Multifaceted coded nuclear data libraries assemblage, verification and validation: TENDL-2019

J.-Ch. Sublet, Arjan Koning[*], Dimitri Rochman[†], Mark R. Gilbert[ǀ], Albert C. Kahler[&]
Cedric Jouanne[''], Jaakko Leppanen[+], Steven C. van der Marck[#] and Paul. Romano[%]

[*]*International Atomic Energy Agency, 1400 Vienna, Austria,* j.c.sublet@iaea.org, a.koning@iaea.org
[†]*Paul Scherrer Institut, 5232 Villigen, Switzerland* dimitri-alexandre.rochman@psi.ch
[ǀ]*United Kingdom Atomic Energy Authority, Abingdon, OX14 3DB, UK,* mark.gilbert@ukaea.uk
[&]*Kahler Nuclear Data Services, LLC, USA,* kahler3ac@gmail.com
''*CEA, Saclay, 91191 Gif-sur-Yvette, France* cedric.jouanne@cea.fr
[+]*VTT Technical Research Centre of Finland, FI-02044 VTT, Finland* jaakko.leppanen@vtt.fi
[#]*NRG, Westerduinweg 3, 1755 ZG Petten, The Netherland,* vandermarck@nrg.eu
[%]*Argonne National Laboratory, 9700 S Cass Ave, Lemont, IL 60439, USA,* promano@anl.gov

INTRODUCTION

The Multipurpose, multifaceted methodical nuclear data libraries coded by TALYS [1], TARES [2], TANES, TAFIS, TEFAL and TASMAN as the Evaluated Nuclear Data Library TENDL [3] have been released nearly every year for the last decade. Considerable experience has been acquired during the production years of such global, truly multifaceted, multiparticle (neutron, proton, deuteron, triton, alpha, helium and gamma induced), and multipurpose nuclear data libraries; based on the feedback from the developers, evaluators, processing experts and, most importantly, end users. The backbone of this achievement is artless but robust: completeness, quality, upgradability and, most of all, reproducibility and methodology. Since TENDL has been comprehensively adopted by many quite different applications (accelerator, astrophysics, fusion, fission, medical, experimental, decommissioning, etc.) that require multifaceted nuclear reaction data in various forms, primary and derived, for not only criticality but shielding, radio-protection, transmutation, experimental interpretation, materials or earth sciences, it is instructive to assess its strengths and remaining weaknesses. The essential knowledge is not the TENDL libraries themselves, but rather the necessary physics databases and methods, processes, codes, tools and know-how that go into the making of each and every evaluations of the libraries. Recent efforts have been focused on a proper assessment of the underlying physics coding and incorporation of databases information and metrics into the scientific T6 system [3].

NUCLEAR OBSERVABLES FOR SCIENCES AND TECHNOLOGIES

Industry recognized traditional nuclear data libraries (ENDF/B-US; JENDL-Japan; JEFF-OECD, CENDL/China, ROSFOND/Russia) have been assembled over decades by hand: 'evaluators' have added nuclides/reactions/energies as and when it was deemed necessary for (principally fission) applications. The methodology is robust when high-quality, differential or integral experimental data is available and can be successfully embedded; but relative to the total set of target nuclides/reactions/energies and derived data needed these libraries are small and incomplete. They generally do not contain any more than a very small fraction of the data and observables needed for other non-operational fission, non-criticality applications: branching ratio, radionuclides production, emitted particles and recoils spectra, etc. Since many (or most) reactions important for advanced systems (fusion shielding, medical, accelerators, instrumentation and manufacturing, security or astrophysics) have few or no experimental differential data, one cannot rely on these traditional libraries, and an alternative is necessary. The TALYS nuclear models code suite uses various physical models (theoretical and semi-empirical; Optical, Hauser-Feshbach, Exciton, Hartree-fock, Distorted Wave Born, Fermi gas, ECIS for the Schrodinger, Dirac equations, etc.) to generate part of a nuclear data library. TENDL is a nuclear data library completely covering the nuclide/reaction/energy sets, preventing errors in simulation due to missing or incomplete data sets. As such it can be used directly in both basic physics and novel, modern applications. The 10^{th} version is TENDL-2019 which is based on both default and adjusted parameters of the most recent T6 codes and databases suite: TALYS-1.95, TAFIS, TANES (Fission observables), TARES-1.4 (Resolved and unresolved resonance parameters handler), TEFAL (ENDF-6 formatter) and TASMAN wrapping them all into a Bayesian Monte-Carlo (BMC) loop for uncertainty quantification. The T6 codes system combines BMC sampling methods according to the weight of its main nuclear model parameters and is uniquely capable of generating a full nuclear data library with complete covariances (model- and/or experiment-based), enabling thorough nuclear data uncertainty analysis that is not always possible using any other libraries or systems.

