Progress in R&D Efforts on Neutronics and Nuclear Data for Fusion Technology Applications

U. Fischer 1), P. Batistoni 2), D. Große 1), A. Klix 1), A. Konobeev 1), D. Leichtle 1), R. L Perel 3), P. Pereslavtsev 1)

1) Association KIT-Euratom, Karlsruhe Institute of Technology, Institut für Neutronenphysik u. Reaktortechnik, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
2) Associazione ENEA-Euratom, ENEA Fusion Division, Via E. Fermi 27, I-00044 Frascati, Italy
3) Racah Institute of Physics, The Hebrew University of Jerusalem, 91904 Jerusalem, Israel

E-mail contact of the main author: ulrich.fischer@kit.edu

Abstract. An overview is presented on the progress achieved over the past two years in the European R&D programmes on neutronics and nuclear data for fusion technology applications. The focus is on the recent achievements in providing consistent high quality nuclear data evaluations including co-variance data, in developing advanced computational tools such as the McCad conversion software for the generation of Monte Carlo analysis models from CAD geometry data, and the MCsen code for efficient Monte Carlo based calculations of sensitivities/uncertainties of nuclear responses in arbitrary geometry. In the experimental field, major progress has been achieved with the conduction of a neutronic benchmark experiment on Pb-Li breeder blanket mock-up employing various techniques for the measurement of the tritium production.

1. Introduction

The nuclear design and operation of any kind of future fusion device relies in a sensitive way on the results provided by neutronics calculations. Validated computational tools and qualified nuclear data are required to ensure high prediction accuracies including reliable uncertainty assessments. Complementary to the application of established standard tools and nuclear data for design analyses, a dedicated neutronics R&D effort is therefore conducted in the EU to develop dedicated computational tools, generate high quality nuclear data and perform integral experiments for their validation.

This paper reports the related progress achieved over the past two years in the R&D programmes on neutronics and nuclear data for fusion technology applications. The focus is on the recent achievements in providing consistent high quality nuclear data evaluations including co-variance data, in developing advanced computational tools such as the McCad conversion software for the generation of Monte Carlo analysis models from CAD geometry data, and the MCsen code for efficient Monte Carlo based calculations of sensitivities/uncertainties of nuclear responses in arbitrary geometry, and in conducting neutronic benchmark experiments on breeder blanket mock-ups.

2. Nuclear data evaluations including co-variance data generation

With the European Fusion File (EFF) and the European Activation File (EAF) projects the EU is conducting a unique effort on the development of nuclear data libraries dedicated to fusion technology (FT) applications [1]. The EFF data evaluations are integrated into the Joint Evaluated Fission and Fusion File (JEFF) [2] which represents a complete data library of general purpose data evaluations satisfying both fission and fusion needs.

Recent efforts were devoted to the consistent evaluation of neutron cross-section data for general purpose applications of $^{50, 52, 53, 54}$Cr up to 200 MeV neutron energy [3]. The evaluations are based on nuclear model calculations, experimental cross-section data and uncertainty information. The nuclear model calculations were performed with an ad-hoc improved version of the TALYS code [4] employing the GDH (geometry dependent hybrid) model for the pre-equilibrium particle emission [5]. The implementation of the GDH model permitted more accurate evaluations of the emission spectra of deuterons, tritons, He-3 and alphas emitted at the pre-equilibrium stage of the nuclear reactions. Fig. 1 illustrates such improvement on the example of example of α- emission spectra for ^{50}Cr.

