Workshop on TALYS/TENDL Developments

13-15 November 2017,
Prague, Czech Republic

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TENDL Development

TALYS and TENDL: Status and future

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International Atomic Energy Agency

Both the TALYS nuclear model code and the TENDL nuclear data library have now reached a certain level of maturity and its combination is used worldwide for the whole range of basic nuclear physics to nuclear technology. My presentation contains two parts:

1. What are TALYS and TENDL, and what has been made possible by them? Several examples of nuclear reaction models implemented in TALYS and their comparison with differential data will be given, as well as a global overview of the applications of TENDL for nuclear applications, including uncertainty propagation.
2. Future possibilities for TALYS and TENDL. Apart from a memory- and speed-efficient revision of the entire TALYS code (opening up entirely new IT possibilities), extension to new physics domains will be suggested. For TENDL, global optimization methods and autonomously powerful data libraries for actinides, and thus criticality-safety, are foreseen.

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FISPACT-II & TENDL Verification & Validation processes

Jean-Christophe Sublet

International Atomic Energy Agency

An essential aspect of a modern simulation software life cycle is the verification and validation which demonstrate the code and nuclear data capabilities and are used to establish its use in regulated analysis. A work in progress aims at collecting and assembling all accessible differential and integral experimental information for nuclear applications with the aim of constructing the most complete validation and verification suite ever assembled. The full capabilities and performance of modern computing, databases, automated scripting and parallelism is beeen deployed to achieve the goal. The FISPACT-II & TENDL libraries simulation software will then become de-facto a standard for nuclear technologies able to answer all needs; from cradle to grave in terms of development and design, plant analysis, operation, fuel management and cycle, decommissioning, dismantling and long term storage/repository requirements.

TENDL-2017: better cross sections, better covariances

Dmitri Rochman

Paul Scherer Institut

This new release of the TENDL library will contain as usually an extensive number of isotopes, all of them with covariance information. But for 2017, dedicated efforts allowed to improve specific cross sections for reactor, fusion and dosimetry applications. As for the previous releases, the covariance information and cross sections are evaluated at once, allowing consistency for the full library, which is a unique feature of TENDL. Some examples will be presented with insights on the evaluation methods.

Important Comments on TENDL-2015

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Japan Atomic Energy Agency, Japan

TENDL (TALYS-based Evaluated Nuclear Data Library) -2015 up to 200 MeV of incident particle upper energy has been used as a standard nuclear data library, particularly in Europe. Recently I tested the TENDL2015 neutron sub-library and its ACE (A Compact ENDF) file and found the following problems.

1) There are no unresolved resonance data in the ACE files except for those of ^{235}U, ^{235m}U and ^{238}U. Thus calculated results are not correct in the case that the self-shielding effect in the unresolved resonance region is large. This issue will be resolved by re-processing TENDL-2015 with the PURR module in the NJOY code.

2) There are no gamma production data in the ACE files except for those of ^{1}H, ^{2}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, ^{12}C, ^{14}N, ^{15}N, ^{16}O, ^{19}F and ^{239}Pu. This is due to an inadequate NJOY input. Thus gamma fluxes in neutron-gamma coupling calculations are not correct, since MCNP calculations uses particle production data in place of gamma production data in ACE files. This issue also occurs in the ACE files of the proton, deuteron, triton, and helium sub-libraries. This issue will be resolved by re-processing TENDL-2015 with an adequate NJOY input.

3) There are no high-energy gamma peaks in the capture reaction of a lot of the TENDL-2015 files. This issue causes incorrect gamma fluxes in neutron-gamma coupling calculations and incorrect DPA cross section data. It is difficult to resolve this issue, because the gamma production data of the capture reaction in TENDL-2015 have to be revised.

The gamma production data in the capture reaction in the TENDL-2015 neutron sub-library should be revised and ACE files in TENDL-2015 should be re-processed with an adequate NJOY input.

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UKAEA work in the verification and validation of TENDL

Michael Fleming

UK Atomic Energy Authority

The pace of TENDL development, with biennial distributions, places significant pressure on the verification and validation process. The UKAEA has developed automated systems to test TENDL (and other international library) databases against a suite of integral data drawn from fusion, fission, accelerator-system and astrophysical measurements. The results of these tests for the most recent TENDL evaluations will be presented with comparisons against other international libraries and previous releases.

