TENDL-2015: Delivering Both Completeness and Robustness

J-Ch. Sublet, A.J. Koning[1], D. Rochman[2], M. Fleming and M. Gilbert

United Kingdom Atomic Energy Authority, Abingdon, United Kingdom
Jean-christophe.sublet@ukaea.uk
Michael.fleming@ukaea.uk
Mark.gilbert@ukaea.uk
[1]*Nuclear Data Section, IAEA, Vienna, Austria*
a.koning@iaea.org
[2]*Paul Scherrer Institut, Villigen, Switzerland*
dimitri-alexandre.rochman@psi.ch

INTRODUCTION

The technologically generated TALYS Evaluated Nuclear Data Library [1] (TENDL) has been released annually since 2008. Considerable experience has been acquired for this yearly production of such unique, truly general-purpose, multi-particle nuclear data libraries based on the feedback from the developers, evaluators, processing experts and, most importantly, users. The backbone of this achievement is simple but robust: completeness, quality, upgradability and, most of all, reproducibility. Since TENDL has been widely adopted in many applications that require nuclear reaction data, it is necessary to understand its strengths and remaining weaknesses. The essential knowledge is not the TENDL library itself, but rather the necessary methods, processes, codes, tools and know-how that go into the making of the libraries. Future efforts must be focused on the evaluation of the underlying physics and incorporation of this information into the technological TALYS system [2]. TENDL-2015 encompasses 2809 target nuclides, including some 543 isomeric states, with seven incident particles up to 200 MeV. By its methodology, TENDL describes all open reaction channels, product yields, emitted spectra, short-lived daughter radionuclides, and includes complete variance-covariance information derived from reference input parameter variation. When fed into a modern simulation platform such as FISPACT-II [3], its enhanced nuclear data forms enable detailed and probing study of the nuclear landscape, even into uncharted territories.

NUCLEAR OBSERVABLES FOR ALL SCIENCES AND TECHNOLOGIES

Industry recognized legacy nuclear data libraries (ENDF/B-US; JENDL-Japan; JEFF-OECD/NEA, CENDL/China, ROSFOND/Russia) are assembled over decades by hand: evaluators have added data for nuclides, reactions and energies as and when it was deemed necessary for (principally fission) user applications. The methodology is robust where high-quality experiments have been performed, but relative to the total set of target nuclides/reactions/energies those libraries are tiny and incomplete. They change only when experiments or reactor feedback explicitly demonstrate errors and they generally do not contain any more than a very small fraction of the data and observables needed for other, non-LWR applications. Since many (or most) reactions important for advanced systems (particularly fusion, but also medical, accelerators, non-proliferation, security or astrophysics) have little experimental data, those legacy libraries cannot be relied upon and an alternative is necessary. The TALYS nuclear models code suite [4] uses various physical models (theoretical and semi-empirical; Optical, Hauser-Feshbach, exciton, Hartree-Fock, distorted-wave-Born, Fermi gas, ECIS for the Schrodinger equation, etc.) to generate the TALYS Evaluated Nuclear Data Library. TENDL is a nuclear data library covering completely the nuclide/reaction/energy sets, preventing incorrect simulation due to missing or incomplete data. The 8th version is TENDL-2015 (http://www.talys.eu/tendl-2015/) which is based on both default and adjusted parameters of the most recent T6 codes: TALYS, TAFIS, TANES, TARES, TEFAL and TASMAN, wrapped into a Total Monte-Carlo loop for uncertainty quantification. The T6 codes system, combined with a Total Monte Carlo (TMC) sampling method of its main nuclear model parameters, is uniquely capable of generating a full nuclear data library with complete (and consistent) covariances, enabling nuclear data uncertainty analysis which is not possible using any other library or systems. The standard release TENDL-2015 contains complete alpha, gamma, deuteron, proton, helium, triton and neutron-incident evaluations for all target nuclides with half-life longer than 1 second, up to 200 MeV, with covariances, emitted spectra, and all reaction and daughter products of half-life greater than 0.1 second.

