# UKFY4.1: A set of prototype fission product yield library for neutron, proton, deuteron, alpha particle, photon and spontaneous fission, developed from UKFY4.0.

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## Introduction

This paper describes the production of the UKFY4.1 fission product yield library which has been developed from UKFY4.0 described in the report Nexia Solutions 7977 (Issue 2).

The UKFY4.0 library included energy dependent fission product yield data resulting from fission induced by neutron, proton, deuteron and alpha particle induced yields for 21 fissioning systems ($^{232}$Th, $^{233}$U, $^{234}$U, $^{235}$U, $^{236}$U, $^{238}$U, $^{237}$Np, $^{238}$Np, $^{238}$Pu, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, $^{242}$Pu, $^{241}$Am, $^{242m}$Am, $^{243}$Am, $^{242}$Cm,$^{243}$Cm, $^{244}$Cm, $^{245}$Cm and $^{252}$Cf). The range of particle energies considered was from $1 \times 10^{-5}$ eV to 150 MeV. The required data were produced using the CYFP code from the Los Alamos National Laboratory in the U.S.A.

The new UKFY4.1 library extends the existing library to include photon induced fission for the above nuclides and spontaneous fission yields for 39 nuclides identified in the JEFF-3.1.1 decay data library as undergoing spontaneous fission ($^{230}$Th, $^{232}$Th, $^{231}$Pa, $^{238}$Pa, $^{232}$U, $^{234}$U, $^{235}$U, $^{236}$U, $^{238}$U, $^{228}$Np, $^{236}$Pu, $^{238}$Pu, $^{239}$Pu, $^{240}$Pu, $^{242}$Pu, $^{244}$Pu, $^{232}$Am, $^{234}$Am, $^{241}$Am, $^{242m}$Am, $^{242n}$Am, $^{243}$Am, $^{234}$Cm, $^{242}$Cm, $^{244}$Cm, $^{246}$Cm, $^{248}$Cm, $^{250}$Cm, $^{238}$Bk, $^{240}$Bk, $^{242}$Bk, $^{249}$Bk, $^{237}$Cf, $^{238}$Cf, $^{240}$Cf, $^{242}$Cf, $^{249}$Cf, $^{250}$Cf and $^{252}$Cf). It should be noted that heavier nuclides exist that spontaneously fission, but due to their short half-lives and extremely low production in applied science it was decided to ignore them. As for UKFY4.0, the data has been produced using the CYFP code, but with some modifications to allow the photon induced and spontaneous fission to be handled easily.

In addition to the extra data, the UKFY4.1 cumulative yields have been made consistent with the JEFF-3.1.1 decay data. It should be noted that this calculation of cumulative yields ignored decays from nuclides with half-lives of greater than 1000 years, as in the JEFF-3.1 fission yield library. This is discussed in more detail below.

The revised library, identified by the name UKFY4.1, has been released to the NEA for distribution to interested parties.

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**Background**

Energy dependent fission yields were requested within the JEFF project for fusion reactor activation and possible accelerator driven systems for transmutation. In fusion reactors; neutrons, protons, deuterons and alpha particles are present with sufficient energy to cause fission and these particles can irradiate trace thorium and uranium impurities in the structure of the fusion device to produce fission products. In accelerator driven reactors usually high-energy protons bombard a target to generate neutrons, thus almost all fissions are from neutrons, although some are at higher energies than found in conventional thermal and fast reactors. Thus to perform these calculations, datasets of fission product yields (amongst other nuclear data especially cross-sections) are required. The scope of the initial work was for all 21 fissioning systems in JEF-2.2 [1] and JEFF-3.1 [2] ($^{232}$Th, $^{233}$U, $^{234}$U, $^{235}$U, $^{236}$U, $^{238}$U, $^{237}$Np, $^{238}$Np, $^{238}$Pu, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, $^{242}$Pu, $^{241}$Am, $^{242m}$Am, $^{243}$Am, $^{242}$Cm,$^{243}$Cm, $^{244}$Cm, $^{245}$Cm and $^{252}$Cf). The range of particle energies is between $1 \times 10^{-5}$ eV to 150 MeV, although it should be noted that some neutron-induced and all charged particle induced fissions will have an energy threshold. To ensure ease of use the UKFY4.0 library was prepared using the international standard ENDF/B format [3].

Following the release of the UKFY4.0 library, requests were received for photon induced fission and spontaneous fission product yields. It should be noted that the new spontaneous fission library supplements the existing $^{242}$Cm, $^{244}$Cm and $^{252}$Cf data released as part of JEFF-3.1 and will enable improved estimates of the small spontaneous fission generated short-lived fission products released from stored spent fuel or reprocessing activities.

<u>Traditional inventory calculation in reactor fuel.</u>

All calculations of the nuclides present in irradiated material whether from a fission reactor, fusion reactor or accelerator driven system are governed by a set of coupled linear differential equations describing the production and destruction of nuclides. These equations are often referred to as the “Bateman equations” [4], although Bateman only considered radioactive decay processes. The nuclide concentration for an individual nuclide can be calculated by integrating all of its production and destruction terms. The destruction terms are only related to the nuclide's concentration and include both radioactive decay and reactions that transform the nuclide. The production terms are related to the concentrations of the other nuclides present that by radioactive decay processes or induced reactions lead directly to the nuclide of interest.

