The Role of Nuclear Data for Fusion Nuclear Technology

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The role of nuclear data for neutronic analyses of Fusion Technology (FT) facilities is presented in this paper. Nuclear data evaluations of high quality are required for transport simulations, uncertainty assessments, activation and radiation damage calculations affecting the design and performance of the FT facilities, as well as safety, licensing, waste management and decommissioning issues. A corresponding programme on the nuclear data development (NDD) and qualification is conducted within the Power Plant Physics and Technology (PPPT) programme of EUROfusion supporting the development of the DEMO fusion power plant and the IFMIF-DONES neutron source. The programme builds on the achievements of pre-ceding NDD activities within the European fusion programme as addressed in the paper. Further needs for design, shielding, activation and radiation dose calculations are discussed, and recommendations are given to further improve and qualify the nuclear data base for PPPT nuclear analyses. This includes dedicated experimental activities tailored to the needs of DEMO and IFMIF-DONES.

Keywords: Neutronics, nuclear data, DEMO, neutron source, activation, radiation damage

1. Introduction

Neutronics simulations play a fundamental role for the design and optimisation of Fusion Nuclear Technology (FNT) facilities, the evaluation and verification of their nuclear performance. Accurate data need to be provided to predict the tritium breeding capability, assess the shielding efficiency, estimate the nuclear power generated in the system, and produce activation and radiation damage data for the irradiated materials/components. Likewise this applies for the radiation dose fields to be provided after shut-down or during maintenance periods. The availability of high quality nuclear data is thus a pre-requisite for reliable design calculations affecting the nuclear design and performance of the facility, as well as safety, licensing, waste management and decommissioning issues.

Accordingly, a dedicated transversal activity on the development of nuclear data was implemented in the European Power Plant Physics and Technology (PPPT) programme of EUROfusion to address the needs of the integrated projects in designing, optimizing and evaluating the DEMO fusion power plant [1] and the IFMIF-DONES neutron source facility [2].

This paper details the new PPPT nuclear data development activities. The status of nuclear data is reviewed, needs for design, shielding, activation and radiation dose calculations are discussed, deficiencies are identified, and recommendations are given to further improve and qualify, also by means of dedicated experiments, the nuclear data base as needed for the PPPT programme.

2. Neutronics simulations for FNT facilities

Neutronics simulations form the basis for providing the nuclear responses which are needed for the engineering design and the performance evaluation of FNT facilities. Suitable computational approaches, tools and data need to be available to provide the required response data with sufficient accuracy. This includes a suitable method for the simulation of neutron transport in complex 3D geometries, high quality nuclear cross-section data to describe the nuclear interaction processes, and simulation models which replicate the real geometry

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without severe restrictions. Such requirements are satisfied with the Monte Carlo (MC) particle transport technique which can handle any complex geometry and employ the nuclear cross-section data without any severe approximations. Suitable radiation transport and activation coupling schemes are required for safety, maintenance and waste related analyses including the assessment of the activity inventories, and the calculation of shut-down dose radiation maps.

Key issues for faithful neutronics simulations are thus related to (i) the reliability of the employed MC particle transport code and its coupling to nuclide inventory calculations which need to be validated with fusion relevant benchmark experiments, (ii) the capability to describe in the simulation the real geometry of the facility with high fidelity and sufficient detail, and (iii) the quality of the nuclear cross-section data available for fusion applications which need to be checked against integral experiments.

All of these key issues are addressed in specific R&D activities of the PPPT programme with the objective to make available, on the medium and long term, the tools and data which are required to ensure a sufficient prediction capability of the neutronic simulations in design applications.

3.Nuclear data for fusion applications

Neutronics simulations need to describe the interactions of neutrons and atomic nuclei including the formation of (stable or radio-active) product nuclei and the emission of secondary particles such as neutrons and photons which are transported through the materials, and charged particles which are locally absorbed. The interactions are governed by quantum mechanical probabilities described by means of neutron cross-section data ("nuclear data") which depend on the nucleus species, the reaction type and on the neutron energy. The availability of high quality nuclear data is thus a pre-requisite for reliable design calculations.

