UCD) prediction for most probable charge; corrected by a term $\Delta Z(A')$, i.e. for the high mass peak:

$$Z_p(A_H) = A_H' \frac{Z_f}{A_f} + \Delta Z(A_H')$$

and for the low mass peak:

$$Z_p(A_L) = A'_L \frac{Z_f}{A_f} - \Delta Z\left(A_f - A'_L\right)$$

Here, A' is the mean fragment mass before prompt neutron emission:

$$A' = A - \bar{\nu}_p(A)$$

where $\bar{\nu}_p(A)$ is the mean number of prompt neutrons from that fragment. (Strictly the argument of $\bar{\nu}_p$ should be A', but approximating it with A causes little error.) For ^{235}U thermal the values for $\bar{\nu}_p(A)$ were taken from Wahl [16], and for other reactions the same function was used but re-normalised to give the appropriate total $\bar{\nu}_p$.

The $N(A)$ can be calculated to better than 1 part in 10^5 from:

$$\frac{1}{N(A)} = 1/2\left[F(A,\text{even } Z) + F(A,\text{odd } Z)\right] + \left[F(A,\text{even } Z) - F(A,\text{odd } Z)\right]\xi(A)$$

where:

$$\xi(A) = (2/\pi)e^{-\pi^2\sigma_2^2/2}\cos\left[\pi Z_p(A)\right]$$

Note that the separate sums of the even Z and the odd Z fractional independent yields are respectively $N(A)F(A,\text{even } Z)[1/2 + \xi(A)]$ and $N(A)F(A,\text{odd } Z)[1/2 - \xi(A)]$.

The factor $F(A,Z)$ giving the combined proton and neutron odd-even effect is defined as follows (here $N = A - Z$ is the neutron number):

Even A, Even Z (Even N)	$F(A,Z) = \bar{F}_Z . \bar{F}_N$
Even A, Odd Z (Odd N)	$F(A,Z) = 1/\left(\bar{F}_Z . \bar{F}_N\right)$
Odd A, Even Z (Odd N)	$F(A,Z) = \bar{F}_Z / \bar{F}_N$
Odd A, Odd Z (Even N)	$F(A,Z) = \bar{F}_N / \bar{F}_Z$

The correction term to Z_p, $\Delta Z(A')$, is composed of linear terms, as shown in Figure 3.2 below representing the heavy mass distribution.

Around the high mass peak:

$$\Delta Z\left(A'_H\right) = \Delta Z\left(A'_H = 140\right) + \left[\frac{\delta\Delta Z}{\delta A'_H}\right]\left[A'_H - 140\right]$$

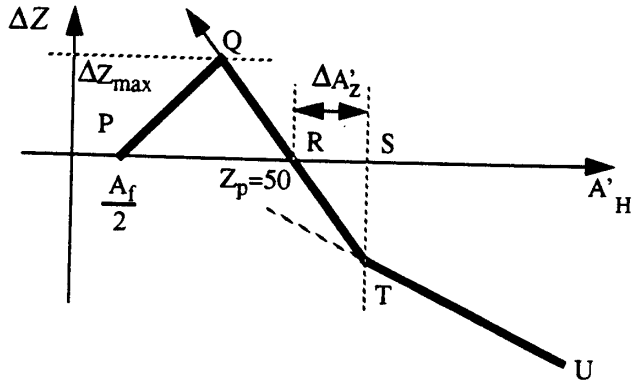
and around the low mass peak:

$$\Delta Z\left(A'_L\right) = \Delta Z\left(A'_H = 140\right) + \left[\frac{\delta\Delta Z}{\delta A'_H}\right]\left[A_f - A'_L - 140\right]$$

where the value of $\left[\frac{\delta\Delta Z}{\delta A'_H}\right]$ is assumed to be constant.

These equations represent the straight line *TU* in Figure 3.2.

Figure 3.2. Assumed variation of $\Delta Z(A')$ with A'



Around symmetrical fission the $\Delta Z(A')$ and σ_z undergo rapid changes described by Wahl [16,17]. Wahl defines the variations with three further parameters σ_{50}, ΔZ_{max} and $\Delta A'_z$ [17].

$\Delta Z(A')$ is assumed to be zero at symmetry A_f and at Z_p = 50 (points *P* and *R* respectively). Between these points, $\Delta Z(A')$ attains a positive maximum ΔZ_{max} at point *Q*.

