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ARTICLE

EASY-II(12): a system for modelling of n, d, p, γ, α activation and transmutation processes

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EASY-II(12) is designed as a functional replacement for the previous European Activation System, EASY-2010. It has extended nuclear data and new software, FISPACT-II, written in object-style Fortran to provide new capabilities for predictions of activation, transmutation, depletion and burnup. The new FISPACT-II code has allowed us to embed many more features in terms of energy range, up to GeV; incident particles: alpha, gamma, proton, deuteron and neutron; and neutron physics: self-shielding effects, temperature dependence, pathways analysis, sensitivity and error estimation using covariance data. These capabilities cover most application needs: nuclear fission and fusion, accelerator physics, isotope production, waste management and many more. In parallel, the maturity of modern general-purpose libraries such as TENDL-2011 encompassing thousands of target isotopes, the evolution of the ENDF format and the capabilities of the latest generation of processing codes PREPRO, NJOY and CALENDF have allowed the FISPACT-II code to be fed with more robust, complete and appropriate data: cross-sections with covariance, probability tables in the resonance ranges, kerma, dpa, gas and radionuclide production and 24 decay types. All such data for the five most important incident particles are placed in evaluated data files up to an incident energy of 200 MeV. The resulting code and data system, EASY-II(12), includes many new features and enhancements. It has been extensively tested, and also benefits from the feedback from extensive validation and verification activities performed with its predecessor.

Keywords: ***high-energy nuclear data; numerical modelling; software; activation; transmutation; depletion; processing; evaluated nuclear data format***

1. Introduction

FISPACT-II [1] is a completely new inventory code designed initially to be a functional replacement for Fispact-2007. This new code is written in object-style Fortran 95 and has extended physical models, a wider range of irradiation options and improved numerical algorithms compared to the old code. Users familiar with the old code will be able for most cases to use the new code with their existing control input files. Some new keywords have been added to deal with the new capabilities, and some of the old keywords have become obsolete.

The major change introduced in this first release of FISPACT-II was the addition of the reading and processing of alternative ENDF-format library data sets. This has caused a major overhaul of the data input parts of the software and a huge expansion of the number of nuclides and reactions that can be treated. Sensitivity and error prediction capabilities have been extended, and better fission yield data and cross-section data in more energy groups up to higher energies can now be used. The present version can also handle more irradiating projectiles (α, γ, n, p, d) and provides additional diagnostic outputs (kerma, dpa and gas appm rates) if the ENDF-format library contains the required input data. The new code can also connect to any version of EAF-formatted libraries [2].

The new inventory code when associated with a set of nuclear data libraries (EAF-2007, EAF-2010 or TENDL-2011 [3]), plus decay, biological, clearance and transport indices libraries, forms the European Activation System EASY-II(12).

2. The models

The FISPACT-II code follows the evolution of the inventory of nuclides in a target material that is irradiated by a time-dependent projectile flux φ, where the projectiles may be neutrons, protons, deuterons, α-particles or γ-rays. The material is homogeneous, infinite and infinitely dilute and the description of the evolution of the nuclide numbers is reduced to the stiff-ode Eq. (1) for N_i the number of atoms of nuclide i

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[4]. The key characteristics of the system of inventory equations are that they are linear, stiff and sparse.

$$\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_i\varphi) + \sum_{j \neq i} N_j(\lambda_{ij} + \sigma_{ij}\varphi) \qquad (1)$$

Here λ_i and σ_i are respectively the total decay constant and cross-section for reactions on nuclide *i*. σ_{ij} is the cross-section for reactions on nuclide *j* producing nuclide *i*, and for fission it is given by the product of the fission cross-section and the fission yield fractions. λ_{ij} is the constant for the decay of nuclide *j* to nuclide *i*.

The stiffness of the system of equations limits the choice of numerical methods. The code uses the Livermore solver for ordinary differential equations LSODES [5] to solve the stiff ode set. LSODES implements Gear's method and uses the Yale sparse matrix package to handle the Jacobian matrices. This numerical solver compares advantageously with the previous EXTRA ode solver, written in 1976, and used in Fispact-2007. FISPACT-II has a wrapper ode module around LSODES that automatically sets storage and parameters for that solver, improving portability and reducing the need for user input.