Various kinds of nuclear data are needed for the different computational steps involved in neutronics analyses of a FNT facility. The neutron transport simulation is the first (and important) step providing the neutron flux distribution in space and energy. The transport simulation takes into account all nuclear interactions of the neutrons with the atomic nuclei including the slowing down process through elastic scattering and the emission of secondary neutrons via inelastic reactions such as (n, n'γ), (n, 2n), etc.. To this end the total nuclear cross-section and the neutron emission cross-section are required, in addition to the angular distributions of neutrons involved in two-particle reactions like elastic scattering (single-differential cross-section data, "SDX") and the energy-angle distributions of neutrons emitted in three-particle reactions like the (n,2n) process (double differential cross-section data, "DDX"). Such general purpose data need to be evaluated, based on nuclear model calculations and experimental cross-section data, and compiled in nuclear data files which can be used, after some preparatory processing, in neutron transport simulations with MC or deterministic codes. The general purpose data evaluations must be complete, i. e. include all data required for a transport simulation and cover the entire energy range of interest which extends for fusion applications from ca. 20 MeV down to thermal energies. Specific response data must be also provided with the data evaluation to enable the calculation of reaction rates such as the tritium and gas production, the nuclear heating, etc.. In addition, general purpose date evaluations must also include photon production cross-sections as function of the incident neutron energy with the related photon emission spectra. Such data are required for the inclusion of photons in the transport simulation, as required for nuclear heating calculations.

The data evaluations are compiled in nuclear data libraries using the international ENDF (Evaluated Nuclear Data File) data format [3]. For fusion applications, tailored to the needs of the ITER project, the Fusion Evaluated Data Library (FENDL) was developed under the auspices of the IAEA/NDS [4.]. The current version FENDL-3.1b [5] includes a set of sub-libraries and covers the neutron energy range up to 200 MeV. The OECD with the NEA Data Bank, Paris, is running the JEFF (Joint Evaluated Fusion and Fission File) project [6] addressing the needs of the European nuclear fusion and fission communities. Data evaluations performed within the European fusion programme are fed into JEFF which serves, among others, as reference data library for PPPT nuclear analyses.

Nuclide inventory calculations represent the second computational step of neutronics analyses providing the radioactive inventory of the facility components as function of the irradiation history and the decay time. Such knowledge is required for assessing the nuclear waste produced in operating the facility, and providing the radioactive sources for safety related analyses including the determination of radiation dose fields during maintenance and shut-down periods of the facility. For such calculations a large amount of activation cross-section data are needed comprising all elements and nuclides of a material/component. This includes, in particular, any impurity or tramp element which might be present in the non-irradiated material. Activation cross-sections represent excitation functions of the nuclides which must be given as function of the incident neutron energy. The activation cross-section data are compiled in special purpose data libraries such as the European Activation File (EAF) with the latest version EAF-2010 [7].

For the calculation of specific responses such as the neutron induced damage to materials, special purpose libraries are produced which include the displacement damage cross-sections, calculated on the basis of general purpose data evaluations and specific radiation damage models, as function of neutron energy. These data can be folded with the neutron flux spectra provided e. g. with a MC transport simulation to get the displacement damage rates in terms of dpa (displacements per atom).

For the nuclear analyses of the accelerator based IFMIF-DONES neutron source facility, deuteron induced reaction cross-section data are required for predicting the neutron generation, simulating – as far as required - deuteron transport in beam facing components of the accelerator, and assessing the radioactive sources produced as result of deuteron interactions with beam facing materials. Such data are provided, for example, with the TENDL data libraries [8] which are based, however, to a large extent on automated nuclear model calculations with the TALYS code [9] using default models and parameters. They need thus be complemented and updated with specific data evaluations to improve the quality for the nuclides of importance to IFMIF-DONES.

4. Nuclear data in the PPPT programme

The development of nuclear data for fusion technology in Europe has been previously organized by Fusion for Energy (F4E), Barcelona, through a framework partnership agreement with the Consortium on Nuclear Data Development (NDD) and Analysis [10]. The related activities addressed the nuclear data needs of the key facilities ITER, IFMIF and DEMO. The activities included the evaluation and validation of relevant nuclear cross-section data, the development/extension of codes and software tools required for nuclear model calculations and sensitivity/uncertainty assessments. The data evaluations performed within this activity are included in the JEFF data libraries maintained and disseminated by the NEA Data Bank, Paris [6]. Special data libraries were produced for activation, gas production and displacement damage calculations.

