Nuclear data for fusion technology – the European approach

Ulrich Fischer[1,a], Marilena Avrigeanu[2], Vlad Avrigeanu[2], Oscar Cabellos[3], Natalia Dzysiuk[4], Arjan Koning[5], Axel Klix[1], Alexander Konobeev[1], Ivo Kodeli[6], Helmut Leeb[7], Dieter Leichtle[8], Elena Nunnenmann[1], Lee Packer[9], Dimitri Rochman[10], Pavel Pereslavtsev[1], Patrick Sauvan[11], and Andrej Trkov[5,6]

[1] Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
[2] Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), 077125 Magurele, Romania
[3] Nuclear Energy Agency (NEA), 46, quai Alphonse Le Gallo, 92100 Boulogne-Billancourt, Paris, France
[4] Nuclear Research and Consultancy Group (NRG), Westerduinweg 3, 1755 Petten, The Netherlands
[5] International Atomic Energy Agency, Vienna International Centre, PO Box 100, 1400 Vienna, Austria
[6] Jožef Stefan Institute (JSI), Jamova 39, 1000 Ljubljana, Slovenia
[7] Technische Universität Wien, Atominstitut, Wiedner Hauptstrasse 8-10, 1040 Wien, Austria
[8] Fusion for Energy, c/ Josep Pla, nº2, Torres Diagonal Litoral, Edificio B3, 08019 Barcelona, Spain
[9] Culham Centre for Fusion Energy, Culham Science Centre, Abingdon OX14 3DB, UK
[10] Paul Scherrer Institut, 5232 Villigen PSI, Switzerland
[11] Universidad Nacional de Educación a Distancia, C. Juan del Rosal, 12, 28040 Madrid, Spain

Abstract. The European approach for the development of nuclear data for fusion technology applications is presented. Related R&D activities are conducted by the Consortium on Nuclear Data Development and Analysis for Fusion to satisfy the nuclear data needs of the major projects including ITER, the Early Neutron Source (ENS) and DEMO. Recent achievements are presented in the area of nuclear data evaluations, benchmarking and validation, nuclear model improvements, and uncertainty assessments.

1. Introduction

The European Fusion Programme aims at the realisation of fusion as energy source for the production of electricity by the year 2050. The Strategic Energy Technology Plan thus assumes the construction and operation of a Fusion Power Plant (FPP) which will provide electricity to the grid. Three major facilities are considered to be required to achieve this ambitious goal: (1) ITER, as a key physics and technology facility for the "next step", (2) a dedicated Early Neutron Source (ENS) for the material development, and (3) an early Demonstration Power Plant (DEMO) to enable a smooth extrapolation to FPP conditions. The European Fusion Roadmap [1] accordingly assumes that all know-how, required to start the construction of DEMO around 2030, can be acquired in time. A central element of this approach is the design of DEMO which is conducted in a dedicated Power Plant Physics and Technology (PPPT) programme of the EUROfusion consortium [2].

The availability of qualified computational tools and nuclear data are pre-requisites for performing the analyses as required for the nuclear design, optimization and performance evaluation of the key facilities, ITER, ENS and DEMO including the assessment of safety, licensing, waste management and decommissioning related issues. The needs for high quality nuclear data are addressed by a Consortium on Nuclear Data Development and Analysis which provides the relevant services on the production of nuclear data evaluations and data files including their validation for neutronics design and activation calculations.

In the following, an overview is presented on the related Nuclear Data Development (NDD) activities of the Consortium with focus on the recent achievements in the areas of nuclear data evaluations, benchmarking and validation, nuclear model improvements, and uncertainty assessments.

2. European NDD programme for fusion

The development of nuclear data for fusion technology in Europe is organized by Fusion for Energy (F4E), the European Joint Undertaking for ITER and the Development of Fusion Energy, Barcelona, Spain.