MAJOR ENHANCMENTS

As the making, assemblage of the libraries is driven by technologies, any enhancement, correction, tweak being at the most basic physics and/or format level is immediately and seamlessly propagated to all targets and data forms. It then can reach the application level forms (processing steps permitting). For this release the following steps have been taken:

- Usage of an enhanced resonance parameter databases instead of on-the-fly statistical simulation
- Major update of the experimental differential and integral databases
- ENDF-6 format frame correction of emitted neutron spectra at the 30 MeV transition energy
- Covariances information on all seven incident particles
- Model simulation energy grid thinning
- Improvements in the branching ratios for isomeric states
- First successful deployment and production outside its birthplace cluster in the Netherland
- Upgrades to TALYS-1.95, TARES-1.4
- etc.

Generally, when issues or errors are found in the format and/or physics of one evaluation, the same issue/error are likely to exist in other evaluations with the same characteristic. Consequently, when corrections are made, they can be propagated to other evaluations in the same manner.

NUCLEAR DATA FORMS FOR APPLICATIONS

The usual ENDF-6 file format in which nuclear data libraries are distributed is typically not sufficient for direct use in many applications. System of processing modules is needed to convert nuclear data in the ENDF-6 format into forms that are usable in practical applications: [3] applications library and Fig. 1-4.

Several processing steps must be taken to satisfy the needs of downstream application codes, some of them being the most basic such as constructing temperature-dependent linearly interpolable pointwise cross sections from resonance parameters and interpolation schemes. Others are more complex and targeted toward a specific application; however those processes always consist of a number of independent, successive, intertwined tasks able to provide direct and derived data forms to simulation codes that need them. It is remarkable and noteworthy to acknowledge that even for the most processed, handled nuclear data forms in terms of steps, specificity, or complexity, a degree of backward compatibility and cross-checking to basic forms exists. This is a very useful remark that fully integrates what may be seem as rather complex quality assurance, QA's or reproducibility processes. Having said that, many end users concentrate on what is defined as cross sections when in fact ones also need emitted particles, residual angular and energy spectra distribution. Other forms such as reaction Q values, energies, prompts, delayed and decay information also co-exist with the above. Different simulations codes usually require different forms, all intended to stem from the same infrastructure.