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On deuteron-induced reactions, with TALYS

Marilena Avrigeanu

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A detailed analysis of the direct-interaction key role in deuteron-induced reactions on target nuclei from Al to U has been carried out. Less considered so far, the specific non-compound processes make substantially different the deuteron-induced reactions than the case of other incident particles. Thus, the deuteron breakup (BU) is particularly important due to the large variety of reactions initiated by the breakup nucleons along the whole incident-energy range. Moreover, the role of the deuteron BU increases with the target-nucleus mass and charge, so that it becomes dominant for heavy target nuclei at deuteron energies particularly around the Coulomb barrier. Otherwise, the deuteron interaction with low- and medium-mass target nuclei below and around the Coulomb barrier proceeds largely through stripping and pick-up direct reactions (DR) while pre-equilibrium emission (PE) and evaporation from fully equilibrated compound nucleus (CN) become important
at higher energies.

However, while the associated models for DR, PE, and CN mechanisms are already settled, an increased attention should be paid to the theoretical description of the BU two components, namely the elastic BU, with no interaction target nucleus–breakup nucleons, and inelastic BU or breakup fusion (BF), where one of these constituents interacts non-elastically with the target nucleus. This is why a comparative assessment of measured data and results of BU microscopic description as well as current parametrization already involved within recent systematic studies is equally useful to basic studies and improved nuclear data calculations. Actually, missing of the suitable BU analysis leads to large disagreement between the more recent studies experimental and calculated deuteron-activation excitation functions. In this respect, the inclusion of an alternative BU formalism in TALYS code upgrades the nuclear modeling capabilities through the parameterization of BU component cross sections as well as the enhancement of the deuteron-induced reaction cross sections due to the variety of reactions induced by the BU nucleons. This goal has been fulfilled in ready-to-implemented form by addition of 3 new subroutines and 2 new databases, while other 8
original subroutines of TALYS were modified.

Actually, an update of the theoretical analysis of deuteron-nuclei interaction within a consistent account of the related reaction mechanisms is highly requested not only by use of deuteron surrogate reactions for (n,gamma) and (n, f) cross sections, of interest for breeder reactors studies, but also by strategic research programs ITER, IFMIF, and SPIRAL-2 as well as by medical investigations using accelerated deuterons. Moreover, as long as powerful computers and available dedicated codes exist, the complexity of deuteron interactions can not motivate the use of, e.g., various Pade approximations for the analysis of measured deuteron-reaction cross sections.

On alpha-praticle induced reactions, too much with TALYS

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The interaction of particles with nuclei has been of special interest from the earliest days of nuclear physics, as well as the optical model potentials (OMPs) involved in this respect. The widely-used phenomenological OMP parameters have been derived from the analysis of either elasticscattering or alpha-induced reaction cross sections below the Coulomb barrier B while then are used to describe also the alpha-particle emission from hot nuclei excited in nuclear reactions. However the later studies are subject of also other various assumptions and quantities. Thus, the alpha-particle OMP seems similar to the so familiar side of the Moon which only is facing always the Earth, in the case of the incident channel, but for the alpha-emission is very like the dark side of the Moon. Moreover, there is a so-called alpha-potential mystery of the account at once of both absorption and emission of low-energy alpha-particles, whereas recent high-precision measurements are still pointing out challenging questions of the alpha-particle OMP even in the case of alpha-induced reaction data below B.

On the other hand, the corresponding statistical model (SM) analysis depends critically on the accuracy of the rest of SM parameters. They could be provided only on the basis of a consistent input parameters, established or validated by analysis of various independent data, against the trial of different combinations of SM ingredients even self-consistent in the sense that they combine only phenomenological or microscopic models, respectively. Thus, e.g., recent (alpha, gamma) reaction data for ^{74}Ge and ^{90,92}Zr isotopes can be well described by the same alpha-particle OMP, following the use of consistent sets of the rest of SM parameters, while their former analysis reported three different OMPs providing their best description by TALYS calculations. However, none of these potentials was the most-physical 3rd version of Demetriou et al. parameter sets, but the former two and the schematic initial approach in TALYS. Similar cases have been proved for Ni isotopes and especially by an investigation of the complete parameter space of the TALYS code using almost 7000 combinations of SM parameters for the analysis alpha-induced reactions on ^{64}Zn below B but with less physical results than use of a consistent-parameter set.