Starting in 2017, the European activities on the development of nuclear data for fusion were integrated into the PPPT programme. Accordingly, the activities focus on the needs of the PPPT neutronics supporting the development of the DEMO fusion power plant and the IFMIF-DONES neutron source through the various projects. In the following sub-sections, a brief overview of these activities is presented including a discussion of the achievements provided to PPPT as result of the preceding development work conducted within the F4E nuclear data gran activities.

4.1 General purpose nuclear data evaluations

The effort in this field focused lately on the evaluation of n + ^{63,65}Cu, $^{54, 56, 57, 58}$Fe, and $^{90, 91, 9294,96}$ Zr neutron cross-section data up to 200 MeV with the inclusion of co-variance data as required for uncertainty analyses. Cu is of high importance for fusion applications. It is used as heat sink material in plasma facing components and for microwave guide tubes and mirrors. Zr is an alloying element of the CuCrZr heat sink material and also a constituent of some breeder materials. Fe is the most important structural element employed in a fusion power reactor in large amounts in all kind of steels including e. g. Eurofer and SS-316. It plays an important role as parasitic neutron absorber in the breeder blanket and as useful neutron shield material. Evaluation work on the Fe nuclides was performed by JSI, Ljubljana, also embedded in the international evaluation activities of the CIELO project [11.]. The Cu and Zr nuclide evaluations were performed by KIT, Karlsruhe, [12] and are now included in the new JEFF-3.3 data library. The Cu evaluation passed several revisions in the high energy and the resonance range to better agree with the integral benchmark experiments relevant to fusion and fission, see section 4.2 below.

The evaluation of these general purpose data is based on an established methodology employing the nuclear model code TALYS [9] for the generation of the high energy neutron cross-section data, most relevant to fusion applications, and adopting resonance data, as needed for a full data evaluation in the lower energy range, from specific other evaluations. The experimental cross-section data available in the EXFOR data base [13] form the basis for checking the calculated cross-sections, adjusting the nuclear model parameters and thus improving the evaluations. As part of the evaluation process, nuclear models are also improved to better simulate, as far as possible, the involved nuclear interaction processes and provide a better agreement with experimental data. This applies e. g. for the modelling of pre-equilibrium emission processes with the geometry dependent hybrid (GDH) model [14.] or an extended break-up model for deuterons (see section 4.5). Fig. 1 shows, as an example, the neutron emission spectrum of Zr evaluated with a modified GDH model (curve labeled KIT).

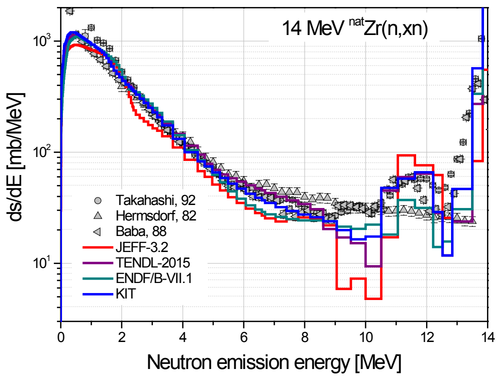

Fig. 1: Neutron emission spectrum for natural Zr at 14 MeV incident neutron energy.

The evaluation includes further the generation of co-variance data which are required for uncertainty analyses and complement the neutron cross-sections on the evaluated data file. Such data are produced, e. g., with KIT's BEKED system [15] which is based on the Unified Monte Carlo approach [16.] and takes into account both nuclear model and experimental uncertainties. This information is used to update the primary model calculation ("prior") with reduced uncertainties. Fig. 2 illustrates this process on the example of the ^{50}Cr(n,2n)^{49}Cr reaction showing the cross-sections with their uncertainties from the nuclear model calculation and after the application of experimental data through the UMC procedure.