ENHANCED MULTIPHYSICS PLATFORM

FISPACT-II is an enhanced multi-physics platform providing a wide variety of advanced simulation methods and employing the most up-to-date and complete nuclear data for both neutron and charged-particle interactions. FISPACT-II has been developed and is maintained by the

United Kingdom Atomic Energy Authority. As a comprehensive, modern object-oriented Fortran code, FISPACT-II fully processes all ENDF-6 nuclear data including the complete TENDL data with full covariance files. This extends the physics up to GeV energy with all channels and incident/emitted particles. Code features include self-shielding factors, broad temperature dependence, thin/thick target yields, robust pathway analysis, Monte-Carlo sensitivity and uncertainty quantification and propagation using full covariance data.

The latest generation of processing codes PREPRO, NJOY and CALENDF are used to provide the user with the most sophisticated incident-particle nuclear data forms from TENDL-2015, but also ENDF/B.VII.1, JENDL-4.0, CENDL-3.1 and JEFF-3.2 international libraries. These are complemented with the latest decay and fission yield data, including the most recent GEF libraries. These yields include 59 incident neutron energies for 119 target nuclides, plus 109 spontaneous fission yields.

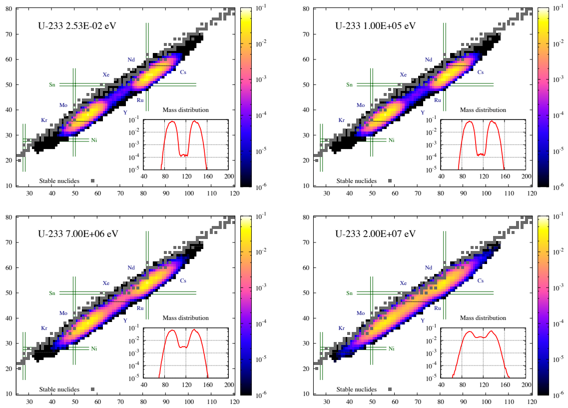

Fig. 1. GEFY-5.2 neutron-induced independent fission yields for U-233. Incident energies shown (read left to right) include 2.53E-2 eV, 100 keV, 7 MeV and 20 MeV, Z over N. Mass distributions are shown in bottom right corners.

The full data forms from TENDL are read and utilized, to generate complete reaction inventories, which include direct, pre-equilibrium and compound products. Above 30 MeV these are handled as total residual production rather than by individual channel, providing inherently consistent reaction yield data.

The maturity of modern, technological nuclear data including TENDL and GEF provides truly comprehensive data for all simulation requirements. The result is a multi-physics platform that can accommodate the needs of all nuclear applications including: activation, transmutation, depletion, burn-up, fuel cycle optimization or denaturing, decays, source definition, full time inventories, dpa, kerma, primary damage (PKA) spectra, gas/radionuclide production, ingestion, inhalation hazards and more.

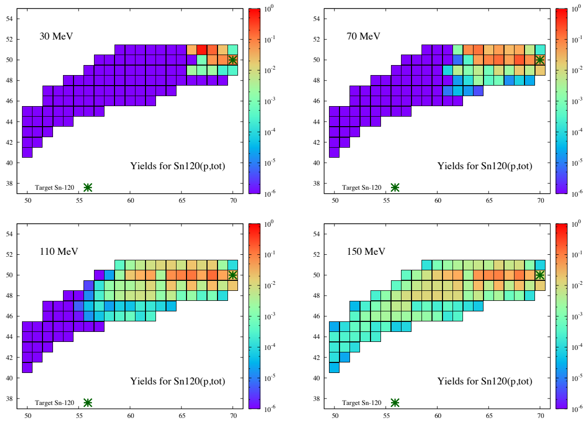

Fig. 2. TENDL-2015 Sn-120 nuclide yields for incident proton energies of 30, 70, 110 and 150 MeV, Z over N. These extrapolate into the 'deep spallation' nuclide production required for accelerator-driven systems.