Note that FISPACT-II differs from Fispact-2007 in that it does not employ the equilibrium approximation for short-lived nuclides, and includes actinides self-consistently in the rate equations (Eq.(1)) rather than as a source term. The new code has been shown to be able to handle short (1ns) time interval and high flux cases that caused problems for older codes.

2.1. Pathways

The reaction network may be described either by the rate equations or as the sum of paths and loops, which we refer to as pathways. The inventory of a given nuclide computed using the rate equations can equivalently be found by a linear superposition of contributions of flows along the pathways to that nuclide. Pathways analysis is used in identifying significant nuclides and reactions, and in performing sensitivity and uncertainty analyses.

Pathways analysis uses directed graph algorithms implemented using breadth-first tree searches with pruning for finding routes from a parent to chosen descendants, and for the assembly and solution of a subset of the rate equations for nuclides on a pathway to get the flow along that pathway. Pathways analyses may be performed for single and multiple step irradiation scenarios, and where the cross-sections are time dependent.

2.2. Uncertainty estimates

Pathways analysis identifies the pathways from the initial inventory nuclides to the (target) dominant nuclides at the end of the irradiation phase, and provides the number of atoms of each nuclide produced by reactions and decays along each pathway. These, together with uncertainties derived from the covariances in the reaction cross-sections and decay half-lives associated with the edges of the pathways are used in FISPACT-II to provide estimates of the uncertainties. The uncertainties are then computed for significant radiological quantities, e.g., number density, decay heat, dose rate, inhalation or ingestion hazards.

More accurate uncertainty estimates that may also include covariance between different reaction cross-sections can be undertaken by combining pathways analysis with monte-carlo sensitivity calculations.

3. Nuclear data libraries

FISPACT-II requires connection to several data libraries before it can be used to calculate inventories. While any libraries in the correct format could be used, the code has been designed to use the European Activation Files, a recommended source of cross-section data in the EAF format. The following libraries are required: cross-section data for projectile-induced reactions, uncertainty data for neutron-induced reactions, decay data, fission yields, biological hazard, legal transport, clearance and gamma absorption data. It is a user choice to select from the 2007 or 2010 library versions. There are nine standard energy group structures that may be used with the EAF libraries.

Alternatively, any libraries in the correct ENDF-6 format could be used. The development of FISPACT-II over the last few years has run in parallel with the development of the TALYS-based Evaluated Nuclear Data Library (TENDL) project and those European libraries are also a recommended source of cross-section data [3]. The TENDL libraries have made possible new predictive capabilities.

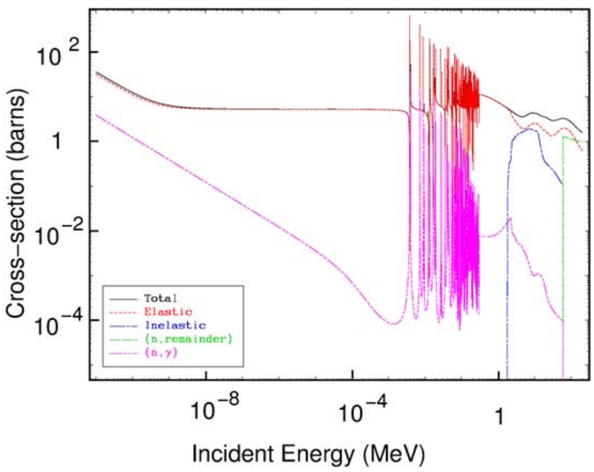

Figure 1. Neutron library cross-sections of ^{90}Zr in the TENDL-2011 pendf, which have all the channels needed for self-shielding to be included.

3.1. Cross-sections

The TENDL-2011 library [3] is the current recommended evaluated data source for use in any type of nuclear technology applications. The principal advances of this new library are in the unique target coverage, 2424 nuclides; the upper energy range, 200 MeV; variance and covariance information for all nuclides; and the extension to cover all important projectiles: neutron, proton, deuteron, alpha and gamma, and last but not least the proven capacity of this type of library to transfer regularly to technology the feedbacks of extensive validation, verification and benchmark activities from one release to the next.