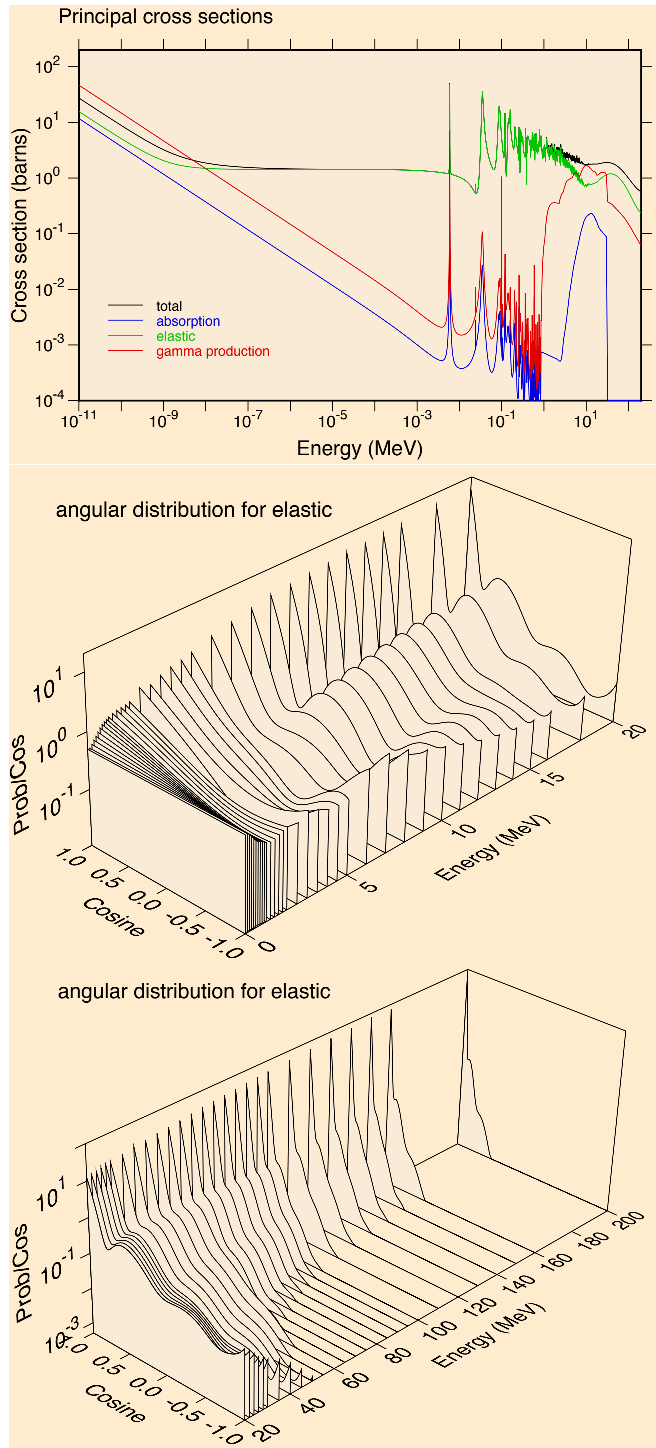

Fig. 1. Al^{27} Principal cross section and angular distribution.