UNCERTAINTY QUANTIFICATION AND PROPAGATION

Nuclear data uncertainty from cross sections, decays, yields and branching ratios are essential for many applications. While FISPACT-II has been designed to accommodate the co-variance data forms of legacy ENDF-6 files, these are often incomplete and occasionally inconsistent. Technological libraries such as TENDL and GEFY offer robust uncertainty quantification with full co-variance treatment. The Total Monte-Carlo (TMC) methodology employs sampling of multiple input parameters to generate many fully consistent files, which can be sampled to calculate co-variances. Alternatively, the many nuclear data files can be used in separate simulations and statistical analysis of the multiple results offers fully propagated nuclear data uncertainty. These approaches have been applied to both reaction rates and fission yields.

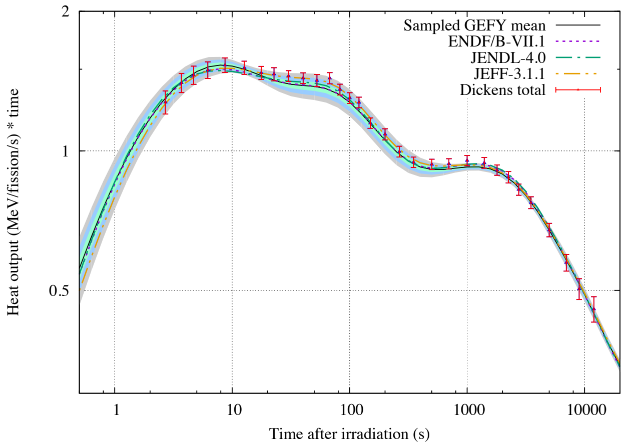

Fig. 3. Total Monte-Carlo fission yield uncertainty for thermal Pu-241 pulse decay heat, generated with GEF-4.2

and compared with ENDF/B-VII.1, JEFF-3.1.1, JENDL-4.0u and experimental data from Dickens *et al*.

PLASMA REACTION RATE VALIDATION

The S-process nucleosynthesis reaction rates have benefitted from significant study and are compiled into the Karlsruhe Astrophysical Database of Nucleosynthesis in Stars (KADoNiS) database. These are given by temperature dependent Maxwellian-averaged cross sections (MACS) for kT=1 keV to 100 keV. Maxwellian-averaged cross sections provide a rare source of high-quality information in the keV energy region, which for many nuclides lack any differential information. For many applications that have to account for neutrons as incident particles this is wholly insufficient and spurious nuclear data may result in unphysical simulations. The standard ENDF utility code inter and the Japanese maxwav codes were used to collapse MACS for ENDF/B-VII.1, JENDL-4.0u and TENDL-2014. The comparisons provide many recommendations for re-analysis of the resonance regions of all considered libraries.