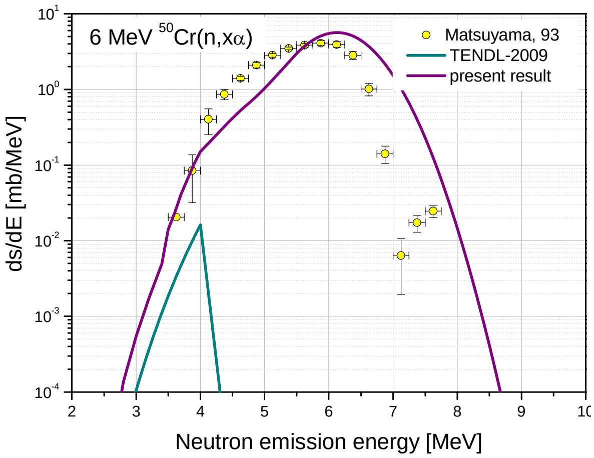

FIG. 1a : 6 MeV incident α– particle energy

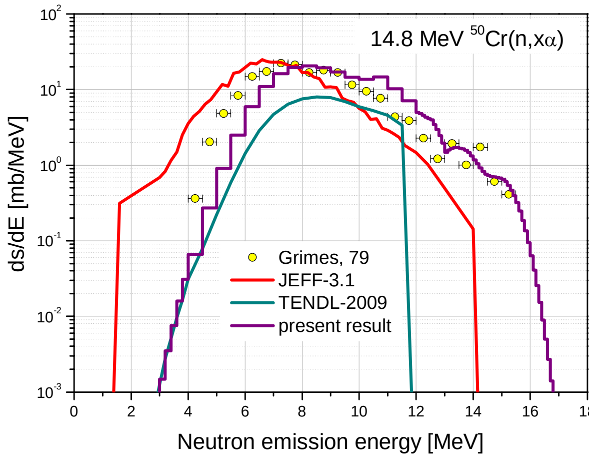

FIG. 1b: 14.8 MeV incident α– particle energy

FIG . 1 a,b: Evaluated and measured α- emission spectra for n + ^{50}Cr.

The calculation of covariances is based on the Unified Monte Carlo (UMC) method [6] and takes into account both experimental uncertainty information and nuclear model uncertainties [7]. Within this approach, the cross-section data are updated in a consistent manner and fed back to the evaluation.

Figs.2 and 3 show examples of cross-sections and their uncertainties obtained from nuclear model calculations before fitting to experimental data and evaluated cross-sections and uncertainties obtained after the application of experimental data through the UMC procedure.

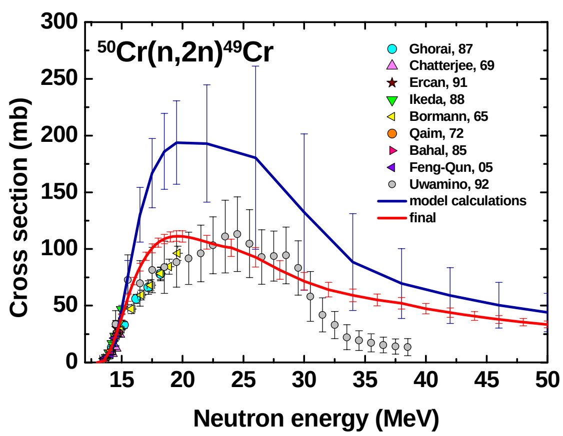

FIG. 2a : ^{50}Cr(n,2n)^{49}Cr

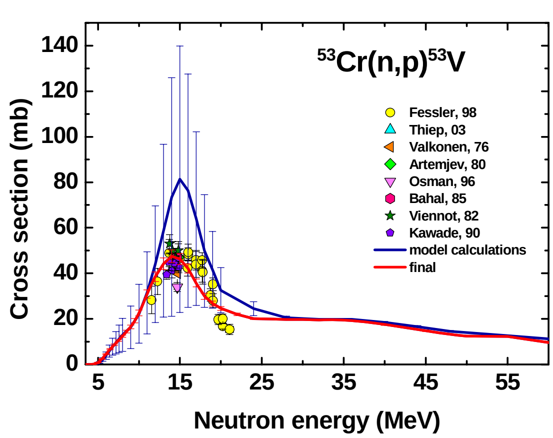

FIG. 2b: ^{53}Cr(n,p)^{53}V reaction

FIG . 2 a,b: Calculated (blue lines) and evaluated (red lines) n + Cr cross-sections.