A dedicated NDD programme is conducted which aims at providing a well-qualified nuclear database and validated computational tools for neutronics and activation calculations as required for the design, licensing and operation of the key facilities ITER, ENS and DEMO. The programme is executed by a Consortium on Nuclear Data Development and Analysis which combines available European expertise on nuclear data evaluation, processing, validation and benchmarking.

The Consortium consists of the research institutions KIT (Karlsruhe, Germany), CCFE (Culham, UK), NRG (Petten, The Netherlands), JSI (Ljubljana, Slovenia), TUW (Vienna, Austria), CIEMAT with UPM and UNED (Madrid, Spain) and IFIN-HH (Bucharest, Romania). The Consortium provides the requested services on nuclear data evaluations relevant to the various fusion applications

[a] e-mail: ulrich.fischer@kit.edu

including nuclear data for neutron, proton and deuteron induced reactions, the generation of associated co-variance data for uncertainty assessments, the development of advanced nuclear models and codes, the processing and benchmarking of the evaluated data against integral experiments, as well as the development of suitable software tools for sensitivity and uncertainty analyses of fusion systems.

According to the actual priorities of the ITER project, ENS and DEMO needs, dedicated NDD work programmes are specified in close agreement of F4E and the Consortium. The requested activities are then conducted by the Consortium through specific grants awarded by F4E. These activities are complemented with a parallel scheme on nuclear data experiments and measuring techniques conducted by another consortium.

3. Recent NDD programme – tasks and achievements

The recent European NDD work programme for fusion extended over a two year period from mid 2014 to mid 2016. It included various activities on the evaluation of nuclear data, the production of data files and libraries, the improvement and development of nuclear models and simulation tools, as well as related verification and validation analyses. Major achievements are detailed in the following sections.

3.1. Evaluation of neutron cross-section data for general purpose applications up to 200 MeV

The activities in this field encompassed general purpose data evaluations on ^{16}O, ^{54,56,57,58}Fe, and ^{90,91,92,94,96}Zr including associated co-variance data, the generation of ENDF data files with checking and processing, and final validation analyses. Fe, O and Zr are important elements for fusion reactor applications. Iron is the most important constituting element of structural and shielding materials. Oxygen is a constituent of water used for shielding purposes and as coolant, and is also a constituent of breeder ceramics and insulating materials. Zirconium is an alloying element of the heat sink material CuCrZr and also a constituent of some breeder materials.

The evaluation work was performed by TUW on ^{16}O [3], JSI on the Fe isotopes [4], and KIT on the Zr isotopes [5]. Each research institution utilized its own specific approach for performing the nuclear model calculations, evaluating the data, and generating the co-variance data. JSI relies on the EMPIRE code [6] for the nuclear model calculations while KIT and TUW utilize the TALYS code [7]. The resulting cross-section data, based to a large extent on model parameters adjusted to experimental data, serve as input ("prior") to the various Bayesan approaches for updating the evaluation and generating the co-variances. With JSI's approach, model uncertainties are treated through tuning parameters within EMPIRE which are defined with uncertainties and implied correlations. The co-variances of the cross sections are produced using the Monte Carlo technique of random sampling of model parameters fed as "prior" into the GANDR system [8], and constrained with experimental data via the generalised least-squares method. KIT employs the Universal Monte Carlo (UMC) approach [9] to generate

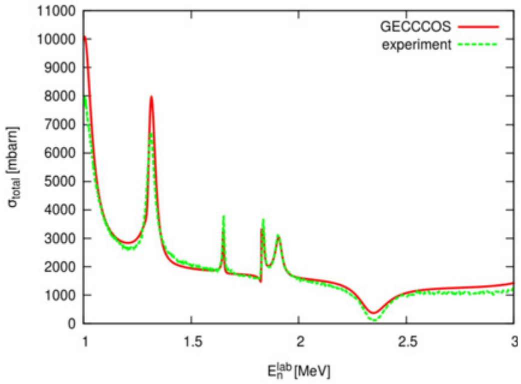

Figure 1. Total cross-section of n + O-16: GECCCOS R-matrix calculation vs. experimental data.

covariance data taking into account both nuclear model and experimental uncertainties as implemented in KIT's BEKED code system [10]. TUW utilizes the Full Bayesian Evaluation Technique (FBET) [11] implemented in the GENEUS system [12] to provide evaluated cross-sections with associated uncertainty information. Model parameter uncertainties are accounted for as well as model deficiencies.

