TENDL-2012 Processing, Verification and Validation Steps

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The goal of a unified, converged format for a truly general-purpose nuclear data library is becoming attainable thanks to a) recent advances and improvements in the proper interpretation and extension of the ENDF-6 format, b) the willingness of the processing communities to interact with applications communities, and c) better physics input. Earlier attempts to move toward a universal format frame for nuclear data files, JEFF-3.0/A, ENDF/B-VI HE, EAF-2010 and TENDL-2011, have paved the way finally to manage to bridge the gap that currently separates general and special purpose file format frames. The unified format exemplified in TENDL-2012, entirely based on the original ENDF-6 format frame, now makes the spine of a new set of nuclear data libraries and forms that are required to feed modern transport and inventory simulation codes. The data structure, also including covariance, is such that it allows the secular processing codes to be used simultaneously and in parallel to process, but also independently verify, all intermediate and final forms useful to the many applications that need them: transport, shielding, inventory and astrophysics. The comprehensive, complete and diverse resulting processed data forms have already been successfully connected, verified and validated when used in conjunction with the inventory code FISPACT-II and the Monte Carlo transport code TRIPOLI-4.9. Criticality, decay heat and inventory integral measurement benchmarking activities are being assessed in order to verify and validate the concatenation of often complex procedures and processes. The results of these assessments will lead to further enhancements for the next generation of the TENDL library.

I. INTRODUCTION

The potential benefits of a unified transport activation-transmutation ENDF-6 file format framework are three-fold: robustness, uniqueness and effectiveness. The main overall result of the conversion or production of evaluated files in this ENDF-6 [1] compliant format framework is that it combines into one single file per target nucleus all that will ever be needed by anybody wanting to access the content of an evaluated file. Extending the nuclear data needed for fusion, high energy applications is also improving the abilities for fission modeling. General information (MF-1), resonance parameters (MF-2), reaction cross sections (MF-3), angular and energy distributions (MF-4, 5), radionuclide multiplicities, production and yields (MF-6, 9, 10), products energy-angle distributions (MF-6), photon data (MF-11, 12, 13, 14, 15) and quite importantly covariance-variances information (MF31-35, 40) can be uniquely stored for incident particles with energy from 10^{-5}eV up to 200 MeV. Furthermore, all the stored information can be understood, manipulated and processed by the three most used processing codes available today:

PREPRO-2012 [2], NJOY-99 [3] and CALENDF-2010 [4]. In fact the most comprehensive processing steps may be achieved by using a combination of data forms extracted from not only one or even two of these codes, but all three of them; each of these codes having unique and pertinent capabilities. The verification and validation processes also immensely benefit from the fact that the outputted forms of the most important and used modules of PREPRO, NJOY or CALENDF can be seamlessly and effortlessly matched up to the highest possible accuracy, adding to the robustness of the interpretation. It also reveals to a knowledgeable and erudite user the different formalisms and interpretations that may be outputted during the processing steps.

II. PROCESSING STEPS

An important aspect of the quality and usefulness of any evaluated files resides in its ability to be properly parsed through a processing code prior to be used generally in a solver of the transport (Boltzmann) or radioactive transformation (Bateman) [5] equations or simply to be displayed to a human eye, perhaps in comparison with experimental information. It is necessary to demonstrate the ability to successfully convert the evaluation into forms useful for the many applications that need them. Depending on the applications, the data-form's

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quantitative and qualitative requirements are not alike or always compatible. The cross section reconstruction accuracy criteria are not as strict when used for simple display to feed pointwise cross section to Monte Carlo Codes.
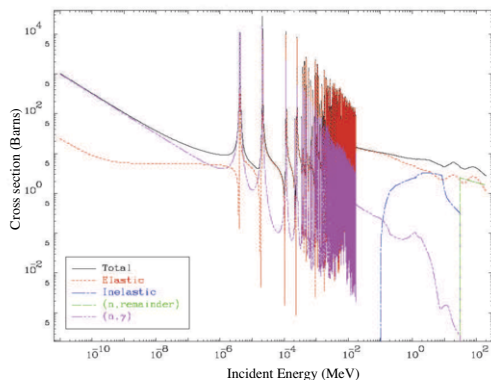
A. PREPRO

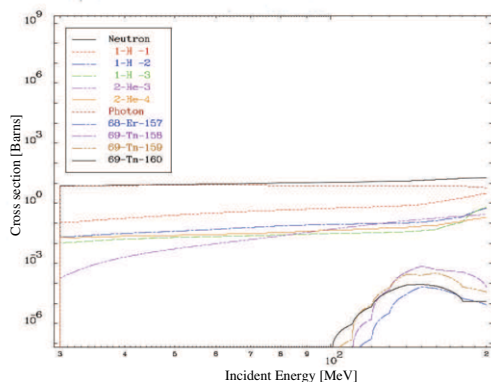FIG. 1. ^{182}W cross sections for dominant neutron induced reactions from TENDL-2012.

FIG. 2. ^{182}W neutron induced particles and radionuclides production cross sections from TENDL-2012.