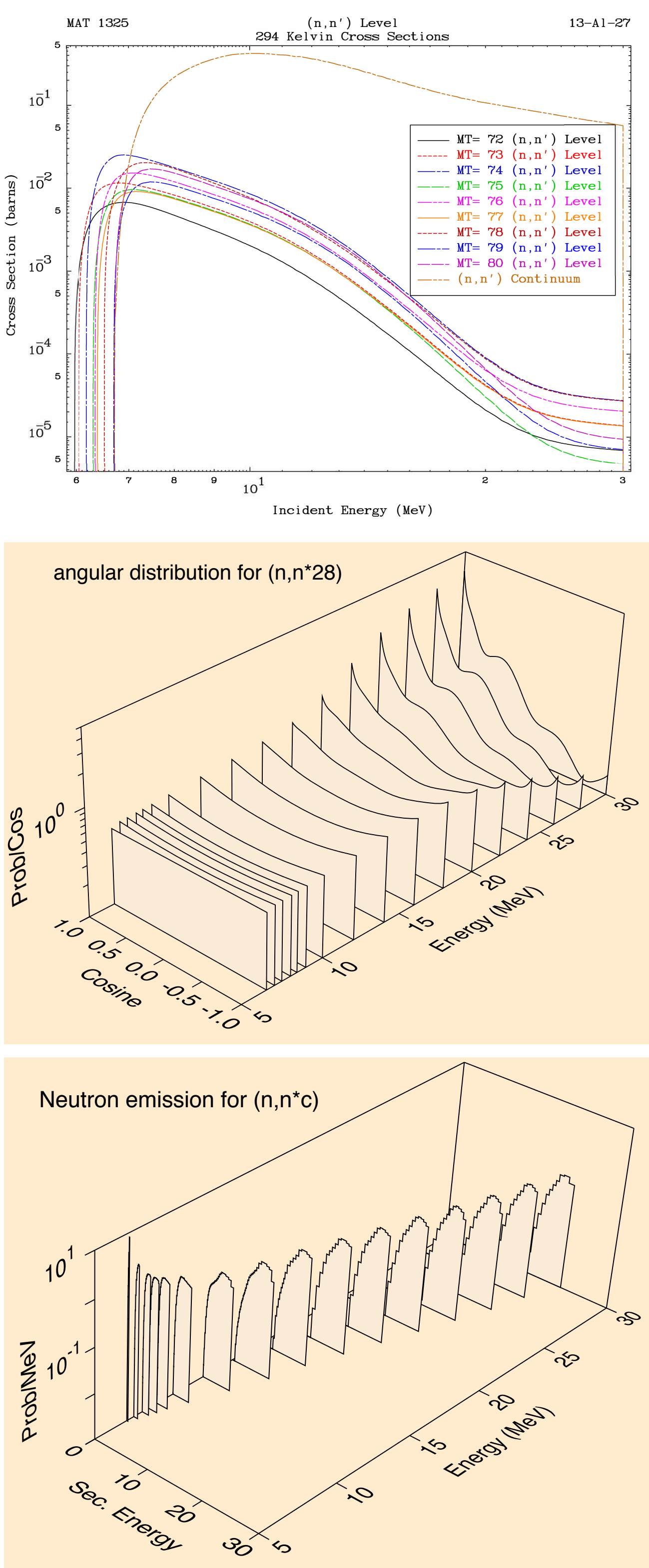

Fig. 2. Al^{27} inelastic cross sections and angular distributions.