TENDL Application

Treating model defects in TALYS to improve TENDL mean values and covariances

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The covariance information in TENDL is obtained by propagating uncertainties of, e.g., TALYS parameters to the observables, and by attempting to match the parameter uncertainties to the experimental data. This results in model driven covariances with strong energy-energy correlations, which can lead to erroneously estimated uncertainties for both differential and integral observables. Further, the model driven approach is sensitive to model defects, which can introduce biases and underestimated uncertainties.

To resolve the issue of model defects in nuclear data (ND) evaluation, models the defect with a Gaussian process. This can reduce biases and give more correct covariances, including weaker energy-energy correlations. In the presented work, we continue the development of using Gaussian processes to treat model defects in ND evaluation, within a TENDL framework. The Gaussian processes are combined with the Levenberg-Marquardt algorithm for non-linear fitting, which reduces the need for a prior distribution. Further, it facilitates the transfer of knowledge to other nuclides by working in the parameter domain. First, synthetic data is used to validate the quality of both mean values and covariances provided by the method. After this, we fit TALYS parameters and a model defect correction to the ^{56}Fe data in EXFOR.

Covariances generation for the cross sections and benchmark responses from the TENDL random files

Stanislav Simakov

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The estimation of uncertainties and energy-energy correlations (covariance matrices) for the aggregate physical quantities or for the observable responses in the macroscopic nuclear systems cannot be done analytically, except the cases when linear propagation of small variation is a valid approximation. The alternative and general solution, which however could be computer time consuming, is a propagation of the basic cross sections uncertainties by multiple repeated calculations on the cross sections ensemble randomly perturbed within physically constrained boundaries.

The present work presents such approach for the neutron damage quantities calculations (gas production, KERMA factors, damage energy and displacement cross section) for Iron. The TENDL-2017 random cross section files and NJOY processing code were employed to generate these quantities and their covariances. The second application demonstrates the propagation of the TENDL-2017 uncertainties to the spectra of neutrons and gammas leaking from the Iron spheres with ^{2582}Cf(s.f.) source in centre. In this case the MCNP transport code was used to propagate the variations of the TENDL-2017 random cross section files to the observables.

TENDL adjustments using integral benchmarks

Henrik Sjöstrand

Uppsala University

Integral experiments can be used to adjust ND-libraries. In this work we show how we can use integral experiments in a consistent way to adjust the TENDL library. A Bayesian method based on assigning weights to the different random files using a maximum likelihood function is used. Emphasis is put on the problems that arise from multiple isotopes being present in a benchmark. The challenges in using multiple integral experiments are also addressed, including the correlation between the different integral experiments.

Improving activation cross section data for TENDL*

Nataliia Dzysiuk

NRG Petten

A new set of cross sections have been improved with the TALYS code. In total more than 350 reaction channels were under consideration. The first part of cross sections is fusion relevant materials which have been re-evaluated in the framework of F4E project. The second part is evaluation of fission products as one of the tasks for the CHANDA project. The fits have been performed by means of nuclear model parameter variation. Mostly for the optical model and level densities, followed by comparison to the recent experimental data taken from EXFOR and other evaluated nuclear databases. The updated cross section data are going to be adopted to the new version of TENDL. The improvements have been performed both for differential as well as integral data sets.

** presented by Arjan Koning*

Facility projects

The Neutrons for Science Facility at SPIRAL-2

Xavier Ledoux

Grand Accélérateur National d'Ions Lourds

The neutrons for science (NFS) facility will be the first experimental area operational at SPIRAL-2. NFS is composed of a well collimated pulsed neutron beam with a flux up to 2 orders of magnitude higher than those of other existing time-of-flight facilities. NFS also offer irradiation stations for irradiation of samples by ions or by neutrons with very intense fluxes. It will open GANIL to new kind of experiments using neutrons beam with energies between a few MeV and a few tens of MeV. Many fundamental topics like reaction mechanisms, measurement of astrophysical reaction rates or the fission process will be studied at NFS. New and reliable nuclear data for applications like the transmutation of nuclear waste, the design of future fission and fusion reactors or the nuclear medicine will also be measured to improve the evaluated databases used in these fields. The development of new detectors or the irradiation of electronic devices will also be covered at NFS. The first experiments were submitted to the GANIL PAC in 2016. After a description of the facility and of its characteristics, the experiments to be performed in the short and medium term will be presented.