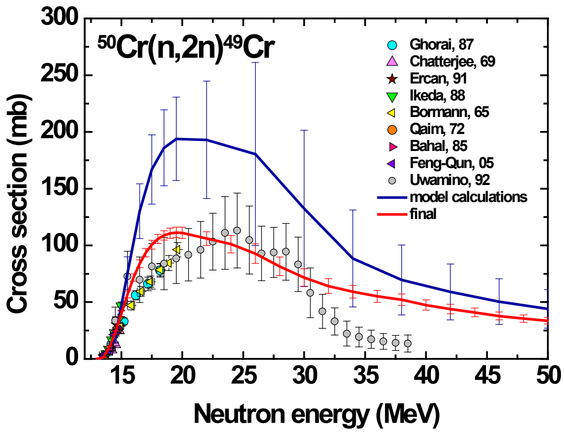

Fig. 2: Calculated (blue line) and evaluated (red line) cross-sections for the ^{50}Cr(n,2n)^{49}Cr reaction.

The evaluation of neutron cross-sections for light mass nuclides like ^{6,7}Li, ^{9}Be, ^{12}C, or ^{16}O (with a small number of nucleons), important to FNT applications, requires the use of models adapted to such few-nucleons systems, in general based on the phenomenological R-matrix approach [17]. For the n + ^{16}O reaction system, an adapted R-matrix approach, based on a coupled-channel model with background potentials, was recently developed by TUW, Vienna [18]. This approach is further developed within the PPPT nuclear data activities with the long-term goal to provide a methodology which can be applied to other low mass nuclei of interest to FNT, including e. g. ^{9}Be.

A major evaluation effort within the PPPT nuclear data activities is on the stable W nuclides starting with a new evaluation of the n + ^{184}W cross-section. Tungsten is of highest importance to FNT since it is used as armour material for the first wall and the divertor. Its shielding efficiency, in particular when combined with a neutron moderating material, is extraordinarily high, and thus may be used as efficient shield material in DEMO. W is also an essential alloying constituent of the Eurofer low activation steel. The current W evaluations in JEFF are considered obsolete and will be replaced by completely revised evaluations using the state-of-the-art evaluation methodology based on TALYS calculations with advanced nuclear models and the UMC procedure for the co-variance data generation.

4.2 Benchmarking

Benchmarking and validation are essential to check the quality of the evaluated nuclear data, identify potential deficiencies and shortcomings, and assess the performance for fusion applications, both in comparison to existing evaluations or model calculations, and experimental data. This is vital for the use of the data in design calculations or safety related analyses within PPPT. Previous important benchmark activities included integral experiments on mock-ups of the HCPB and HLL breeder blankets performed at the Frascati Neutron Generator [19], and, most recently, the benchmark experiment on a copper assembly [20] which prompted a revision of the ^{63,65}Cu general purpose data evaluation performed within previous F4E nuclear data grant activities. Fig. 3 shows a, as example, C (calculation)/E (experiment) ratios of the ^{27}Al(n, alpha)^{24}Na reaction rate measured at several positions in the Cu block by the activation foil technique.

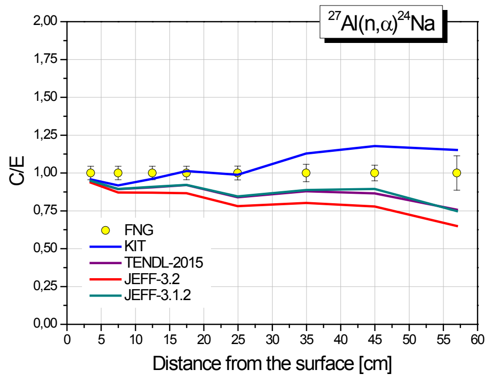

Fig. 3: C (calculation)/E (experiment) comparison of the^{27}Al(n, alpha)^{24}Na reaction rate in Cu block (the blue line labelled KIT denotes the revised ^{63,65}Cu evaluation).

The benchmark activities started within the new PPPT nuclear data programme are focusing in the first phase on the recent and running Fe and O data evaluations using available experimental data as provided e. g. with the SINBAD data base for 14 MeV neutron and shielding experiments [21]. Experimental benchmark activities are planned for inclusion in the PPPT programme after the completion of the running experimental activities supported by F4E. The focus will be on benchmark shielding experiments for DEMO, and on measurements of radio-nuclides and gas productions in the high energy range relevant to IFMIF-DONES.