The point *R* is determined by the value A'_H for which Z_p = 50 (a closed shell for protons), if the correction term is ignored (i.e. ΔZ = 0.) The point *S* is a distance $\Delta A'_z$ along the A'_H axis from *R*. *T*, which is vertically below, is then fixed by this value of A'_H and by the equations above of the line *TU*. *T* and *R* define a straight line which crosses the horizontal line $\Delta Z = \Delta Z_{max}$ at the point *Q*. *Q* and the point *P* of symmetrical fission define the final straight line of the set.

The Gaussian width $\sigma(A)$ has either of two values. Near symmetry, between the points *P* and *S* (i.e. for $1/2\ A_f \le A'_H < A'_H\ (Z_p = 50) + \Delta A'_z$), and in the corresponding region for light masses, $\sigma(A) = \sigma_{50}$. For other masses, that is, over the regions of the chain yield peaks, $\sigma(A) = \sigma_z$.

The Z_p model was initially fitted to our weighted average fractional independent and cumulative yield sets using a general non-linear least squares procedure (NAG routine E04FCF). Errors (1 standard deviation) were calculated from the χ^2 and the covariance matrix output by the routine. To simplify the fitting, the cumulative yield weighted averages were converted to sum yields. This conversion used our chain yields and the recommended experimental P_n values from Lund, *et al*. [18], by removing additions to and losses from the chain due to delayed neutron emission. The converted sum yields were thus just the sum of the previous independent yields in the relevant chain and the independent yield of the nuclide itself.

The input yields to the least-squares fit were constrained to have uncertainties of 5% or greater, to stop a few highly-weighted values dominating the fit. As small yields in a chain are difficult to measure, a lower limit was set on the fractional yields that were fitted, at the point where the reduced χ^2 rapidly diverged.

For ^{235}U thermal it was possible to fit all the parameters. However, for other reactions it was not possible to fit parameters σ_{50}, ΔZ_{max} or $\Delta A'_z$ as there are no significant data in the region of near symmetric fission. Therefore the ^{235}U thermal values for these parameters were used and only the five other parameters varied in the fits.

When this was first attempted [19] many systems were fitted. However most of the data were fractional cumulative yields near 1.0 in value (i.e. for nuclides near the stable ends of chains). Also, it was not certain whether complete P_n, values were available for some chains with small yields. It was therefore decided to ignore the fractional cumulative yields. This left only four systems with sufficient data to be fitted, but the uncertainties on the derived parameters were considerably reduced. The results for the four fission reactions are given in Table 3.4.

Table 3.4. Parameters for the Wahl Z_p model

Parameter	^{233}U T	^{235}U T	^{239}Pu T	^{235}U F
$\Delta Z(A') = 140$ +/-	-0.511 0.013	-0.523 0.012	-0.4854 0.0076	-0.3758 0.0205
$\frac{\delta \Delta Z}{\delta A'}$ +/-	-0.0153 0.0027	-0.0078 0.0017	-0.0143 0.0014	-0.01883 0.00446
$\overline{\sigma}_z$ +/-	0.5735 0.0104	0.5460 0.0112	0.5506 0.0080	0.5206 0.0238
$\overline{\sigma}_{50}$ +/-	(0.35)	0.35 0.02	(0.35)	(0.35)
$\overline{F}_Z$ +/-	1.267 0.031	1.2776 0.026	1.144 0.015	1.121 0.036
$\overline{F}_N$ +/-	1.075 0.025	1.077 0.022	1.0509 0.0139	1.002 0.031
$\Delta A'_Z$ +/-	(0.941)	0.941 0.260	(0.941)	(0.941)
ΔZ_{max} +/-	(0.693)	0.693 0.238	(0.693)	(0.693)
Reduced χ^2	3.8	2.61	1.86	2.08
Minimum fission yield used	0.005	0.05	0.05	0.1
Number of measurements	132	145	81	42

Parentheses denote quantities fitted for ^{235}U T only and then used as constants for other systems.
One standard deviation in brackets; insufficient data to fit parameter, assumed same as ^{235}U T.

Reduced $\chi^2 = \left\{ \frac{1}{no.\,of\ \ po\,int\,s} \sum_i \left[\frac{(EXPT_i - CALC_i)^2}{\sigma_i^2} \right] \right\}^{0.5}$

For ^{235}U thermal, probably the most measured system, there were a total of 145 values after data for isomers had been combined. Of these, 47 were discrepant. However the agreement between fit and measurement is good for most masses, particularly for results for the low mass peak where considerable data is available from recently-developed mass separator measurements.