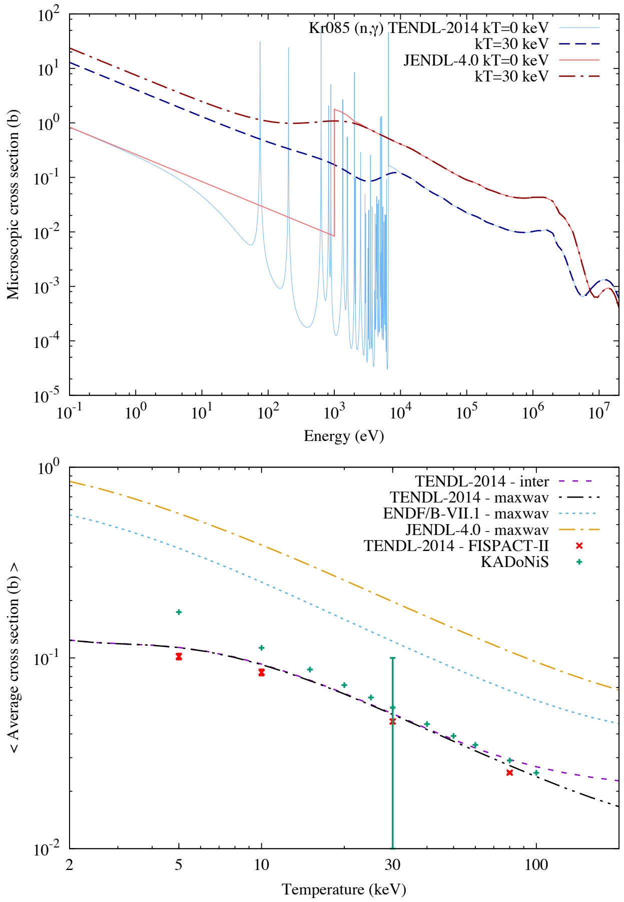

Fig. 4. Microscopic 0K and 30 keV broadened cross sections (top) and Maxwellian-averaged Kr-85 capture cross sections compared with KADoNiS data (bottom).

FUSION DECAY HEAT VALIDATION

With the 2014 release of TENDL, a complete validation was performed against the JAEA FNS decay-heat benchmark [6], resulting in an extensive report [7]. Figures 5 and 6 show example plots of this validation for nickel and niobium, respectively. In both examples, TENDL-2014 out-performs other international libraries because it includes data for a more complete set of nuclides, including metastable (isomeric) states. In Figure 6, for niobium, the match to the experiment is particularly good, with the simulation result generally falling within the experimental uncertainty, and vice-versa. This shows that TENDL correctly models the four metastable states: ^{89m}Y, ^{94m}Nb, ^{92m}Nb, and ^{90m}Y; that contribute significantly to the response.

Even in Figure 5, where the match between TENDL and the experiment is not as good, TENDL is still out-performing the other libraries by a significant margin again because of a more complete set of nuclides and associated cross-section data.

From the overall results, a set of inadequacies, not only in the cross sections but also in the associated decay libraries, have been identified that will require some corrective actions to be taken. These corrections and/or amendments will benefit the next generation of the TENDL library cross-sections, associated variance and covariances, and decay data files. As expected, they impact both the production paths and/or decay data of some specific radionuclides without impairing the overall picture. A large proportion of the decay powers calculated in such validation exercises with TENDL-2014 are in good agreement (within a few %) with the experimental values for cooling times spanning from tens of seconds up to more than a year.

CONCLUSIONS

Due to the methodology behind TENDL, the libraries are continuously updated and upgraded. This has resulted in a technologically generated nuclear data system that, within eight years of development, has outperformed the well-known legacy libraries for a large variety of applications. Those technological processes and mass data mining enable TALYS to be self-healing, responding quickly, physically and reproducibly to any new challenge it faces.

Non-proliferation applications that benefit from spontaneous, neutron induced fission on minor actinides, exotic material source terms characterization, nuclear forensics, isotopic denaturing and probing unchartered nuclear landscape can be conducted with predictive power.