4.3 Displacement damage and gas production data

The assessment of neutron induced radiation damages in fusion reactor materials builds on displacement cross-section data, in general based on the simple NRT damage model for the calculation of the number of lattice defects [22]. To enable damage calculations for a wide set of materials, a complete dpa cross-data library was produced within the previous NDD activities supported by F4E. The library contains dpa cross-sections for 53 elements up to 200 MeV neutron energy based on JEFF-3.2 data with suitable extensions using TENDL-2015 [8]. The library is available from the NEA data bank as special purpose sub-library of JEFF-3.2. Both ACE formatted files for use with MCNP and multi-group damage energy cross sections in the VITAMIN-J+ (211 groups) energy group structure are available. Fig. 3 shows the damage cross-section produced for ^{56}Fe on the basis of JEFF-3.2 data below 20 MeV and a smooth extrapolation to 200 MeV based on TENDL-2015.

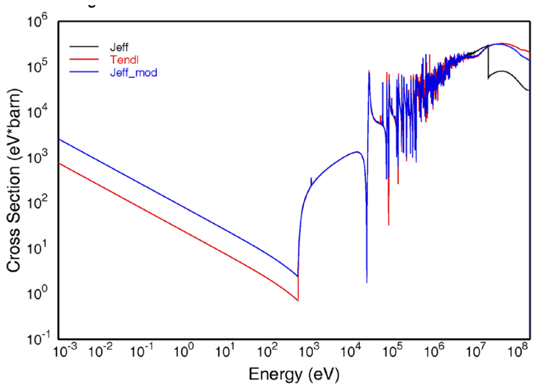

Fig. 3: Displacement damage cross-section of n + ^{56}Fe (Jeff_mod denotes the data included in the dpa library).

For the main structural materials in DEMO, Eurofer and SS-316 steel, dedicated displacement damage cross-section data were evaluated using advanced modelling approaches based on Binary Collison (BC) and Molecular Dynamics (MD) simulation results for the calculation of the number of lattice defects. The resulting dpa cross-sections are significantly lower as compared to the standard NRT damage model approach. Related cross-section data files were prepared for the two steels and made available to the international community through the IAEA, Vienna. They are used as reference data for the calculation of displacement damages to steel components in the PPPT programme.

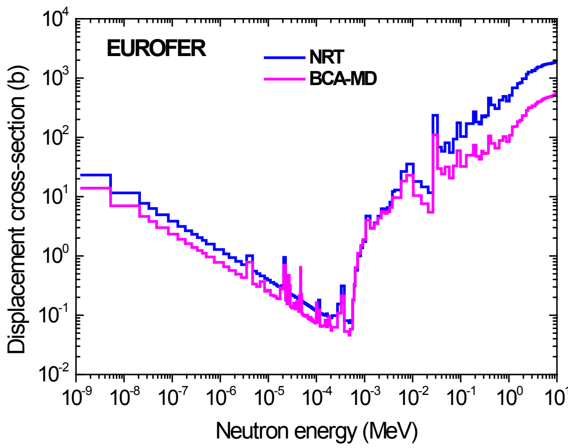

Fig. 4: Displacement damage cross-section evaluated for Eurofer steel with BCA-MD and NRT damage models.

The efforts to improve the data base and modelling capabilities for radiation damage calculations is continued within the PPPT programme with the extension of the NRT model to the athermal recombination corrected (arc) dpa formalism [23]. Arc-dpa take into account lattice defects surviving thermal annealing and thus enable the estimation of the actual damage production in irradiated materials. Formally, the arc-dpa concept is a modification of the NRT formalism with additional parameters to describe the defect generation efficiency. These parameters can be derived from available experimental data, molecular dynamics simulation results and systematic inter- and extrapolations. This feature enabled to generate a large set of arc-dpa cross-section data for the elements from Li to U utilizing neutron cross-section data from JEFF-3.3, ENDF/B-VIII, JENDL-4 and TENDL-2015 [24] which complement the previous JEFF-3.2 damage data library. Fig. 5 shows such dpa cross cross-section for tungsten.