The focus of TUW's recent work was actually on the development of a consistent evaluation procedure for neutron-induced reaction data of light nuclei. An adapted R-matrix approach was developed, based on a coupled-channel model with background potentials [13]. This allows a continuous matching of the reaction data with statistical model calculations as provided e.g. by TALYS. Thus a smooth transition from the R-matrix regime to the statistical model regime can be achieved. A generalized R-matrix code has been developed and integrated as module in the general reaction code system GECCCOS [14]. Several verification tests were performed showing perfect agreement with results of the FRESCO code [15] for elastic and inelastic reactions.

The ability to describe the resonance region with a smooth transition to pure potential models was demonstrated for the total, elastic and (n,α) cross-section of ^{16}O in the energy range 1–6.2 MeV. As an example, Fig. 1 shows the total cross-section in the energy range 1 to 3 MeV as predicted by the adapted R-matrix representation with a background potential.

A prototype ENDF data file was produced for ^{16}O comprising the R-matrix generated data in the energy range 1 to 3 MeV, data associated with the background potential between 3–6 MeV, and TALYS evaluated data above 6 MeV up to 200 MeV. The file is a complete ENDF data file ready for processing and applications tests in neutron transport calculations. TUW's work related to the modelling of ^{16}O reaction data and JSI's evaluation of ^{56}Fe cross-section data are also part of the international CIELO project [16].

In KIT's evaluation of the Zr cross-section data [5], an improved description of the pre-equilibrium emission of particles has been employed. It is based on a modified version of Blann's geometry depend hybrid (GHD) model, as implemented in an extended version of the TALYS code [17] (see Sect. 3.9). This is reflected in a better reproduction of the neutron emission spectra as shown in Fig. 2 for incident 14 MeV neutrons.

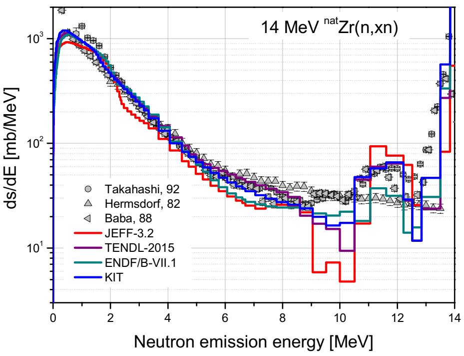

Figure 2. Neutron emission spectra for natural Zr at 14 MeV neutron incidence energy.

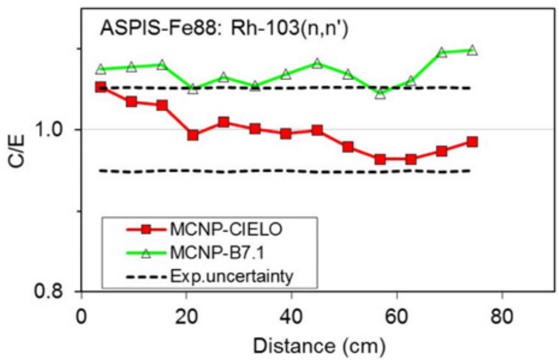

Figure 3. C/E ratios for the ^{103}Rh(n,n′) reaction rate measured in the “ASPIS IRON-88” experiment.

3.2. Benchmark analyses for specific shielding and tritium breeding calculations

With these activities the status of the available nuclear data evaluations was assessed with regard to their use in shielding and tritium breeding calculations.

