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JEFF fission product yield evaluation methodologies

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Summary

- JEFF-3.1.1 fission yields (JEF Report 20) (Slides from JEF/DOC-1343)
  - Scope
  - Data and Analysis
  - Models to fill gaps
  - Constrains/Adjustment, cumulative yields
- Cumulative yields
- Q matrix
- Error propagation / covariance

Definitions

The **independent yield** y(A,Z,I) is the number of atoms of (A,Z,I) produced directly from one fission, but after the emission of prompt neutrons (but before any radioactive decay and hence the emission of delayed neutrons). It can be written as the product of 3 factors:

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

where the **sum yield** or **mass yield** Y(A) is the total of the independent yields (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.

Definitions

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The **cumulative yield** c(A,Z,I) of nuclide (A,Z,I) is the total number of atoms of that nuclide produced over all time after one fission. If the nuclide is stable the cumulative yield is the total number of atoms of that nuclide remaining per fission after all precursor decays (ignoring the effects of other nuclear reactions e.g. neutron capture). However, for a radioactive nuclide for which this is not the case, some atoms will have decayed before all have been produced.

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.

The **chain yield** Ch(A) is equal to the sum of all stable or long-lived cumulative yields for a given mass chain. It should be noted that the chain yield, Ch(A), and the sum or mass yield, Y(A), for a mass chain A may differ by a few per cent because the former applies after, and the latter before, delayed neutron emission.

History of JEF(F)/UK FY evaluations

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- 1960-1981 Crouch
  - Atomic and Nuclear Data Tables (1977)
- 1981-1987 James and Banai
  - UKFY1 / JEF1 (1986)
- 1988-1995 Mills, James and Weaver
  - UKFY2 / JEF-2.2 (1993)
- 1995-present Mills
  - UKFY3.x series - JEFF-3.1.1 (UKFY3.6A)
  - (UKFY4 photon, neutron and charged particle induced energy dependent or spontaneous fission using Wahl code)

Fissioning systems in UKFY2/3

Maximum fraction of fission rate			Spontaneous fission
>10%	1-10%	0.1-1%	
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.