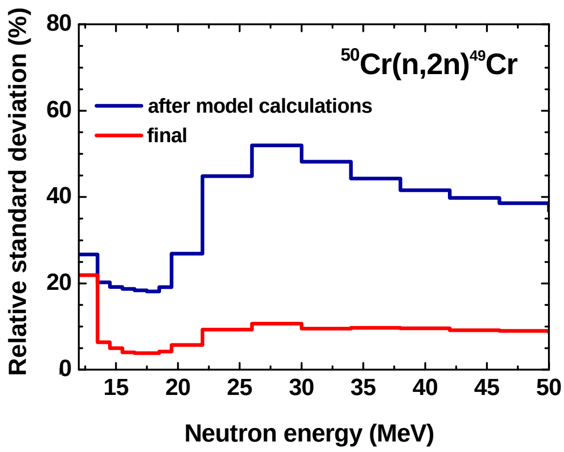

FIG. 3a : ^{50}Cr(n,2n)^{49}Cr

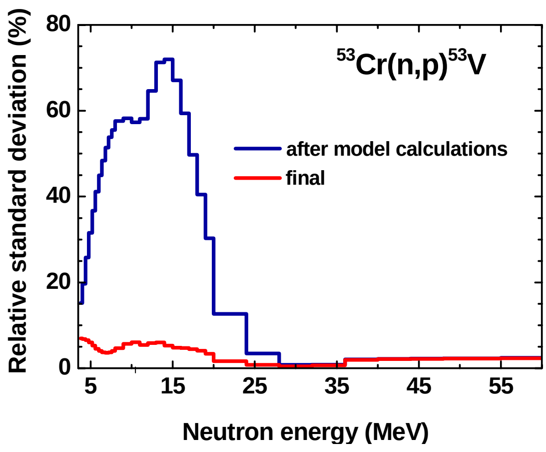

FIG. 2b: ^{53}Cr(n,p)^{53}V reaction

FIG . 3a,b: Evaluated cross-section uncertainties due to nuclear model uncertainties (blue lines) and uncertainties obtained after the evaluation taking into account experimental data (red lines)

3. McCad geometry conversion tool

The Monte Carlo method is the preferred computational technique for particle transport simulations in fusion technology applications. A major drawback of the method is related to the high human effort needed for developing complex 3D geometry models. A promising way to overcome this bottleneck is to make use of available CAD geometry data in the Monte Carlo calculations. This can be achieved by converting the CAD data into the geometry representation used in Monte Carlo simulations.

The McCad conversion tool [8] has been developed to enable the CAD geometry conversion for the Monte Carlo code MCNP [9]. McCad is entirely based on open software, in particular the use of the Open Cascade CAD kernel and the Qt4 libraries for the graphical user interface (GUI). It is realized in a framework like library based on object oriented design patterns. McCad is programmed in C++ and is implemented on the Linux platform. The GUI, displayed in Fig. 4, provides tools for visualization, data exchange and basic CAD modelling operations.

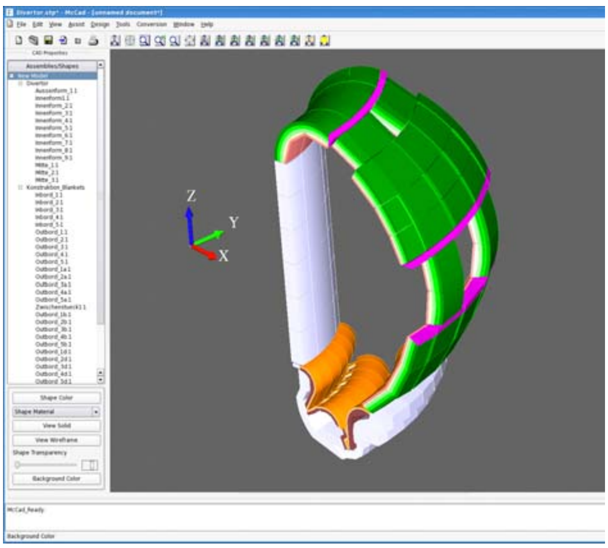

FIG 4a: GUI with ITER model in display window

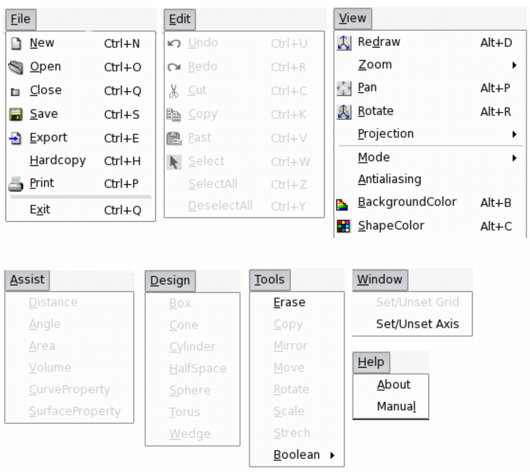

FIG. 4b: GUI components

FIG. 4 a, b: Graphical User Interface (GUI) of McCad conversion software

The CAD geometry data are imported via data files in the STEP, IGES or BREP format. Converted geometry models can be exported in the MCNP and the TRIPOLI [10] syntax. McCad is also capable of reading MCNP input decks and converting the data into CAD geometry in the STEP format. McCad currently integrates a simple material management system for MCNP that allows the assignment of material and density information not available in the free CAD formats. An advanced material management system based on a material library is under development.