Relevant iron shielding benchmarks from the recently updated SINBAD compilation [18] were utilized to check the Fe data evaluations. These included the “ASPIS IRON-88”, “JANUS phase I”, “ASPIS NESDIP 3”, and the “EURACOS Fe” experiments. The analyses revealed a general good performance of the new iron data evaluations (Sect. 3.1). As an example, Fig. 3 shows the C/E (calculation/experiment) ratios obtained for the ^{103}Rh(n,n′) reaction rate measurements in the “ASPIS IRON-88” experiment. (The red curve labelled “MCNP CIELO” stands for the recent Fe nuclide evaluations provided in the frame of the NDD programme for fusion technology, see Sect. 3.1).

The HCPB and HCLL benchmark experiments, performed previously at the Frascati Neutron Generator (FNG) [19] were re-analyzed with the state-of-the-art nuclear data libraries JEFF-3.2, FENDL-3.1b, and ENDF/B-VII.1 with focus on the tritium production. It was found that all three evaluations produce similar results. The tritium production in the HCPB mock-up is underestimated while it is well predicted in the HCLL mock-up for most measurement positions. Similar results were previously obtained with FENDL-2.1, the FENDL.3.1 pre-cursor library FENDL-3.0/SLIB4 and JEFF-3.1.1 [20]. The underestimation of the tritium production in the HCPB mock-up experiment is attributed

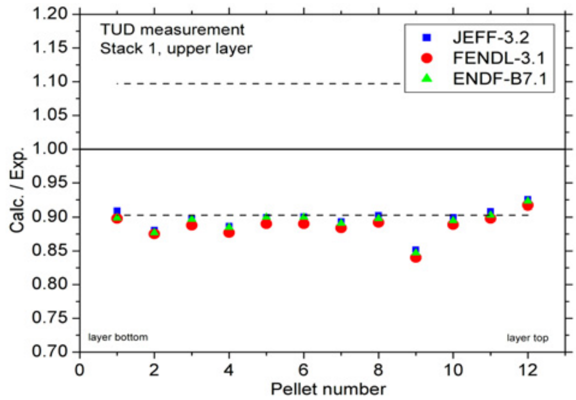

Figure 4. C/E comparison of the tritium produced in Li_2CO_3 pellets placed in a stack in the HCPB mock-up.

to the Be data which need to be checked again and possibly updated.

3.3. Sensitivity/uncertainty tools and application analyses

The issue of sensitivity/uncertainty (S/U) assessments, including related tool developments and application analyses, is also addressed within the NDD activities. The aim is to enable the identification of important reactions for relevant responses such as the tritium production, and quantify associated uncertainties on the basis of available co-variance data. In the framework of previous NDD activities, related development work has been conducted on the deterministic S/U code SUSD3D [21] by JSI, and on the MCNP based Monte Carlo sensitivity code MCSEN [22] by KIT with the Hebrew University of Jerusalem, including the adaptation of MCSEN to MCNP5.

Within the recent NDD activities, the coupling of SUSD3D with the 3D discrete ordinates / finite elements code ATTILA [23] was investigated. ATTILA offers advanced features such as the use of unstructured 3-D tetrahedral meshes and the possibility to import CAD geometry data through the translation to a mesh grid. On the basis of a simple one-group test case it was shown that coupling of ATTILA and SUSD3D is feasible although additional development effort is required to provide a fully tested general coupling scheme.

With the MCSEN code it is possible to use for the sensitivity calculations the same MCNP model as applied in design calculations. On this basis, uncertainty estimates can be obtained for a real fusion reactor configuration without approximation in the geometry representation. This capability was tested for a DEMO model developed within the PPPT programme [24].