It is difficult to extrapolate this model to other systems, due to the small group of systems fitted (three thermal and one fast) and the large associated errors in the parameters. The σ_z are similar and show no apparent trend, so the average of 0.554 was used. The F_Z shows a trend in fissioning charge and energy, and we assume a value of 1.0 at 14 MeV. Using the values for two atomic numbers (92 and 94) and two energies (thermal and fast), we assume:

$$\overline{F}_Z(\text{thermal \& spont.}) = \begin{cases} 1.2723 - 0.06415\left(Z_f - 92\right) & \text{if } Z_f \le 96 \\ 1 & \text{if } Z_f \ge 97 \end{cases}$$

$$\overline{F}_Z(\text{fast}) = 0.88\overline{F}_Z(\text{thermal})$$

$$\overline{F}_Z(\text{high energy}) = 1.0$$

For $\overline{F}_N$ the value becomes 1.0 for fast and 14 MeV energies, the thermal values showing a charge dependency:

$$\overline{F}_N(\text{thermal \& spont.}) = 1.0758 - 0.01245\left(Z_f - 92\right)$$

The parameters $\Delta Z(A' = 140)$ and $\frac{\delta \Delta Z}{\delta A'_H}$ are small additions to the *UCD* estimate and thus means of the fitted values were chosen as being reasonably adequate, that is -0.494 and -0.01266 respectively.

The fractional independent data for all the systems of interest were then produced using the parameters either from the fit where appropriate or from the above extrapolations. For most mass chains, the agreement between calculated and measured data is moderately good; the exceptions are sufficiently few for them to be studied in detail in the next round of evaluation.

Ternary yields

The main requirement in UKFY2 for ternary yields was for yields for ^{4}He and ^{3}H for all the systems. The yield of ^{4}He at different incident neutron energies shows little discernible difference from that for thermal neutron fission for ^{233}U, ^{235}U and ^{239}Pu, and therefore the yields were considered energy independent. This disagrees with Thomas and Whetstone's work described by Madland and Stewart [20] which suggested a linear dependence on the excitation energy of the system. The graphs in James, *et al*. [5] show possible structure but well within the uncertainties of the current measurements.

For extrapolation to nuclides for which there were no ternary yield measurements, two methods described by Madland and Stewart [20] were tried. These fit the yield as linear functions of respectively (i) Z_f^2/A_f and (ii) $(4Z_f - A_f)$. Figures 24 and 25 in James, *et al*. [5] show the data for ^{4}He

plotted against these functions. Choosing Z_f^2/A_f as the independent variable gave the better fit and thus this was used for prediction of missing yields. The least-squares line is given by:

$$Y(^4\mathrm{He}) = 0.0647\, Z_f^2/A_f - 2.1292$$

where a reasonable estimate of the uncertainty in $Y(^4\mathrm{He})$ is ±20%.

For ^{3}H both variables were tried but it is difficult to justify anything other than a constant ratio of ^{3}H to ^{4}He yields. Therefore:

$$Y(^3\mathrm{H}) = 0.06554\, Y(^4\mathrm{H})$$

was used for unmeasured tritium yields. A reasonable estimate of the uncertainty in the predicted $Y(^3\mathrm{H})$ is ±25%.

The energy dependence of ^{3}H yields remains uncertain, there being considerable discrepancies between the few measurements available. Tritium yield against energy for ^{235}U and ^{239}Pu include considerable discrepancies. Most of the differences are due to the method of separating α-particles and tritons; early work considered only the energy of the fragment, but more recent work by, for example, Ouasti [21] measured also the energy loss, allowing different particles to be more precisely distinguished. Ouasti's results show very little variation with energy, but no measurements were made between thermal energy and 0.5 MeV, which is the most important region for averaging over a "fast" neutron spectrum.

Fitting to constraints

Using the evaluation methods described above, a library in ENDF/B-V format was produced. However, as was pointed out above, there are constraints that must apply to the yields due to the conservation of nucleons and charge:

$$\sum_A Y(A) = 2$$

$$\sum_A A.Y(A) = A_f - \bar{\nu}_p$$

$$\sum_{ZA} Z.\, f(A,Z).Y(A) = \sum_A Z_p(A).Y(A) = Z_f$$

The first two conditions together imply the third.