Technology exploitation at JET: recent and planned activation experiments, and supporting analysis using TENDL

Lee Packer

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The planned experiments over the coming years at the Joint European Torus (JET) is expected to produce large neutron yields of up to 1.7×10^{21} neutrons in total. A range of plasma operations are forseen, including DD, TT and most importantlt at DT phase expected towards the end of 2019, which will produce significant fluxes 14 MeV neutrons. The scientific objectives of the these operations at JET are linked with the WPJET3 technology programme, with the aim to deliver the maximum scientific and technological return with particular emphasis on technology exploitation via the aforementioned high neutron fluxes predicted in and around the JET machine. Importantly, the programme aims to extract experimental data relevant to the international effort to design, construct and operate ITER, the international tokamak device being constructed in Cadarache, France, that is designed to produce significant fusion power of up to 500 MW with corresponding DT neutron emission rates of 1.77×10^{20} neutrons per second. The data retrieved under the JET experimental program will support, develop and improve the radiation transport and activation simulation capabilities via benchmarking and validation in relevant operational conditions, which are applied extensively to predict a wide range of nuclear phenomena and impacts associated with components and materials that will be used in ITER operations.

This paper outlines the progress on experimental characterisation work using dosimetry foils, conducted as part of the ACT sub-project under WPJET3. The aim of the subproject is to take advantage of the JET neutron fluxes to irradiate samples of materials that will used in the manufacturing of main ITER tokamak components, such as Nb3Sn, SS316L steels from a range of manufacturers, SS304B, Alloy 660, W, CuCrZr, OF-Cu, XM-19, Al bronze, NbTi and EUROFER. Measurement and predictions are detailed of the nuclear environment at the relevant irradiation locations at JET, measured using a range of dosimetry foils (Ti, Mn, Co, Ni, Y, Fe, Co, Sc, Ta). Experimental results are compared to the latest simulations using MCNP6 JET models with FISPACT-II for activation quantity predictions. These are performed with TENDL, and also other nuclear data libraries for comparison.

Projected fast neutron facilities at CANAM-NPI cyclotrons

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At the Cyclotron laboratory (LC) of the Centre of Accelerators and Nuclear Analytical Methods (CANAM), two cyclic accelerators are at disposal: U-120M cyclotron (p, d, ^{3}He and α beams, K = 40) and recently commissioned high-power proton cyclotron TR-24 (300 µA, maximum beam energy 24 MeV).

Various neutron generators are operated at the U-120M cyclotron (based on proton reactions on liquid and solid targets), providing neutrons of continuous and quasi-monoenergetic spectra with energy up to 36 MeV. A long-term program of cross-sections measurement takes advantage of variable energy of incident particles, activation and scintillation techniques reflecting natural time structure of incident beam (limited rate T/ΔT ~ 7). The development of TOF technique for fast neutron spectrometry on the U-120M cyclotron is rather advanced. The original principle of internal multi-orbital extraction of protons on Be target is applied to produce time-selected neutron bursts. Projected parameters (20 µA /36 MeV of pulsed protons, repetition rate T/ΔT ≥ 100, ΔTFWHM ~ 3ns) are close to those of TOF neutron source at NFS SPIRAL-2 in pBe version and will offer some synergy option in selected tasks of neutron data measurement.

The high-power neutron generator is under development also at the TR-24 cyclotron. White spectrum neutrons ($E_n \leq 22$ MeV) with flux up to 3×10^{12} n/sr/s produced in the Be(p,xn) reaction will be available. Static version of the Be target has been chosen taking into account the irradiation requests. Since extreme heat power density (up to 4 kW/cm^2) is expected, the impingement submerged jet for target cooling is currently developed. Fast neutrons of high-intensity are an important tool for measurement of neutron data relevant for fusion-technology. In comparison with research fission-reactors, the TR-24 neutron generator will offer some advantages regarding the irradiation tests of ITER components, too.

Project SPIRAL2-CZ in NPI CAS

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The project SPIRAL2/GANIL has recently received a support from Czech Republic as an international infrastructure SPIRAL2-CZ. In the first period the efforts are concentrated on SPIRAL2/NFS (Neutrons For Science). An irradiation chamber (IC) for charged particles was developed in NPI CAS and together with Pneumatic Transfer System (PTS) from KIT Karlsruhe is currently installed in the site. Details of operation and experiences from tests in beam on U120M cyclotron in NPI CAS will be shown as well as an overview of the SPIRAL2-CZ project and ND research plans.