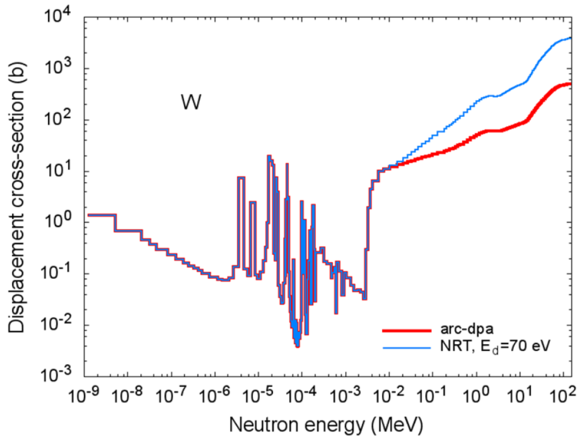

Fig. 5: Displacement damage cross-section of tungsten calculated with arc-dpa and NRT damage models and evaluated ENDF/B-VIII cross-section data[24].

4.4 Activation cross-section data

Activation cross-section data are of highest importance to FNT applications since they form the basis for the calculation of the radioactivity inventories generated in the components/materials of the facility upon irradiation. The quality of activation cross-section data directly determines the accuracy of the predicted radiation sources and thus affects safety and licensing issues, decommissioning and waste management.

A major evaluation effort is therefore conducted on the production of a qualified activation data library for fusion inventory calculations. This has led to the various versions of the European Activation File with the latest version EAF-2010 [7] including 816 different targets nuclides from ^{1}H to ^{257}Fm with 66,256 excitation functions up to the neutron energy of 60 MeV, thus covering the needs of the IFMIF neutron source facility.

The EAF series of activation data libraries for fusion applications was terminated with EAF-2010. The strategy in the PPPT programme is to adopt the TENDL data library [8] as source data library for activation cross-sections. Significant efforts were thus undertaken in the preceding work 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 on a large set of integral experiments actually showed that TENDL-2014 is outperforming EAF-2010 as data library for fusion relevant activation calculations [25].

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 [26]. The list was prioritised with regard to the importance of reactions for fusion applications including IFMIF-DONES, resulting in a set of 97 reaction cross-sections to be improved. These cross-sections were updated on the basis of nuclear model calculations with TALYS and recent experimental data whenever available. Fig. 6 shows the example of the $^{16}O(n,p)^{16}N$ activation cross-section which in the high energy range above 20 MeV was reduced as compared to TENDL-2015.

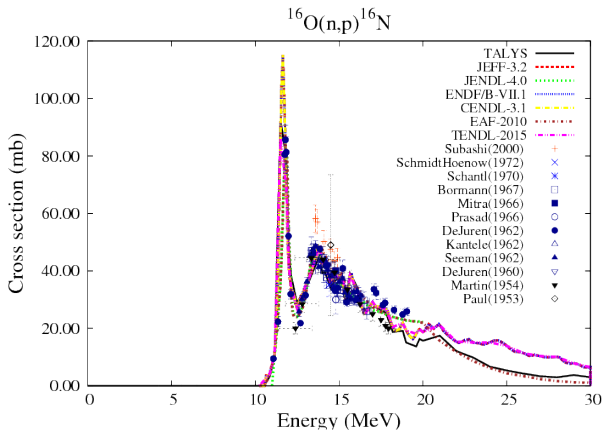

Fig.6: Evaluated and measured cross-sections for $^{16}O(n,p)^{16}N$.. (The curve labelled "TALYS" refers to the updated cross-section)

Within the new PPPT nuclear data activities, these improved activation cross-sections are integrated into the upcoming release of the TENDL-2017 data library. The integration is performed using the elaborated set of new TALYS parameters for the adjustments of the cross sections, after verification of the physics consistency for the competing channels. Verification and validation analyses are performed on the entire TENDL-2017 data library using the most extensive differential and integral experimental data bases and including resonance integrals, thermal cross-sections and astrophysical data. TENDL-2017, validated on such a basis for fusion inventory calculations, will then serve as basis for the generation of a dedicated activation data following the EAF format standards. This library will include all cross-section data improvements mentioned above and will serve further-on as reference activation data library in the PPPT programme of EUROfusion. It will be usable by any activation code compatible with the EAF data format and thus supersede EAF-2010 as activation data library for fusion applications.