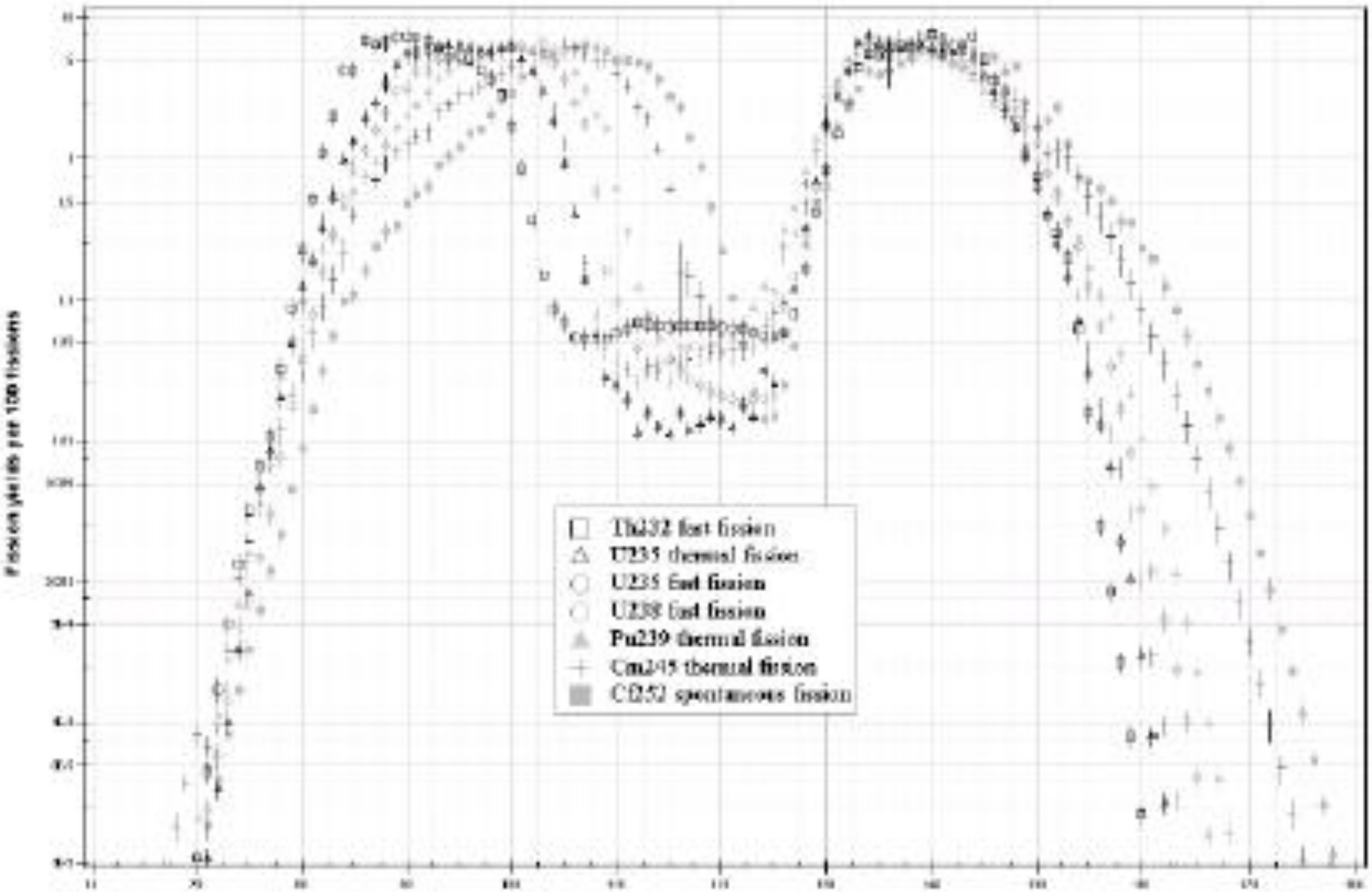
Evaluation – Data Analysis

- UKFY3 based upon experimental data from >2000 papers, reports etc.
- Measurements analyzed to given "best estimates" of each measured yield

Table 1: Number of data items in the UKFY3 experimental database

Absolute measurements	ratio measurements	ratio of ratio measurements	Total
11887	1352	1471	14710

Measured – Mass Distribution



Models – Mass Distribution

Historically empirical fitting of Gaussian distributions have been used to model chain yields. Work in the 1960s showed that the best results were obtained using five Gaussians. Due to physical constaints there were only 7 free parameters to fit:

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

Note that $N_3=2(1-N_1-N_2)$.

Models – Charge distribution (Wahl Zp)

- **The independent yield is calculated as the integral of a normal distribution**

$$FI(A,Z) = \frac{1}{2}F(A,Z)N(A)(\mathrm{erf}(V) - \mathrm{erf}(W))$$

where

$$V = \frac{Z(A) - Z_p(A) + 0.5}{\sigma_Z(A)\sqrt{2}} \qquad W = \frac{Z(A) - Z_p(A) - 0.5}{\sigma_Z(A)\sqrt{2}}$$

F(A,Z) describes the odd-even effect and N(A) is a normalization constant

- **The integral of a normal distribution between a and b is given by:**

$$\frac{1}{2}\left(erf\left(\frac{a}{\sqrt{2}.}\right) - erf\left(\frac{b}{\sqrt{2}}\right)\right)$$

Models – Charge distribution (Wahl Zp)

- **$Z_p(A)$ is the most probable charge for mass A**

This is calculated as the "unchanged charge distribution" corrected for prompt neutron emission with a term describing the variation of the charge offset ΔZ

In the heavy mass peak this is:

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

In the light mass peak, by conservation of mass and charge

$$Z_p(A_L) = A'_L \frac{Z_f}{A_f} + \Delta Z(A'_{Hc}) \qquad A'_{Hc} = A'_f - A'_L$$

