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EASY-II Renaissance: n, p, d, α, γ-induced Inventory Code System

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The European Activation SYstem has been re-engineered and re-written in modern programming languages so as to answer today's and tomorrow's needs in terms of activation, transmutation, depletion, decay and processing of radioactive materials. The new FISPACT-II inventory code development project 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 and covariance, so as to cover all anticipated application needs: nuclear fission and fusion, accelerator physics, isotope production, stockpile and fuel cycle stewardship, materials characterization and life, and storage cycle management. In parallel, the maturity of modern, truly general purpose libraries encompassing thousands of target isotopes such as TENDL-2012, the evolution of the ENDF-6 format and the capabilities of the latest generation of processing codes PREPRO, NJOY and CALENDF have allowed the activation 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 (n, p, d, α, γ), are placed in evaluated data files up to an incident energy of 200 MeV. The resulting code system, EASY-II is designed as a functional replacement for the previous European Activation System, EASY-2010. It includes many new features and enhancements, but also benefits already from the feedback from extensive validation and verification activities performed with its predecessor.

I. 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. The new inventory code when associated with a set of nuclear data libraries EAF-2010& 2007 [2] or TENDL-2012& 2011 [3], plus decay, biological, clearance and transport indices libraries, forms the European Activation System EASY-II.

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

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

Here λ_i and σ_i are respectively the total decay constant and cross-section for reactions on nuclide i. σ_{ij} is the

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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 (1 ns) time interval and high flux cases that caused problems for older codes.

III. NUCLEAR DATA LIBRARIES

FISPACT-II requires connection to several data libraries before it can be used to calculate inventories. 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 2003, 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 latest European libraries are also a recommended source of activation cross-section data [3].

A. Cross Sections

The TENDL-2012 library [3] libraries processed in line with the ENDF format framework brings new activation prediction capabilities. The principal advances are in the unique target coverage, 2434 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. Gas production, dpa and kerma cross-sections are used to give gas appm, displacement per atom and kerma diagnostics in activation calculations. Gamma and alpha reaction cross-sections introduce new classes of calculations. TENDL-2012 is the fifth generation of such a library and as such has benefited from the previous releases and from the EAF-2010 V&V processes [2].

B. 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 [2] 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-6.12, 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.

C. Self Shielding of Resonant Channels

The CALENDF-2010 [6] 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).

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 2314 isotopes of the TENDL-2012 library. These data are used to model dilution self-shielding effects from channel, isotopic or elemental interferences. 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.

D. Verification and Validation

Verification and Validation (V&V) is a critical, yet often overlooked, part of scientific 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 [2].

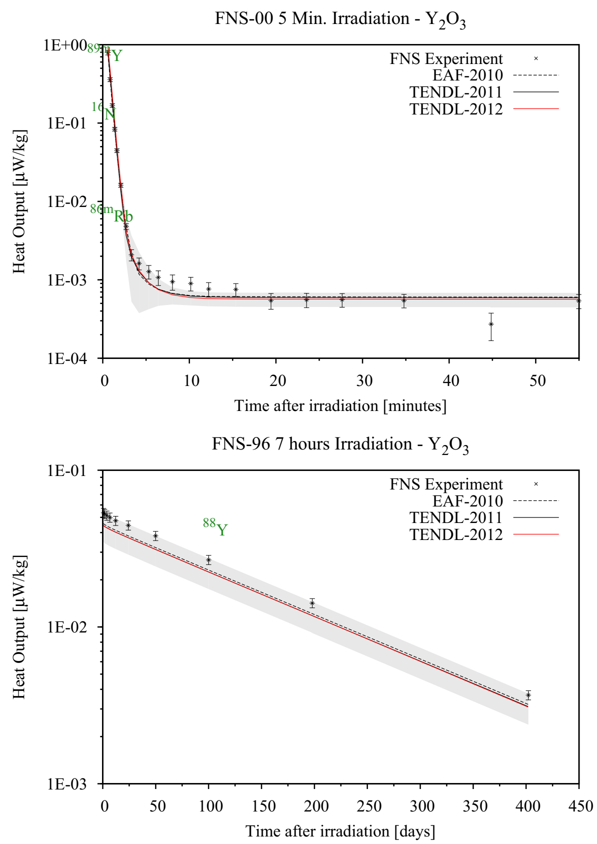

FIG. 1. Yttrium oxide decay heat comparison, TENDL derived uncertainty as gray area.

Reaction rates, effective cross-section validation, integral validation are very useful, when simulated integral values are compared against experimental measurements. For that the JAEA FNS assembly where 14 MeV neutrons are generated by a 2 mA deuteron beam impinging on a stationary tritium bearing titanium target has proven most beneficial [7].

More than seventy different material samples have been irradiated in sequence to have their decay heat measured in a whole energy absorption spectrometer. The value of those integral results reside mainly in the well characterized and stable neutron spectra at the target position, but also to the time scale of the measurements from a few seconds after irradiation up to 400 days. All experimental results have been compared with values derived from the EASY-II simulation. For both calculated and experimental values uncertainty estimates are also provided. Figure 1 demonstrates the validation results for two samples of Yttrium oxide irradiated for 5 minutes and 7 hours at JAEA FNS. Decay heat was measured for both samples at many cooling time ranging from 36 s to 400 days. The short term decay heat, including an isomer, is well predicted, but the code prediction seems to underestimate the long term one by around 20%. Further V&V processes are being actively deployed and demonstrated in support of EASY-II and the associated TENDL libraries.

IV. EASY-II CAPABILITIES

- Large number of targets: 2434 from H^1 to Ds^{281}
- Broad energy range: 1.0×10^{-5} eV to 1 GeV
- Five incident particles: α, γ, d, p, n
- Covariance, uncertainty
- Pathways analysis, dominant nuclide
- Self-shielding effects: channel, isotopic, elemental
- Sensitivity analysis (Monte Carlo)
- DPA, Kerma, gas and radionuclide production
- Thin, thick target yields

V. CONCLUSIONS

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, homeland security.

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