Figures 1-3 show for ^{90}Zr some of the data that brings the new activation prediction capabilities. Similar data are available for all nuclides in the library. Figure 1 shows the pointwise data available from 10^{-5}eV to 200 MeV, including resonance ranges. Elastic cross-section data are available for the self-shielding corrections (see Sec 3.4). Gas production (Figure 2) and kerma cross-sections are used to give gas appm and kerma diagnostics in activation calculations. Gamma reaction cross-sections (Figure 3) introduce a new class of calculations.

TENDL-2011 is the fourth generation of such a library and as such has benefited from the previous releases and from the EAF-2010 V&V processes.

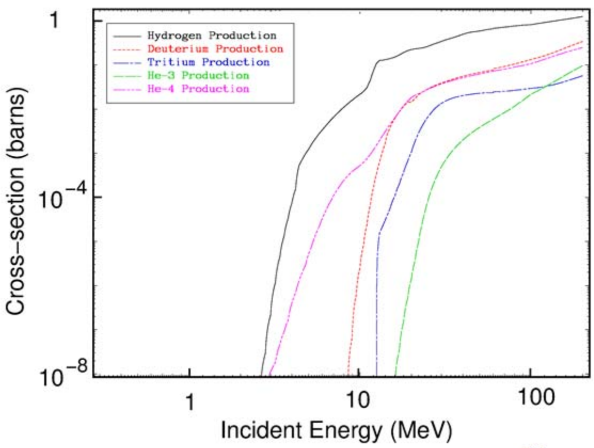

Figure 2. Gas production cross sections of ^{90}Zr in TENDL-2011 pendf, which make possible new gas appm predictions.

The cross-section data are provided in two universal group structures: a CCFE (709) scheme for the neutron-induced cross-sections and a CCFE (162) scheme for the non-resonant p, d, α and γ-induced cross-sections. The data format used is fully compliant with the ENDF-6 manual specification handled on an isotopic basis and so allows many existing utility codes further to manipulate, visualise or check any aspects of the pre-processed files. The data files are produced using a complex but robust, complementary sequence of modules of the processing codes NJOY-99, PREPRO-2010 and CALENDF-2010.

3.2. Fission yields

The fission yield data need to be provided for each actinide and incident particle. Only 19 of the many nuclides that undergo fission have any fission yield data in JEFF-3.1.1 and these cover only a reduced energy range. For the remainder the UKFY4.1 library [6] then further extends the range before a neighbouring fission yield is used. This UKFY4.1 library using Wahl's systematics is also used for all other particle-induced fission yields.

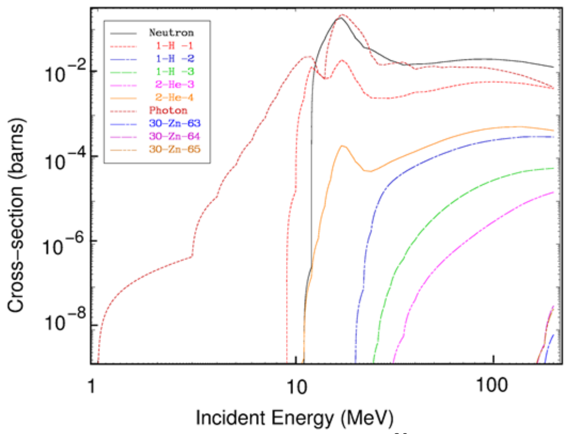

Figure 3. γ-induced cross-sections of ^{90}Zr in TENDL-2011 pendf, which allow a new class of activation calculations.

3.3. Variance-covariance

Above the upper energy of the resolved resonance range, for each of the 2424 isotopes a Monte Carlo method in which the covariance data come from uncertainties of the nuclear model calculations is used. In the TENDL-2011 library, all information on cross-section covariance is stored in the MF=33 or 40 formats, starting at the end of the resonance range up to 200 MeV. Short-range, self-scaling variance components are also specified for each MT type. The data format used to store the variance-covariance information has been made fully compliant with the ENDF-6 format description and the files are read directly by FISPACT-II(12) without any further intermediate processing. Variance and covariance data are used by FISPACT-II to create uncertainty predictions and sensitivity analyses.