The modular set of computer codes are named preprocessing because they are designed to pre-process ENDF-6 formatted data into forms useful for applications. Each code performs one or more independent operations on the data while, and this is particularly important, reading and writing evaluated nuclear data files respecting the ENDF-6 format framework at any stage. The high-energy part of the file as MF-3*MF-6 is handled by the *sixpack* module before being embedded as an MF-10:MT5 into the original evaluation. Furthermore, gas production, kerma and dpa information produced by NJOY from the same data file are also carefully stacked into the ENDF-6 formatted file before the relevant data forms, while the cross sections and other derived quantities, are group averaged by the groupie module. The ENDF-6 format MT's extension required only minimal modifications to any of the PREPRO modules. The dis-

play modules *evalplot* and *complot* have been amended to account for the new channels. The *sixpack* module has been further extended to handle the single particle, gas and many radionuclide productions though the MF-3*MF-6 format frame, shaping then into useful MF-10:MT5 forms. Figs. 1-2 produced by *evalplot* illustrate the different nuclear data forms that come out of the PREPRO modules sequenced processing steps.

B. NJOY

The nuclear data evaluations are physics representations of the data encoded in the above-described unified computer-readable format called ENDF-6. They need to be converted into suitable forms for applications, such as transport or activation-transmutation calculations using multi-group, pointwise, deterministic or Monte Carlo techniques. The Fortran-77 style form of NJOY in its 99.393 version is perfectly able to handle this unified format and so feed in the many nuclear codes that rely on the data format of its numerous and pertinent modules. NJOY also has the unique capability, amongst the three processing codes, to process photon, neutron and kinematic kerma, total and partial damages, as well as the five gas production rates. It is also possible to output pointwise MCNP Ace data forms with *purr* probability table in the unresolved resonance range. Such data forms are available in this fully-fledged and comprehensive MCNP style formatted library file.

C. CALENDF

The CALENDF Nuclear Data Processing System is used to convert the evaluation defining the cross sections in ENDF-6 format (i.e. the point-wise cross sections and/or 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 quadratures and effective cross sections. The code accesses the data stored in MF-2 (resonance parameters) and MF-3 (point wise cross sections) of the ENDF-6 data file provided as input, ignoring all other MF. Ladders of resonance parameters are generated into some energy "zones"in the unresolved range, which are then treated as the resolved range. Checks of the consistency of the evaluated data MF-2 parameters are performed and messages emitted. In the Unresolved Resonance Range (URR) the basic idea is to generate random ladders of resonances. The treatment of these ladders is then the same as that of the Resolved Resonance Range (RRR), except, for the treatment of external or far-off resonances. For each group, or several groups in case of fine structure, an energy range is defined, taking into account both the nuclear properties of the nuclei and the neutronics requirements (accuracy and grid). By default, in CALENDF, the energies are taken from a sequence of eigenvalues of a random matrix. A stratified algorithm, improved by an antithetic method, creates the partial widths. In the URR range

CALENDF applies the "statistical hypothesis" based on the fact that the resonances can be statistically described.

III.   NUCLEAR DATA LIBRARIES

Out of the three processing codes come a set of data forms that feed the different codes; Boltzmann or Bateman solvers. The structural framework of the ENDF format allows numerous codes and solvers to access the processed data forms, that may be divided into three classes:

- Pointwise data forms; pendf, ace, anisotropy,

- Groupwise data forms; gendf, uncertainty, matrice,

- Probability tables forms; pt tables.

The Monte Carlo code, MCNP, TRIPOLI or SERPENT connect to the pointwise forms while deterministic and inventory code FISPACT-II [6] interface with groupwise sets. The format and physics of the probability tables advantageously complement both classes.

IV.   VERIFICATION AND VALIDATION

Verification and Validation (V & V) is a critical, yet often overlooked, part of scientific computer code development. Careful software life-cycle management under configuration control need to be used, as well as unit, integration and validation tests. These terms are similar, yet subtly different. Verification is the process of determining whether or not the products of a given phase in the software life-cycle fulfill a set of established requirements. In contrast, Validation is the stage in the software life-cycle at the end of a development process where software is evaluated to ensure that it complies with the requirements. This is a more comprehensive effort which is intended to test code and data in aggregate to ensure that the package is obtaining the correct results for the required quantities.

A.   Data Visualization and Comparison

Being able to visualize excitation functions, angular distributions and emitted spectra, understand their shape, and compare them with differential experimental information is an important aspect of any proper validation and verification V & V process. Only in the recent past have independent tools been sufficiently developed to allow thorough and accurate verification processes to take place. Such processes have already highlighted many defects, deficiencies and weaknesses either at the numerical value or format frame level. They contributed tremendously the robustness and the interpretation of the TENDL-2012 data files. Quality assurance also benefits from the ability to access and assess the data forms with similar but truly independent tools, showing the limitations and strengths of each of them.

B.   Differential Validation

The EXFOR [9] library contains an extensive and unique compilation of experimental nuclear reaction data. Neutron reactions have been compiled systematically since the discovery of the neutron. It is possible to compare the cross section, angular distribution data and the differential experimental information from EXFOR. However, only around 1700 cross sections may be compared in such a manner, but not always in the right, application relevant, energy range.