Data measurements

The benchmark of the EAF-2010 Fe and Cr neutron cross-sections with various neutron spectra

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In the frame of the program F4E-FPA-395 (Fusion 4 Energy) the NPI is involved in the experimental benchmark of the neutron cross-section database with the focus on the gas production reactions, eg. (n,p), (n,d), (n,a).
In 2015, the EAF-2010 experimental cross-section benchmark was performed on elements Fe and Cr (published as F4E report and as INDC(CZR)-0003 proceeding), the cross-sections elements Cu and V were benchmarked aside (ND2016 proceeding). The benchmark of the cross-sections for elements Ta and W is currently being performed.
Within the benchmark, the activation foils made of the studied material are irradiated with quasi-monoenergetic and continuous neutron spectra. The residual radioisotopes are measured by the means of the gamma spectrometry. The obtained production rates are compared with the predictions from the EAF-2010 (as well as JEFF and TENDL) databases. The experimental benchmarks mostly confirm the validity of the database with few exceptions which will be discussed.
Finally, new experimental facilities currently at construction at the NPI (evacuated chamber dedicated to direct measurement of gas production cross-sections, neutron generators upgrade) and future research topics will be mentioned (experimental measurement of the material damage).

Comparison of two independent neutron spectrometry methods, proton-recoil and time-of-flight, used for iron Nuclear Data Libraries validation

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Research Centre Řež

The measurements (M) of leakage neutron spectra from the iron spherical assemblies of approximately the same diameters have been done by two independent methods. The neutron source was always positioned in the center of iron spheres.
In the first case an encapsulated Cf-252 neutron source and proton recoil (PR) method for neutron spectrum measurement were used (hydrogen proportional counters and stilbene).
In the second case the thin fission chamber served as a neutron source whereas the neutron spectrum was measured by the Time- of-Flight (TOF) technique.
The neutron spectra leaking from these assemblies were calculated (C) in both cases with the same data library, as well as the ratios C/M in the proper wide neutron energy groups.
Finally these quantities obtained from the two independent measurements PR and TOF were compared to derive conclusion about the validity of the neutron transport library.

Proton and deuteron activation measurements on the NPI and future plants at SPIRAL2/NFS

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The proton and deuteron induced reactions at low and medium energies have a great importance within several on-going strategic research programs for international large-scale facilities. It was shown that the global reaction models used in design, validation and assessment of the facilities can have significant deviation, where the experimental data were not present for the database verification. A determination related activation cross-sections of proton and deuteron induced reactions up to 20MeV are performed using CANAM infrastructure – NPI energy variable cyclotron U120M and ion-beam irradiation chamber. A methodical approach and some results will be presented. The comparison of present results to data of other authors and to predictions of evaluated data libraries is discussed. The investigation shall continue for higher energy interval 20-35 MeV at SPIRAL2 NFS facility using a charged-particle irradiation chamber being developed presently at NPI.

LA150H library for the reaction 7Li(p,n) and new experimental data on neutron production

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Quasi-monoenergetic neutrons, produced with the reaction ^{7}Li(p,n) are used for the measurements of the neutron cross-sections above 20 MeV. Good knowledge of the produced quasi-monoenergetic neutron spectra is crucial for the extraction of reliable neutron cross-sections.
The neutron spectra for three different p+^{7}Li generators (NPI Řež, CYRIC Tohoku, TSL Uppsala) were simulated using the MCNPX code with the LA150H library and compared to the experimental measurements. The disagreements were studied and the update of the LA150H library with the inclusion of the experimental data is discussed.

Studies of cross-sections of (n,xn) reactions on Au and Y

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Knowledge of the excitation function of neutron reactions is important part for the ability to develop and to model advanced nuclear system facilitating fast neutrons such as accelerator driven systems, spallation neutron source etc. Unfortunately the experimental knowledge of neutron reactions with energy of the primary neutron in range of tens of MeV is insufficient. And this fact propagates even in the ability of calculation these date with various codes using existing nuclear models. We measured several cross-sections of (n,*x*n) reactions on Y and Au using ^{7}Li(p,n)^{7}Be quasi-monoenergetic neutron source at the Nuclear Physics Institute of the Czech Academy of Sciences. Bigger part of obtained results are new data in unmeasured energy interval.