3.4. Self shielding of resonant channels

The CALENDF-2010 [7] nuclear data processing system is used to convert the evaluation defining the cross-sections in ENDF-6 format (i.e., the resonance parameters, both resolved and unresolved) into forms useful for applications. Those forms used to describe neutron cross-section fluctuations correspond to “cross-section probability tables”, based on Gauss quadrature and effective cross-sections. FISPACT-II iteratively solves for the dilution cross-section (which depends on mixture fractions and total shielded cross-section) and the shielded cross-section for nuclides in the mixture (which depends on dilution cross-section and probability table data) [1,7].

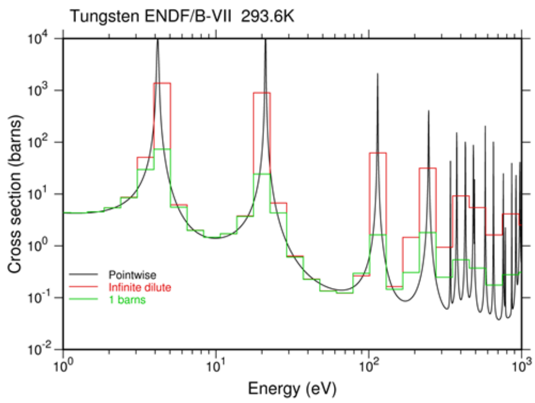

Figure 4. Self-shielding effects for different dilutions, which show that changes to effective groupwise cross-section may be large.

CALENDF-2010 provides probability tables in the energy range from 0.1 eV up to the end of the resolved or the unresolved resonance range. Probability table data in 709 energy group format are provided for 2143 isotopes of the TENDL-2011 library. These data are used to model dilution self-shielding effects from channel, isotopic or elemental interferences (c.f. **Figure 4**). Doppler broadening effects are included and the tables are given at three temperatures: 293.6, 600 and 900 degree Kelvin.

The dilution cross-sections computed using the CALENDF data are applied either as scaling factors to the library cross section data or as replacements over the energy ranges for which the probability table data are available [1]. This ability to self-shield, in much the same manner as is done in deterministic transport codes and in Monte Carlo codes for the unresolved resonance range (URR) depicted is believed to be unique amongst inventory codes.

3.5. Decay data

In addition to cross-sections the other basic quantities required by an inventory code are information on the decay properties (such as half-life) of all the nuclides considered. FISPACT-II is able to read the data directly in ENDF-6 format; it requires no pre-processing to be done. The now well-verified and validated EAF_dec_2010 library based primarily on the JEFF-3.1.1 and JEF-2.2 radioactive decay data libraries, with additional data from the latest UK evaluations, UKPADD-6.10, contain 2233 nuclides. However, to handle the extension in incident particle type, energy range and number of targets many more decay data are needed. A new 3873-nuclide decay library dec_2012 has been assembled from EAF_dec_2010 complemented with all of JEFF-3.1.1 and a handful of ENDF/B-VII.1 decay files.

3.6. Radiological data

The radiological data for the increased number of nuclides present in the TENDL-2011 data are computed in the same manner as described for the EAF data. The new hazards, clearance and transport data are respectively for 3647, 3873 and 3872 nuclides, compared to 2006, 2233 and 2233 for the EAF data.

4. Verification and Validation

Verification and Validation (V&V) is a critical, yet often overlooked, part of scientific computer code development. Careful software lifecycle management under configuration control has been used for the code, unit and integration tests and validation tests. FISPACT-II is distributed with over 400 input/output regression tests that preserve and extend the validation heritage of Fispact-2007. Further V&V processes are being actively deployed in support of EASY-II.

5. Conclusion

EASY-II (12) is a new versatile multi-particle inventory code and nuclear data package aimed at satisfying all activation-transmutation requirements for facilities in support of any nuclear technology: stockpile and fuel cycle stewardship, materials characterization, and life cycle management. It has been developed and tested for: magnetic and inertial confinement fusion, fission Gen II, III, IV plant generations; high energy and accelerator physics; medical applications, isotope production; earth exploration and astrophysics.

Acknowledgements

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