In traditional inventory calculations of nuclear reactors the destruction terms considered are radioactive decay of the nuclide and the neutron induced reactions of the nuclide (n,γ), (n,f), (n,2n) etc. The production terms include radioactive decay of the parent, fission products from the fission of actinides and the neutron reactions of all nuclides that generate the nuclide of interest. The fission product yields are given for a specific neutron spectrum e.g. thermal or fast.

The nuclide inventory can be determined in several ways. The first and most commonly used is a numerical solution to the complete set of differential equations (e.g. FISPIN [5], ORIGEN [6], etc.). An alternative is an analytical solution of simplified nuclide chains (e.g. FISP [7]).

In all of these calculations, the neutron induced fission product yields are from a limited set of actinides that significantly contribute to the fission rate during the irradiation. The fission rates are calculated from the neutron flux, spectra and fission cross-sections. The production rate for each fission product is calculated by summing over the product of the independent yield and the fission rate for each significant fissioning nuclide.

Requirements for fission product yield data for novel applications

The requirement for fission product nuclear data was considered, by this author, in his contribution to an IAEA collaborative research programme on minor actinide transmutation [8]. Different particles with differing kinetic energies will give rise to different fission product yield distributions; hence it is necessary to determine number densities of fissionable species in the system and the energy spectra of incident particles. Using these parameters with the particle fission cross-sections it is possible to calculate the fission rates from each fissionable nucleus and thus determine the fission rate weighted average yield distribution. This requires energy dependent yields for each important fissionable nuclide. For charged particles, a code that can model charged particle transport and secondary particle production is required to do this (such as MCNPX [9]).

**Possible formats to store energy dependent fission product yields**

In previous work contributing to an IAEA Collaborative Research Project (CRP) on minor actinide transmutation [8], the author proposed three ways of storing energy dependent fission yields. However, the existing ENDF/B-6 format allows for the storage of fission product yields for neutrons, photons and charged particles at multiple energies with interpolation laws between energies being defined within the format and thus it was decided to use this format rather than develop another non-standard format.

It should be noted that existing codes cannot use this new extended data and there are no codes to process this data into a suitable form for future application codes. However, now a preliminary library exists in this format, application developers can begin consideration of possible uses and implementation of the data.

**Production of the UKFY4.1 library.**

In this work, the production of the required library has been automated using Wahl's CYFP code [10] and a set of internal Nexia Solutions Ltd codes. The process is in two steps.

1. The CYFP code is used to generate yields at a range of energies (1.e-11, 2.5e-8, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.5, 2, 3, 4, 5, 6, 7, 8, 9, 10, 14, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120, 130, 140, 150 MeV) for the list of fissionable nuclides and fission inducing particles specified by the JEFF project and listed above. Two approximations were made. Firstly, in the case of spontaneous fission it is assumed that this is equivalent to zero energy photon induced fission. Secondly, the CYFP code only considers ground state fissioning nuclides. However, as the yield distributions in this model vary very little below excitations of several MeV it was decided to approximate the yields of fissioning meta-stable states nuclides as being the same as the ground state yield distributions.
2. The data from the CYFP code was formatted in ENDF/B-6 format using the material numbers (MAT) from the JEFF-3.1.1 decay data library. Also the cumulative yields were regenerated from the independent yields using the JEFF-3.1.1 decay data. The CYFP code uses a simplification to generate cumulative yields; it assumes each mass is a separate decay chain leading to a stable nuclide and uses a hard-wired set of decay data to generate the cumulative yields. Thus, some cumulative yields will be dominated by alpha decay from long-live parents that have millions of year half-lives and will not have any effect over practical human timescales. Thus in this work, like the JEFF-3.1 library, nuclides with half-lives over 1000 years are considered not to decay. As these cumulative yield distributions are usually used for the analysis of experiments rather than for inventory calculations this should not give rise to any significant problems. Care needs to be exercised in the use of cumulative yields for practical applications involving long cooling times (e.g. repository modelling).

The CYFP code was chosen for this work, as it is publicly available and can generate fission product independent and cumulative yield distributions from zero to ~200 MeV for mass, charge and isomeric state. It should be noted that the Wahl parameterisation is an empirical fit to a very sparse set of experimental data and thus large uncertainties are expected from the method. The empirically determined systematic relationships in the CYFP code vary only slowly with energy and thus the list of energies given above allows the accurate interpolation of the data within this model. If an improved model is used a more extensive list of energies may be required.

### Testing of UKFY4.1

The Brookhaven ENDF format checking code CHECKR v7.02 [11] was downloaded from the Brookhaven website and used to check the generated library. Apart for the MAT numbers being different from that of the general-purpose library, no errors were found.

### Limitations of the UKFY4.1 library

The UKFY4.1 library, like the UKFY4.0 library, is intended as a proof of principle as the empirical methods used to estimate the yield distributions are based upon the currently available limited experimental data and requires testing of the results against integral experiment to validate its accuracy. The large uncertainites on this data means that these data cannot be recommended for use in accurate applied nuclear physics calculations. However, it may be suitable for applications where crude estimates are acceptable, e.g. initial scoping calculations to design future experiments in areas where no experience currently exists.

### Conclusion

A set of spontaneous fission and alpha, neutron, proton, deuteron and gamma-ray induced fission yield data in an ENDF library have been produced that are consistent with the JEFF-3.1.1 decay data. These have been released to the NEA Data Bank for distribution.

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