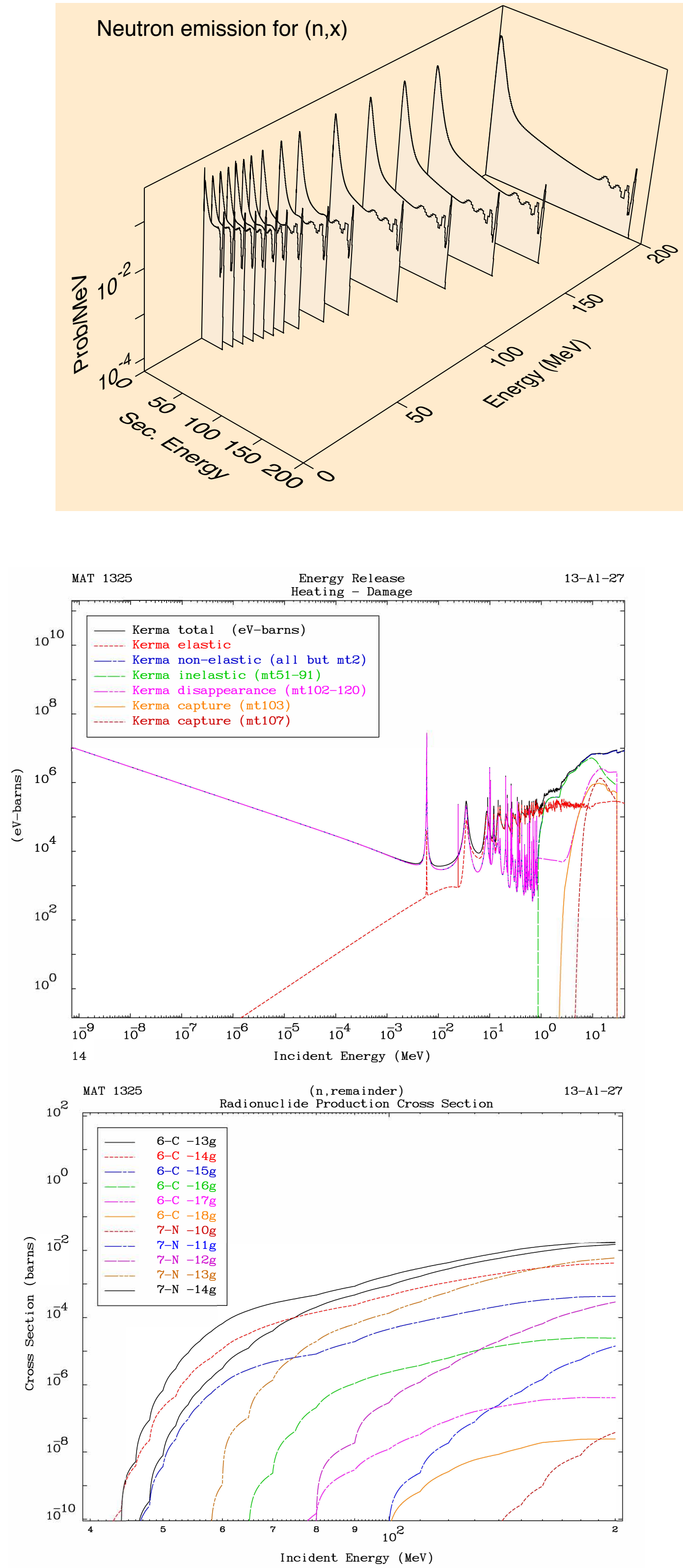

Fig. 3. Al^{27} high energy neutron emission, kinetic energy releases in material and transmutation yields.