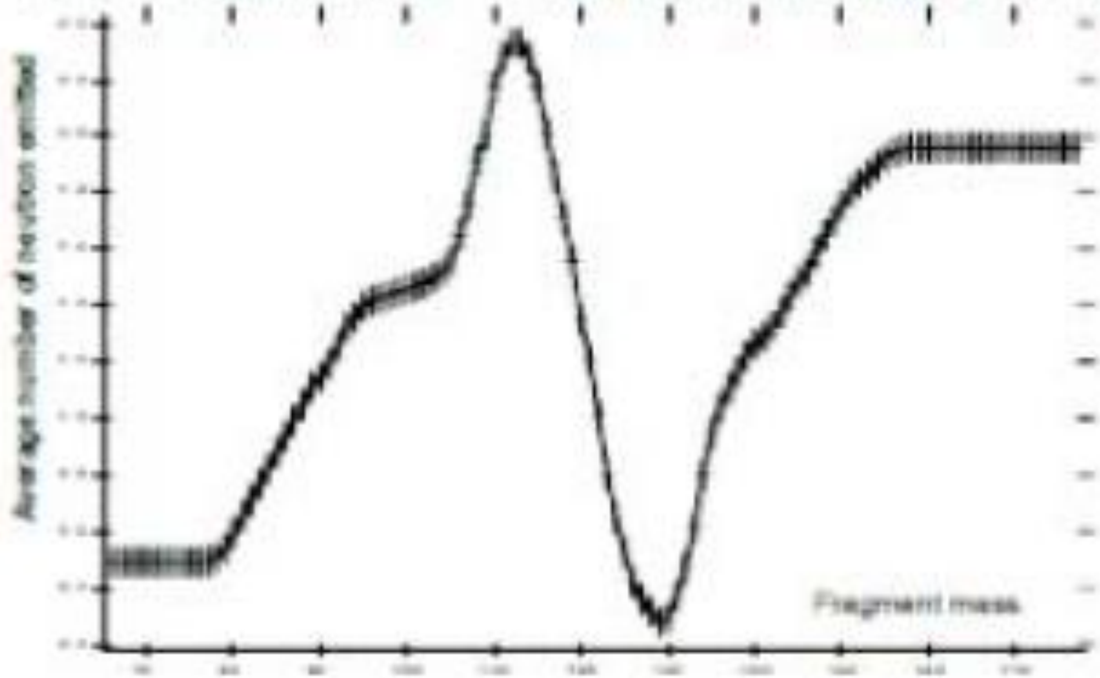
The mass after prompt neutron emission is A' and the mass before is A. Thus

$$A' = A - \nu(A)$$

Models – Charge distribution (Wahl Zp)

- $\nu(A)$ **can be estimated using chain yields by the method of Terrell.**

The $\nu(A)$ distribution for ^{235}U thermal neutron induced fission is:



Models – Charge distribution (Wahl Zp)

- **The odd-even effect, F(A,Z) is defined by two parameters** $\bar{F}_Z$ and $\bar{F}_n$.

  Where F(A,Z) is given by:

F(A,Z)	proton number Z	neutron number N
$\bar{F}_Z\bar{F}_n$	even	even
$\frac{\bar{F}_Z}{\bar{F}_n}$	even	odd
$\frac{\bar{F}_n}{\bar{F}_Z}$	odd	even
$\frac{1}{\bar{F}_Z\bar{F}_n}$	odd	odd

Isomeric splitting of yields

- There exists 388 nuclides with two long-lived isomeric states and 21 with three or more.
- Only small number of measurements.
- The main predictive model available is that of Madland and England that assumed the fragments with a spin near a long-lived isomer would feed that isomer. Model used in UKFY2.
- Rudstam proposed a modification that included energetic feasibility. Results used in UKFY3.

Ternary fission

- The emission of protons, deuterons, tritons, alpha particles and other light fragments up to 30 amu have been observed from fission.
- The most common emission is an alpha particle followed by tritons.
- The light charged particles are produced between the two heavy fragments very close in time to the scission of the nucleus.
- In UKFY2 empirical relationships were used to fill gaps, but in UKFY3 improved model results published by Serot et al at ND2004 were used.

Conservation laws

- $$\sum_A Y(A) = 2.0$$
- $$\sum_{A>\frac{A_f}{2}} Y(A) = 1$$
- From conservation of mass
$$\sum_A A\,Y(A) = A_f - \overline{\nu}_p - A_{LCP}$$
- From conservation of charge
$$\sum_{ZA} Z\ f(A,Z)\ Y(A) = Z_f - Z_{LCP}$$

and as $Z_1 + Z_2 = Z_f$
then

$$\sum_A f(A,Z)Y(A) = \sum_A f(A,Z_f - Z)Y(A)$$

for all $Z < \frac{Z_f}{2}$

Cumulative yields

- **The cumulative yield can be calculated from the independent yields and the decay data branching fractions**

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

or in matrix form

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

which can be rearranged to give

$c = Qy$ where $Q = (1 - \bar{b})^{-1}$

Fission Product Yields- Q matrix method

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- Given the individual decay branches for all nuclides in the decay paths from one nuclide to a distant daughter it is possible to calculate the fraction of j that decays to i

$$Q_{j,i} = \sum_{allpaths} \left(\prod_{eachj \to i} B_{j,j+1} B_{j+1,j+2} \ldots B_{i-1,i} \right)$$

- If $Q_{i,i}$ is defined as 1 and $Q_{k,i}$ =0 (where k does not decay to i), Thus any cumulative yield can be calculated from the independent yield.

$$Y_i^c = \sum_j Y_j^i Q_{j,i}$$

Uncertainty propagation

- As this is a weighted sum, the variance of the result is given by

$$var(Y_i^c) = var(\sum_j Y_j^i Q_{j,i})$$
$$= \sum_j var(Y_j^i) Q_{j,i}^2$$
$$+ 2 \sum_j \sum_k Q_{j,i} Q_{k,i} cov(Y_j^i, Y_k^i)$$

- As all terms expect the covariance are known, these can be calculated.