The sensitivity and uncertainty of the TBR were calculated for the reactions on the major nuclides including ^{1}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{16}O, ^{28,29,30}Si, ^{54,56}Fe, ^{52}Cr, ^{58}Ni, and ^{182,183,184,186}W. The related covariance data were taken from JEFF-3.2 whenever available, from FENDL-2.1 for ^{7}Li, from EFF-3 for ^{9}Be and from JENDL-3.2 for ^{16}O. For comparison purposes, covariance data from the TENDL-2014 library were also used. The TBR was shown to be predominantly sensitive to the ^{16}O data, followed by ^{6,7}Li, ^{28}Si, ^{9}Be and ^{56}Fe. An overall uncertainty of ±3.2% was obtained for the TBR when using JEFF-3.2 covariance data with the mentioned additions. The uncertainty is

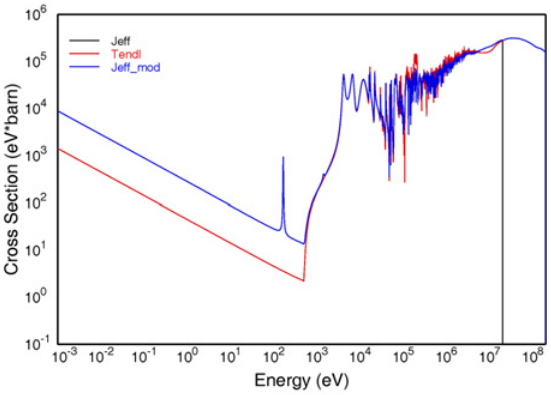

Figure 5. Displacement damage cross-section processed for ^{51}V.

dominated by the uncertainties coming from the ^{16}O, ^{6}Li and ^{7}Li cross-sections. When using TENDL-2014 covariance data, the uncertainty estimate increases to ca. ±10%.

3.4. DPA cross-section data library based on JEFF

To enable radiation damage calculations for a wide set of materials up to 200 MeV neutron energy, a complete dpa (displacement per atom) cross- data library was produced for 53 elements based on JEFF-3.2 data with suitable extensions using TENDL-2015 [25]. Missing cross sections and recoil spectra were added to the JEFF-3.2 data and unphysical data replaced. The library was processed into PENDF and ACE formatted files using NJOY [26] with the standard NRT model for the calculation of the number of lattice defects [27]. Multi-group damage energy cross sections have been also produced in the VITAMIN-J+ (211 groups) energy group structure. The dpa cross-section data library includes 16 nuclides with JEFF-3.2 data without modifications, 109 nuclides with JEFF-3.2 data below 20 MeV and TENDL-2015 above 20 MeV, 28 nuclides with fixed JEFF-3.2 data up to 150 MeV, and 18 nuclides with fixed JEFF-3.2 data below 20 MeV and TENDL-2015 data above 20 MeV. For ^{9}Be, a dedicated evaluation of the dpa and gas production cross-section has been performed [28]. Figure 5 shows the damage cross-section produced for ^{51}V on the basis of slightly fixed JEFF-3.2 data below 20 MeV and a smooth extrapolation to 200 MeV based on TENDL-2015.

3.5. Gas production cross-section data for Z = 12 to 83 nuclides

In addition to the displacement damage, the production of gases like hydrogen and helium strongly affects the behaviour of materials under irradiation. In particular this applies for the material irradiation with high energy neutrons in fusion devices and the IFMIF/ENS facility. To enable a reliable assessment of the gas production in these facilities, a systematic evaluation of gas production cross-sections was performed for nuclides ranging from Z=12 to 83. This evaluation is based on available experimental data, nuclear model calculations and systematics [29]. Figure 6 shows, as example, the helium gas production cross-section evaluated for Cr including the available experimental data. The curve labelled "after correction

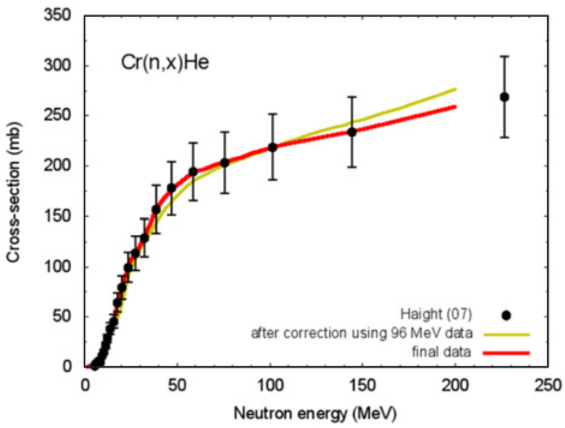

Figure 6. Evaluated and measured He production cross-sections for ^{nat}Cr.

using 96 MeV data" applies for the prior evaluation using mass dependent cross-section data obtained for a wide range of nuclei at 96 MeV on the basis of experimental data.