C.   Integral, Decay Heat Benchmarking

In nuclear plants, decay power arises after shutdown from the energy released in the decay of the products of neutron activation-transmutation from alpha, gamma and beta rays. Computation of the decay power is performed by the inventory code FISPACT-II which solve the large number of coupled differential equations which govern the generation and decay chains for the many nuclides involved. The code relies on a large volume of nuclear data, both neutron activation-transmutation cross sections based on TENDL and other radioactive decay data.
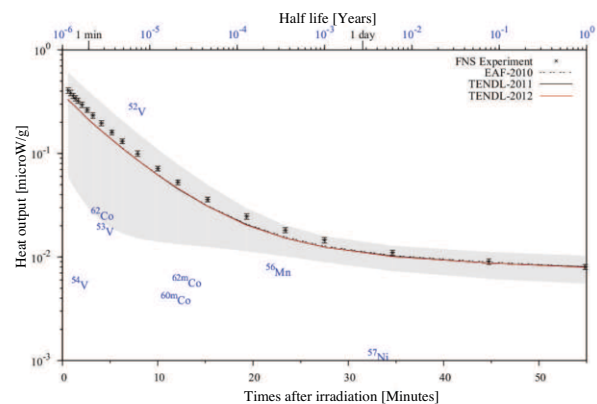

FIG. 3. JAEA FNS Inconel decay heat benchmarking.

Validation of decay power code predictions by means of direct comparison with integral data and measurements of sample structural materials under high energy fusion relevant neutron spectra generate confidence in the decay power values calculated. It also permits an assessment of the adequacy of the methods and nuclear data and indicates any inaccuracy or omission that may have led to erroneous results. A series of experiments were performed using the Fusion Neutron Source FNS facility at the Japan Atomic Energy Agency, JAEA [10]. Many elements and some alloy samples we irradiated in a simulated D-T neutron field for times up to 7 hours and the decay power so generated measured for cooling times from seconds up to a year. Using the highly sensitive Whole

TABLE I. ICSBEP's TRIPOLI-4.9 & JEFF-3.1.2, BRC-09, ENDF/B-VII.1 and TENDL-2012 k_{eff} results, BRC-09 corresponds to Bruyere le Chatel 2009 actinide evaluations, St. Dev. for all simulations.

Library				JEFF-3.1.2	BRC-2009	ENDF/B-VII.1	TENDL-2012	
ICSBEP		k_{eff}	Unc.	k_{eff}	k_{eff}	k_{eff}	k_{eff}	St. Dev.
Big Ten	deta.	1.0045	70	0.99878	1.00610	1.00479	1.00666	13
	simp.	1.0045	70	0.99770	1.00527	1.00419	1.00585	13
Δ (C-E)				-626	119	-1	175	
Jezebel	c-1	1.0000	200	0.99999	1.00033	0.99960	1.00022	15
Δ (C-E)				-1	33	-40	23	
Hiss		1.0000	600	1.00978	1.01152	1.01050	1.01160	13
Δ (C-E)				978	1152	1050	1160	
Godiva	c1	1.0000	100	0.99658	1.00015	1.00016	1.00503	11
Δ (C-E)				-342	15	16	503	

Energy Absorption Spectrometer (WEAS) method, both β and γ rays decay energies were measured at selected cooling times as early as a few tens of seconds after the irradiation ended. Fig. 3 exemplifies a graphical representation of the calculated versus experiment (C vs E) results for an Inconel 600 alloy sample when irradiated during 5 minutes. Simulations with three libraries (EAF-2010, TENDL-2011, -2012) are shown, the grey shaded area corresponds to the calculation uncertainty, mainly related to the production routes of the dominant isotopes ^{52}V and ^{56}Mn, which are plotted as their decay heat at shutdown versus their half-life (following the top log X-axis). The smaller vertical error bar represents the uncertainty associated with the measured decay heat. It is around 5% for the 21 measured decay times steps, starting as early as 30 seconds after the end of the irradiation.

V.   CRITICALITY BENCHMARKING

A TRIPOLI-4.9 critical assembly suite has been set up as a collection of 130 major benchmarks taken principally from the International Handbook of Evaluated Criticality Benchmarks Experiments (2012 Edition). It contains cases for a variety of U and Pu fuels and systems, ranging from fast to deep thermal solutions and assemblies. It covers cases with a variety of moderators, reflectors,

absorbers, spectra and geometries. The results presented (see Table I) show that while the most recent major library ENDF/B-VII.1, which benefited from the timely development of JENDL-4 and JEFF-3.1.2, produces better overall results, TENDL-2012 also performs well. It clearly suggests also that improvements are still needed.

VI.   CONCLUSIONS

The unified format exemplified, entirely based on the original ENDF-6 format framework, now makes the spine of a new set of nuclear data libraries and forms that are required to feed modern transport and inventory codes. The data structure is such that it allows the secular processing codes to be used simultaneously to process all the forms useful to the many applications that need them. The comprehensive and diverse resulting processed data forms have already been successfully connected and tested with the inventory code FISPACT-II and the Monte Carlo codes TRIPOLI and MCNP.

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