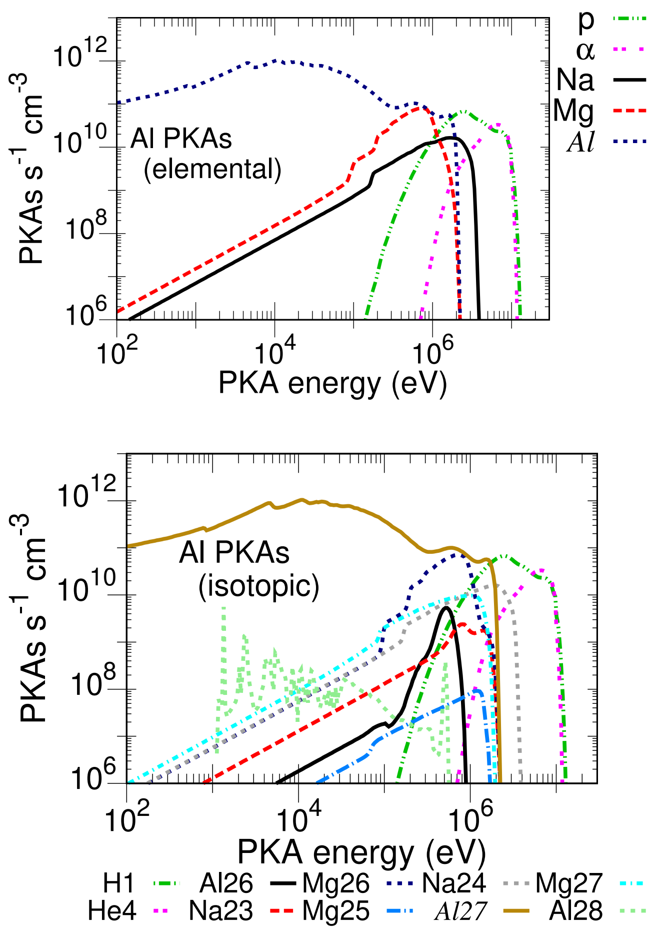

Fig. 4. Al^{27} primary knock on atoms spectra events

RESULTS

TENDL-2019 encompasses 2813 target nuclides, Z=1-115, Hydrogen to Moscovium, including as target some 513 m (1^{st}), 30 n (2^{nd}) isomeric states (T½ > 1s), for seven incident particles: alpha, gamma, deuteron, proton, helium, triton and neutron up to 200 MeV. Through its making, TENDL describes all open reaction channels, product yields, emitted spectra, and short-lived daughter radionuclides (T½ > 0.1s) as product and includes complete variance-covariance information derived from reference input parameters variation. When used in conjunction with EXFOR, the primary differential and integral data forms and interpretation can be compared with available experimental information. When fed through application libraries into modern simulation platform such as FISPACT-II [4] (a Bateman [5] solver) or MCNP [6], TRIPOLI [7], SERPENT [8], OpenMC [9] and CASMO [10] (as particle transport solvers), SPECTRA-PKA (primary knock-on atom evaluator) [11], its enhanced nuclear data primary and derived forms enable detailed, consistent and probing studies of the nuclear application landscape [3] V&V, like no other, leading the way scientifically and technologically into chartered and uncharted territory.

REFERENCES

1. A. J. KONING, S. HILAIRE, and S. GORIELY, "TALYS-1.95, User Manual," (2019). http://www.talys.eu/
2. D. ROCHMAN, A. J. KONING, J.-Ch. SUBLET, "A Statistical Analysis of Evaluated Neutron Resonances with TARES for JEFF-3.3, JENDL-4.0, ENDF/B-VIII.0 and TENDL-2019," Nucl. Data Sheets 163 (2020) 163-190
3. A. J. KONING and D. ROCHMAN, "TENDL-2019: TALYS-based Evaluated Nuclear Data Library," (2019) https://tendl.web.psi.ch/tendl_2019/tendl2019.html
4. J.-Ch. SUBLET, J. W. EASTWOOD, J. G. MORGAN, M. R. GILBERT, M. FLEMING, W. ARTER, "FISPACT-II: An Advanced Simulation System for Activation, Transmutation and Material Modelling," *Nuclear Data Sheets* 139 (2017) 77-137 and https://fispact.ukaea.uk/
5. H. BATEMAN, "The Solution of a System of Differential Equations Occurring in the Theory of Radio-active Transformations," *Proc. Camb. Phil. Soc.*, **16**, 423 (1910)
6. C.J. WERNER (editor), "MCNP Users Manual - Code Version 6.2", (2017) LA-UR-17-29981
7. E. BRUN, F. DAMIAN, C.M. DIOP, E. DUMONTEIL, F.X. HUGOT, C. JOUANNE, Y.K. LEE, F. MALVAGI, A. MAZZOLO, O. PETIT, J.C. TRAMA, T. VISONNEAU, A. ZOIA,"Tripoli-4®, CEA, EDF and AREVA reference Monte Carlo code," Annals of Nuclear Energy **82**, 151-160 (2015) and http://www.cea.fr/tripoli-4/
8. J. LEPPANEN et al, "The Serpent Monte Carlo code: Status, development and applications in 2013." Ann. Nucl. Energy, *Annals of Nuclear Energy* 82 (2015) 142-150 (2015)
9. P.K. ROMANO, N. E. HORELIK, B. R. HERMAN, A. G. NELSON, B. FORGET, and K. SMITH, "OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development," *Ann. Nucl. Energy*, **82**, 90–97 (2015) and https://docs.openmc.org/en/stable/
10. Studsvik, "CASMO5," https://www.studsvik.com/our-solutions/products/casmo/
11. M. GILBERT and J.-Ch. SUBLET, "Differential dpa calculations with SPECTRA-PKA," J. Nucl. Mater. 504 (2018) 101-108 and http://fispact.ukaea.uk/wiki/Spectra-PKA