Also there should be equality of yields of complementary elements:

$$\sum_A f(A,Z).Y(A) = \sum_{A'} f(Z_f - Z, A').Y(A') \text{ for all } Z < \frac{Z_f}{2}$$

These relationships ignore ternary fission, which introduces errors of less than 1%.

As in the previous evaluation UKFY1, the first three constraints were applied for all *A*. However, whereas in UKFY1 the fourth was applied for the 15 pairs of elements nearest symmetry, in UKFY2 this was applied to those pairs of elements with the greatest yields. The number of pairs was increased until the reduced χ^2 did not excessively exceed unity or, where reduced χ^2 was always greater than 1.0 the number of pairs was chosen to be that which gave a minimum value.

The values of $\overline{\nu}_p$, used in the fitting are given in James, *et al*. [5]. The number of elements pairs fitted and the subsequent χ^2 per degrees of freedom and summation of fitted element yields are also given in Table 6 of the same reference.

The details of the least-squares fit are given in the Appendix to James, *et al*. [5]. It gives, of course, not only the adjusted yields for each fissioning system but also their covariance matrix. The diagonal terms of each matrix give the standard deviations which are required by the ENDF/B-V format, but the complete matrices (39 symmetric matrices each of order approximately 900×900) would be too large to store in the library. However the fitting program FITFYS is quick enough for it to be reasonably incorporated as a sub-routine in any program that needs the covariances; the authors have supplied both the code and the input (unadjusted) yields and uncertainties to the NEA Data Bank.

The adjustments in both chain and independent yields were mostly less than one standard deviation. Figures 31-34 of James, *et al*. [5] show examples of the adjustments in chain yields relative to the experimental (and predicted) chain yields, and Figures 35 and 36 display the distributions of the adjustments relative to the standard deviations for all chain yields and all fractional independent yields respectively. Except for a few extreme cases in the latter, with changes greater than two standard deviations, the adjustments will be seen to be relatively small.

It is worth noting that the formulae for interpolation and extrapolation of chain and fractional independent yields described above are designed to satisfy the first three constraints. Consequently it was generally the case that greater adjustments were needed for those fissioning systems that had more measured yields and thus more experimental noise in the data.

Isomeric yields

Except in the initial interrogation and averaging of the database, the evaluated yields have been those of complete nuclides and we have ignored the division of the independent yield of a nuclide between its isomers. To allow for such a division for a nuclide with excited state *m* and ground state *g*, we define the isomeric yield ratio *r*(*A*,*Z*):

$$r(A,Z) = \frac{y(A,Z,m)}{y(A,Z,m) + y(A,Z,g)}$$

Where possible, experimental data were used for the *r*(*A*,*Z*). These are of two types. Preference was given to direct measurements of the ratio, as these are free of normalisation problems. Failing these, the independent yield evaluations contained a number of pairs of isomers for each of which there was an averaged value, so that the above equation could be used to calculate *r*. However, measurements of either kind were found to be sparse, so that recourse had to be made to theory. We used the method of Madland and England [8], as that requires minimal information (the spins of the excited and ground states) about the nuclide; even that was sometimes uncertain, but generally we relied on the spin data in a preliminary version of JEF-2.

Nuclides with three isomeric states (including the ground state) were considered using a simple extension of the Madland and England model.

The calculation of cumulative yields

The concept of the cumulative yield $c(A,Z,I)$ of the nuclide (A,Z,I) has been introduced already, where two equivalent definitions were given. Although these definitions may be applied with no difficulty to short-lived fission products, there is some ambiguity with the decay products of nuclides having very long half-lives. First, it is reasonable to ignore the very long-lived α decays (^{144}Nd [half-life 2.4×10^{15} years] and ^{147}Sm [half-life 10^{11} years]), as these will lead to an apparent approximate doubling of the cumulative yields of the daughters (^{140}Ce and ^{143}Nd) which, because of the times involved, is absurd. Other similarly long-lived β decays should also have been removed but are still in the present library. These however are easily detected; greater problems arise with half-lives of say 1-100 years, i.e. of the same order as irradiation or storage times. Because of these problems we would recommend that cumulative yields should be used only rarely; the safer method is to use independent yields with an inventory code that correctly treats all relevant types of decay, and also permits the consideration of neutron capture. As has already been stated, cumulative yields are useful in some special applications: in delayed neutron calculations, only short-lived nuclides are of importance. In calculations of total energy emission, corrections should be made for the contribution emitted after long decay times.