The evaluated gas production cross-sections are available as ENDF data files using the standard MT-numbers 203, 204, 205, 206, and 207 for proton-, deuteron-, triton-, ^{3}He-, and α-particle production cross-sections, respectively.

3.6. Improved TENDL activation cross-sections

The EAF (European Activation File) series of activation data libraries for fusion applications was terminated with EAF-2010 [30]. The strategy in the European Fusion Programme is to adopt in future TENDL as reference data library for activation calculations. Significant efforts were thus undertaken to ensure that TENDL can actually preserve or increase the quality of EAF-2010 by including the variety of validated cross-sections and improving deficient data. Validation analyses performed by CCFE on a large set of integral experiments showed that TENDL-2014 actually is outperforming EAF-2010 as data library for fusion relevant activation calculations [31].

To further increase TENDL's quality as an activation data library, a priority list of relevant reactions was elaborated for which discrepant or deficient cross-sections were found, either with regard to differential or integral experimental data, or unphysical characteristics. The list was prioritised with regard to the importance of reactions for fusion applications including, in particular, the activation of concrete in ITER and the IFMIF facility. The related analyses on the ITER bio-shield showed that TENDL-2014 produces consistently higher activity and dose rate values than EAF-2010. Some discrepancies were also found for the concrete irradiation in IFMIF. The final list of reactions to be improved encompassed 97 reactions. All of these cross-sections were updated on the basis of nuclear model calculations with the TALYS-1.8 code and recent experimental data whenever available.

Figure 7 shows the example of the ^{16}O(n,p)^{16}N activation cross-section which in the high energy range above 20 MeV had to be reduced as compared to TENDL-2015 (The curve labelled "TALYS" refers to the updated cross-section).

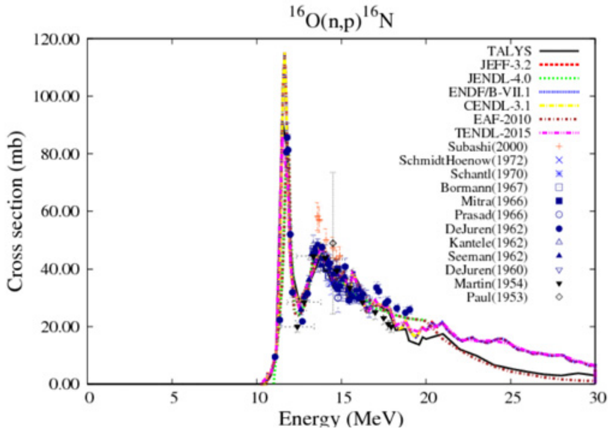

Figure 7. Evaluated and measured cross-sections for $^{16}O(n,p)^{16}N$.

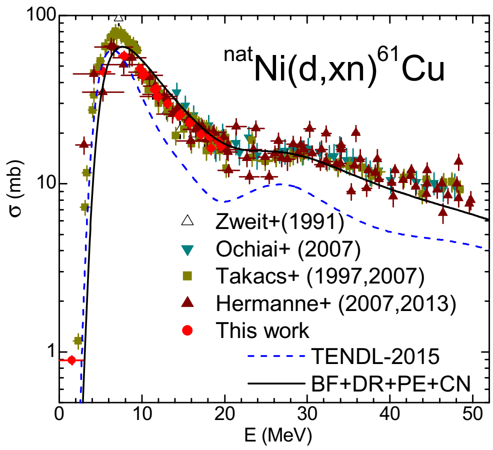

Figure 8. Measured and evaluated $^{nat}Ni(d,xn)^{61}Cu$ cross-sections taking into account BF (burn-up fusion), DR (direct reactions), PE (pre-equilibrium) and CN (compound nucleus) contributions [32].