4.5 Deuteron induced cross-section data

Deuteron induced cross-section data are required for nuclear analyses of the IFMIF-DONES neutron source facility which utilizes the interactions of deuterons, accelerated up to 40 MeV energy, and $^{6,7}Li$ nuclei in a liquid lithium target, to produce high energy neutrons (up to 55 MeV) at high intensity.

The neutron generation, which is described with the McDeLicious Monte Carlo code [27], employs evaluated d+ $^{6,7}Li$ cross-section data [28] which were extensively validated against thin and thick Lit target experiments. The MCUNED Monte Carlo code [29] is used for nuclear analyses of the accelerator facility. MCUNED can handle deuteron cross-section data in the transport simulation for any material, including, as latest enhancement, the capability to represent in the deuteron transport simulation directly the deuteron break-up process based on an analytical formalism proposed by Kalbach [30]. Two additional parameters need to be stored on the nuclear data files used by MCUNED. Based on available deuteron induced TENDL 2015 data, a dedicated library has been produced for all stable isotopes and successfully tested for Al and Cu targets [31].

Deuteron induced activation cross-sections are of high importance for safety, licensing and radiation protection of the IFMIF-DONES accelerator and target facilities. Such data are available with the TENDL library. They are, however, largely based on automated TALYS calculations with default models and parameters and in general do not show sufficient accuracy. There is also a significant lack of experimental data. An advanced modelling approach has been therefore elaborated within the previous NDD activities supported by F4E [32]. This approach enables a better prediction of deuteron induced reaction cross-sections. It takes into account contributions from all involved reaction mechanisms, including break-up, stripping, pick-up, pre-equilibrium and evaporation processes. The resulting improvement was demonstrated with the recent evaluations on the deuteron induced cross-sections of the stable Ni isotopes $^{58,60-62,64}Ni$, see Fig. 7 for the $^{nat}Ni(d,xn)^{61}Cu$ reaction.

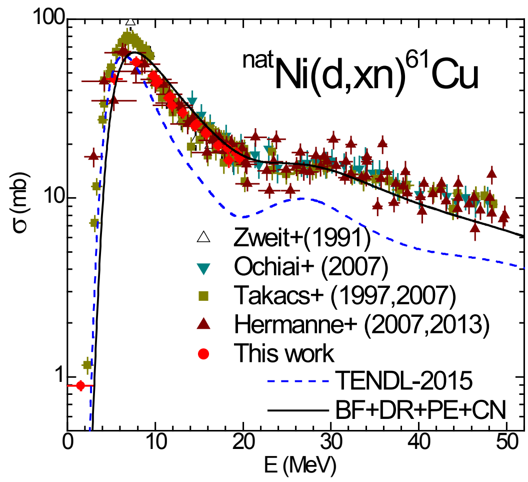

Fig. 7: Measured and evaluated $^{nat}Ni(d,xn)$ ^{61}Cu cross-sections taking into account BF (burn-up fusion), DR (direct reactions), PE (pre-equilibrium) and CN (compound nucleus) contributions [32].

Within the new PPPT nuclear data activities, the TENDL deuteron data library is going to be updated with such improved data evaluations on a larger scale.

5. Conclusions

The role of nuclear data for neutronic analyses of Fusion Technology (FT) facilities has been presented in this paper. Nuclear data evaluations of high quality are required for transport simulations, uncertainty assessments, activation and radiation damage calculations affecting the design and performance of the

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A corresponding programme on the nuclear data development (NDD) and qualification is thus conducted within the Power Plant Physics and Technology (PPPT) programme of EUROfusion supporting the development of the DEMO fusion power plant and the IFMIF-DONES neutron source. The programme builds on the achievements of pre-ceding NDD activities within the European fusion programme as addressed in the paper. Further needs for design, shielding, activation and radiation dose calculations were discussed, and recommendations were given to further improve and qualify the nuclear data base for the PPPT nuclear analyses. This includes dedicated experimental activities tailored to the needs of DEMO and IFMIF-DONES.

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