From the definition given of cumulative yields:

$$c(A,Z,I) = y(A,Z,I) + \sum_{(A',Z',I')} b(A',Z',I' \rightarrow A,Z,I)c(A',Z',I')$$

where $b(A',Z',I' \rightarrow A,Z,I)$ is the fraction of decays of (A',Z',I') that go to (A,Z,I).

As has already been explained, the rare and slow α decays are ignored in this context. This leaves two complications that prevent a cumulative yield equalling simply the sum of independent yields up to and including the nuclide under consideration. First, the occurrence of isomers splits decay chains. Secondly, (β^-,n) decays destroy to a small extent the independence of individual mass chains. If it were not for these delayed neutron decays, the cumulative yield of the stable nuclide at the end of a mass chain would equal the sum of independent yields along the chain. Their presence means that there are small differences between the two, which were tabulated first for the earlier UKFY1 evaluation in Ref. [4] and for UKFY2 in Ref. [5]. In using the above equation, note must also be taken of the small fraction of fission products that decay by other modes which change the mass of the nucleus.

All these types of decay can be considered in sequence if we number each fission product so that each decay goes to a nuclide with a larger number than the parent. This entails:

- Ordering by decreasing mass number *A*.
- Ordering β^- nuclides by increasing *Z*, and *EC*/β^+ nuclides by decreasing *Z*. Stable nuclides come last in each chain.
- Ordering ground states after first isomeric states after second isomeric states, etc.

Then, if we denote nuclides numbered in such a sequence by *i*,*j*,..., the above equation becomes:

$$c_i = y_i + \sum_j b_{j\to i} c_j$$

or in matrix form (with a bar denoting a transposed matrix):

$$c = y + \bar{b}c$$

Since the only non-zero values of $b_{j\to i}$ are those for which $j < i$, this equation can be readily used to compute cumulative from independent yields. However, the calculation of the variances (and covariances) of the cumulative yields from those of the independent yields is more complicated. From the above:

$$\left(I - \bar{b}\right)c = y$$

or:

$$c = Qy$$

where:

$$Q = \left(I - \bar{b}\right)^{-1}$$

Then if a change δy in y produces a change δc in c:

$$\left\langle \delta c \delta \bar{c} \right\rangle = Q \left\langle \delta y \delta \bar{y} \right\rangle \bar{Q}$$

In particular, the variance of c_i is given by:

$$\left\langle \delta c_i^2 \right\rangle = \sum_{j,k} Q_{i,j} Q_{i,k} \left\langle \delta y_j \delta y_k \right\rangle$$

The covariances of the independent yields y_i are calculated by the adjustment program FITFYS described in the appendix of James, *et al*. [5]. The matrix Q can be calculated from radioactive decay branching ratios; its definition in above implies that it is a lower triangular matrix with $Q_{ij} = 0$ if $j > i$, diagonal terms $Q_{ii} = 1$, and, for $j < i$:

$$Q_{ij} = \sum_{k=j+1}^{k=i} b_{j\to k} Q_{ik}$$

If, for a given value of i, Q_{ij} is calculated successively for j the values of Q_{ik} on the right hand side of this equation will already be known. At most 30 nuclides will contribute to the variance of c_i so it suffices to calculate and store $Q_{i(i-m)}$, where $m = \mathrm{Min}(i,30)$.

Production of the JEF-2.2 libraries

Following the completion of UKFY2 in 1990, the library was submitted to the JEF technical working groups. In July 1993, a revision of the library was produced using the decay data branching ratios from the final frozen JEF-2.2 decay data. However, in producing this library it became apparent that some short-lived nuclides were not present in the JEF-2.2 decay data, some of these contributed greater than 10% of the yield in some mass chains for some fissioning systems. Thus a correction term was applied to adjust the independent yields for each mass such that a calculation of the chain yields would arrive at the recommended chain yield values.

Subsequent to the adoption of the JEF-2.2 fission product yield library a few cases were found where the calculation of individual correction terms had failed to converge to a physical value, as the missing yield was the majority of that in the mass chain. For UKFY3 an improved method of calculation of the correction terms has been implemented and decay data evaluation has been sponsored to produce data for the most significant missing nuclides.

Conclusions

We have described the recent UK work in the producing the JEF-2.2 fission product yield evaluation. The chief remaining task is the testing of the new library by comparison with others, and also by calculation of decay heat and of delayed neutron emission rates. Some preliminary tests have been carried out and are described by Mills [22]. This reference also includes work towards a new fission yield evaluation, UKFY3.

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