Mass 85 example

- What does the Q matrix look like

$Q_{i,j}$	^{85}Ge	^{85}As	^{86}Ga	^{86}Ge	^{86}As	^{85}Se	^{85}Br	^{85m}Kr	^{85}Kr	^{85}Rb
^{85}Ge	1.00	0.85				0.67	0.67	0.67	0.14	0.67
^{85}As		1.00				0.78	0.78	0.78	0.17	0.78
^{86}Ga			1.00	1.00	1.00	0.33	0.33	0.33	0.07	0.33
^{86}Ge				1.00	1.00	0.33	0.33	0.33	0.07	0.33
^{86}As					1.00	0.33	0.33	0.33	0.07	0.33
^{85}Se						1.00	1.00	1.00	0.22	1.00
^{85}Br							1.00	1.00	0.22	1.00
^{85m}Kr								1.00	0.21	1.00
^{85}Kr									1.00	1.00
^{85}Rb										1.00

Effect on cumulative yield uncertainties

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- The following shows the JEFF-3.1.1 file data and a calculation of Yc and its uncertainty **<u>without the covariance terms.</u>**

Quantities	^{85}Ge	^{85}As	^{86}Ga	^{86}Ge	^{86}As	^{85}Se	^{85}Br	^{85m}Kr	^{85}Kr	^{85}Rb
JEFF-3.1.1 Y^i	2.44e-5	1.41e-3	1.82e-6	2.85e-6	4.42e-4	9.58e-3	2.19e-3	1.12e-5	4.85e-5	3.30e-8
JEFF-3.1.1 Y^i 1sd	9.08e-6	4.69e-4	6.65e-11	1.04e-6	1.59e-4	9.47e-4	7.14e-4	4.18e-6	1.81e-5	1.23e-8
JEFF-3.1.1 Y^c	2.44e-5	1.43e-3	1.82e-10	2.85e-6	4.45e-4	1.08e-2	1.30e-2	1.30e-2	2.86e-3	1.31e-2
JEFF-3.1.1 Y^c 1sd	9.06e-6	4.19e-4	6.66e-11	1.04e-6	1.55e-4	2.10e-4	1.19e-4	1.19e-4	2.10e-4	1.19e-4
Calculated Y^c	2.44e-5	1.43e-3	1.82e-10	2.85e-6	4.45e-4	1.08e-2	1.30e-2	1.30e-2	2.86e-3	1.31e-2
Calculated Y^c 1sd	9.08e-6	4.69e-4	6.65e-11	1.04e-6	1.59e-4	1.02e-3	1.24e-3	1.24e-3	2.68e-4	1.24e-3
Y^c ratio file/calc	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Y^c 1sd file/calc	0.998	0.893	1.000	1.000	0.978	0.206	0.096	0.096	0.785	0.095

- The results show that without the covariance terms the yields are over-predicted.

Effect on cumulative yield uncertainties

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Quantities	^{85}Ge	^{85m}Kr	^{85}Kr	^{85}Rb
JEFF-3.1.1 Y^i	2.44e-5	1.12e-5	4.85e-5	3.30e-8
JEFF-3.1.1 Y^i 1sd	9.08e-6	4.18e-6	1.81e-5	1.23e-8
JEFF-3.1.1 Y^c	2.44e-5	1.30e-2	2.86e-3	1.31e-2
JEFF-3.1.1 Y^c 1sd	9.06e-6	1.19e-4	2.10e-4	1.19e-4
Calculated Y^c	2.44e-5	1.30e-2	2.86e-3	1.31e-2
Calculated Y^c 1sd	9.08e-6	1.24e-3	2.68e-4	1.24e-3
Y^c ratio file/calc	1.000	1.000	1.000	1.000
Y^c 1sd file/calc	0.998	0.096	0.785	0.095

- The results show that without the covariance terms the yields are over-predicted.

Thank you for your attention