Validation analyses performed on available integral measurements revealed a good performance of the improved cross-sections with C/E values around 1.0 for 40 of the considered reactions.

The updated cross-sections will be integrated into TENDL-2017 which will then be adopted as reference data library for activation calculations in the European Fusion Programme and thus supersede EAF-2010.

3.7. Deuteron induced activation cross-sections

High quality cross-section data of deuteron induced reactions are required to assess the generation of activation products and secondary neutrons in the accelerator facility of IFMIF/ENS. The recent evaluation effort in this field was on the deuteron cross-sections of the stable Ni isotopes $^{58,60-62,64}$Ni to up to 60 MeV. In the evaluation, contributions of all involved reaction mechanisms were taken into account including break-up, stripping, pick-up, pre-equilibrium and evaporation processes [32]. The comparison to TENDL-2015 and experimental data (Fig. 8) demonstrates the improvement obtained with this approach.

3.8. Improved α-particle optical model potential

The systematic analysis of the optical-model potential (OMP) for incident and emitted α-particles for target nuclei in the mass range 40 to 209 resulted in a superior OMP which was included as default option in the TALYS code and submitted to the IAEA for inclusion in the RIPL-3 data base. Global model calculations, performed with TALYS over a wide nuclei and energy range, showed that this OMP provides the highest accuracy for the cross-sections of α-induced reactions as well as for the emission of α-particles in neutron-induced reactions [33].

3.9. Improved modelling capabilities for TALYS

The improvements developed for the TALYS nuclear model code within the recent NDD programme refer to an improved description of the pre-equilibrium emission of particles and a new formalism for the deuteron break-up process.

A modified version of Blann's geometry depend hybrid (GDH) model, as coded in the ALICE/ASH code [34], was implemented as option in a local version of TALYS at KIT [35]. There are various projectile-energy-target combinations where a clear improvement for the emission spectrum is obtained. The implementation of the GDH option into an official TALYS release, following strict QA rules, is still pending.

The deficiencies found in the prediction of deuteron-induced cross sections with TALYS, in particular evident for the (d,p) and (d,n) break-up cross sections as included in TENDL, prompted to include in TALYS a new break-up model as developed by IFIN-HH [36]. A working version of TALYS has been modified for the inclusion of the basic mechanisms. The model needs to be further developed to avoid the dependence on pre-calculated external cross-sections such as TENDL data files. A new official TALYS version with the new deuteron break-up model built in is expected for the 2017 TALYS release.

3.10. MCUNED code extension for deuterons

MCUNED is an extension to the MCNPX Monte Carlo code including the capability to handle deuteron data libraries in the transport simulation with the production of secondary particles [37].

Within the recent NDD activities, MCUNED was further enhanced to represent in the deuteron transport simulation directly the deuteron break-up process based on the recent Kalbach formalism. This allows representing the angular distribution of the secondary particles emitted in the break-up reactions with analytical formula including two parameters which need to be stored on the evaluated ACE-type data files used by MCUNED. A new compliant TENDL data library has been produced for all stable isotopes. Test calculations performed with MCUNED for Al and Cu targets showed a significant improvement as compared to previous simulation results with a very good agreement to the measured emission spectra.

4. Conclusions and outlook

The strategic approach adopted in the EU for the development of nuclear data for fusion technology was outlined and the major recent achievements were presented. The related R&D activities have been conducted so far by the Consortium on Nuclear Data Development within a Partnership Agreement with F4E, Barcelona. The NDD activities will be transferred to EUROfusion and implemented in the PPPT programme to directly serve the nuclear data needs for neutronics analyses of DEMO and IFMIF/ENS.

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