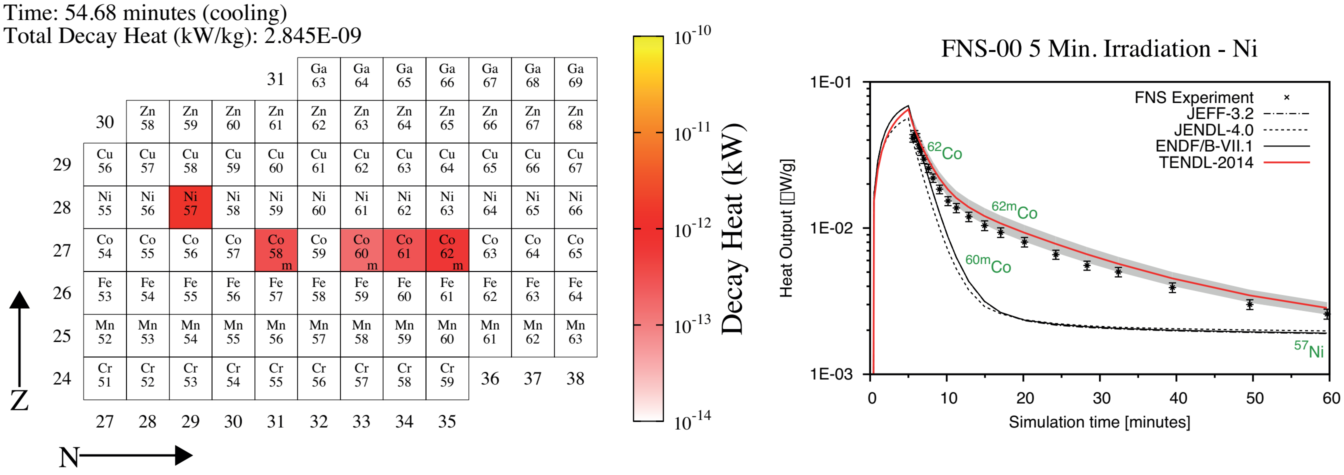

Fig. 5 Simulation of nickel irradiated for 5 minutes in JAEA FNS. On the right the complete simulation result of the total decay heat with four different nuclear data libraries in comparison to the experimentally measured decay heat. Only TENDL-2014 includes the necessary metastable states to properly reflect reality. The left figure is a "chart of the nuclides" tableau, showing the dominance of the metastable nuclides at the end of the experimental cooling period. An *m* in the box of a particular nuclide indicates that the decay heat contribution is dominated by a *m*etastable state.

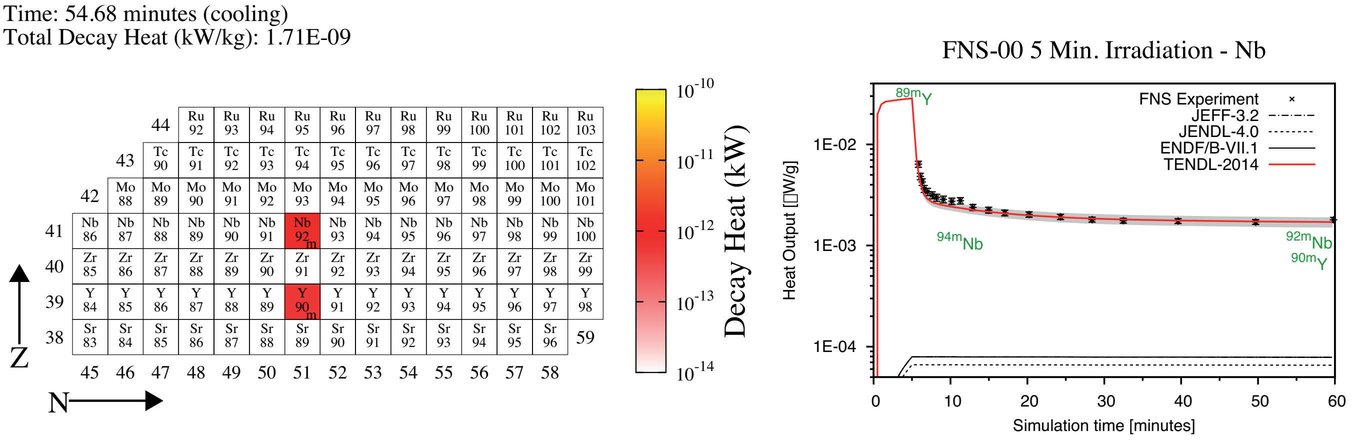

Fig. 6 Simulation of niobium irradiated in JAEA FNS. On the right the complete simulation result of the total decay heat with four different nuclear data libraries in comparison to the experimentally measured decay heat. Only TENDL-2014 includes the necessary metastable states to properly reflect reality. The left figure is a "chart of the nuclides" tableau, showing the dominance of the two metastable nuclides at the end of the experimental cooling period.

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