Technical note on producing energy dependent fission product yield files.

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EXECUTIVE SUMMARY

This paper has been prepared to describe a study into implementing energy-dependent fission-product yield files in ENDF/B formatted files. The study consists of three parts; a review of possible ways to store energy dependent fission product yields, the production of neutron, proton, deuteron and alpha particle induced yields for 21 fissioning systems requested by the JEFF project and testing of the files using the standard ENDF checking code CHECKR.

The energy dependent fission yields have been requested within the JEFF project for fusion reactor activation and possible accelerator driven systems for transmutation. The scope of this work is for all 21 fissioning systems in JEF-2.2 and JEFF-3.1 (^{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 $1x10^{-5}$ eV to 150 MeV. The required sets of files were produced using the CYFP code. These have been identified by the name UKFY4.0 (Issue 1). These files have been released to the JEFF project for testing. The limitations of these files are discussed.

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1 Introduction

The energy dependent fission yields have been 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 are bombarded on a target to generate neutrons, thus almost all fissions are from neutrons, although some are at higher energies than found the conventional thermal and fast reactors. Thus to enable these calculations datasets of fission product yields (amongst other nuclear data especially cross-sections) are required. The scope of this work is 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 1×10^{-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.

This paper has been prepared to describe a study into implementing energy-dependent fission-product yield files in ENDF/B formatted files [3]. The study consists of three parts; a review of possible ways to store energy dependent fission product yields, the production of neutron, proton, deuteron and alpha particle induced yields for 21 fissioning systems requested by the JEFF project and testing of the files using the standard ENDF checking code CHECKR.

Associated with this work, a set of files has been produced using the CYFP code [12]. These have been identified by the name UKFY4.0 (Issue 1). These files have been released to the JEFF project for testing. The limitations of these files are discussed.

2 Background

2.1 Traditional inventory calculation in reactor fuel.

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 reactor 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 defined at a single energy either 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.

2.2 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]. As different particles with differing kinetic energies will give rise to different fission product yield distributions, 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]).

The fission rate averaging of the yield distributions are similar to the condensation of cross-sections by the NJOY [10] code used to generate cross-sections for radiation transport and reactor physics codes, although time dependent effects have to be considered. It should be noted that fission product yields could be represented as products of the fission reaction using either MF=6 or MF=10 in the ENDF/B-6 format, and thus could be processed by NJOY. However, these formats both require cross-section data that is not available at this time. Thus this work will only consider the current ENDF/B-6 fission product yield formats within MF=8.

3 Possible formats to store energy dependent fission product yields

In a contribution to an IAEA Collaborative Research Project (CRP) on minor actinide transmutation [8], the author proposed three ways of storing energy dependent fission yields. The existing ENDF/B-6 format allows for the storage of fission product yields for neutrons and charged particles at multiple energies with interpolation laws between energies being defined within the format. It should be noted that such files are large and the format requires cumulative yields that are unnecessary for most purposes, as only independent yields are required for most calculations.

A second method would be to store a well known single energy fission product yield distribution and give parameters for variation of energy. However, the parameterisation of the odd-even effect and isomeric splitting [11] introduces complications that would require a non-trivial set of equations.

A third method would be to store a set of parameters required to reconstruct the yield distributions with energy, for example Wahl's systematics of the yield distributions [12]. However, although this would be a much smaller set of parameters to store it would introduce a considerable amount of processing to produce the required yields and would risk different codes producing different yields unless a comprehensive set of test results were supplied for comparison.

It is thus decided that the first option, the existing ENDF/B-6 format is currently the best solution.

4 Production of a demonstration file, UKFY4.0.

In this work, the production of the required libraries has been automated using Wahl's CYFP code [12] and a set of internal Nexia Solutions Ltd codes. The process is in three steps. Firstly, 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 in the introduction above. Second a list of nuclides produced for fissionable nuclide and incident particle is produced so that the yields can be specified for the same nuclides at each energy. Thirdly, the data is formatted in ENDF/B-6 format using the material numbers (MAT) from the JEFF-3.1 decay data.

The CYFP code was chosen for this study, 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. In addition, 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 does not use a set of decay data to generate the cumulative yields. Thus, cumulative yields dominated by delayed neutron emission or alpha decay will be incorrectly calculated. In addition, nuclides shielded by very long-lived parents will have cumulative yields that may not be observed in practice for thousands of years. However, as cumulative yields will not be used directly for inventory calculations this will not be a significant problem.

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 extrapolation of the data. If an improved model is used a more extensive list of energies may be required.

5 Testing of UKFY4.0

The Brookhaven ENDF format checking code CHECKR v7.02 [13] was downloaded from the Brookhaven website and used to check the generated files. Apart for the MAT numbers being different from that of the general-purpose file no errors were found.

6 Further work

As mentioned above the cumulative yields are not calculated by a set of decay data thus it would be possible to improve this calculation using the JEFF-3.1 decay data.

The JEFF-3.1 thermal, fast yields and 14 MeV fission product yield data could be used to normalise the yield predictions to give a set of yields that is suitable for reactor physics calculations as well as a crude estimate of high-energy particle induced fission.

7 Conclusions

The ENDF/B-6 format has been shown to be suitable for producing energy dependent neutron and charged particle fission yield distributions, and a demonstraion file, UKFY4.0 (issue 1), has been produced.

The UKFY4.0 file 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 files cannot be recommended for use in accurate applied nuclear physics calculations. However, it may be suitable for applications where order of magnitude estimates are acceptable.

8 Acknowledgements

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