As result of various benchmarks performed, McCad is considered sufficiently mature for practical design applications [11]. At KIT, McCad is routinely used for the generation of MCNP analysis models from engineering CAD models generated with CATIA V5. Recent applications include the model generation for the European DEMO reactor study [12], ITER components such as the Test Blanket Modules [13], the ECRH launcher [14], and the IFMIF neutron source facility [15]. As an example, Fig. 5 shows the CAD model of the European TBM system, developed for irradiation tests in ITER, and the corresponding MCMP model converted by employing McCad. The converted TBM model has been integrated into the horizontal test blanket port of the ITER Alite MCNP model for nuclear performance analyses.

The McCad conversion software has been conceived as open source project and is available upon request in a beta testing version under a dedicated GPL type licence agreement.

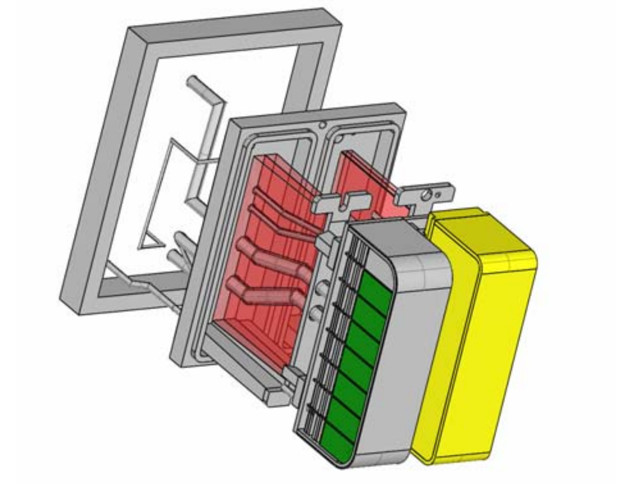

FIG 5a: CAD model of European TBM system developed for testing in ITER

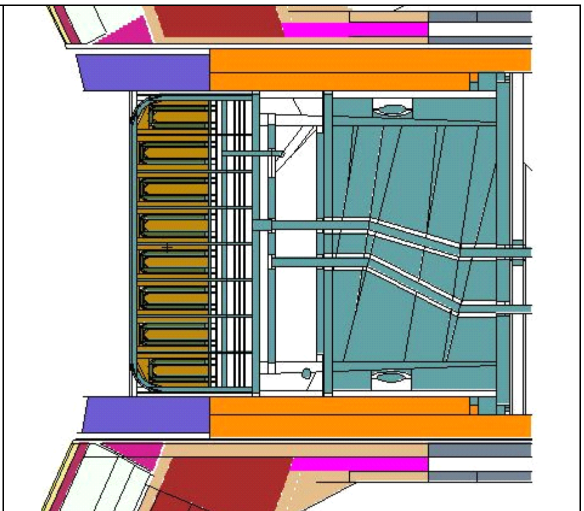

FIG. 5b: Converted MCNP model integrated in ITER test blanket port (2D cut by MCNP)

FIG. 5 a, b: Comparison of CAD and MCNP models converted by the McCad interface

4. MCsen Monte Carlo code for sensitivity/uncertainty calculations

The Monte Carlo based calculation of uncertainties is a powerful means to assess uncertainties of nuclear responses in arbitrary 3D geometry and track down these uncertainties to specific nuclides, reaction cross-sections and energy ranges. Suitable algorithms based on the differential operator method were previously developed and implemented into MCsen, a local extension to the MCNP Monte Carlo code, to enable the efficient calculation of sensitivities based on the track length estimator approach [16]. The MCsen code has been upgraded to enable the calculation of sensitivities to nuclear cross sections of nuclides contained in different materials in a complex 3D geometry. A release version of the MCsen code package has been recently prepared and submitted to the NEA Data Bank of the OECD for dissemination among member countries. This will allow the user to create an MCsen executable using a patch to the standard MCNP code package.

MCsen has been first applied to detailed sensitivity/uncertainty analyses of the HCPB neutronics mock-up experiment [17] and the HCPB TBM in ITER [18]. Recent MCsen applications include sensitivity/uncertainty analyses of the benchmark experiment on a neutronics mock-up of the Helium Cooled Lithium Lead (HCLL) Test Blanket Module (TBM) [19] as well as corresponding analyses on the HCLL TBM integrated into a dedicated Test Blanket port in ITER [20]. Fig. 6 shows cross-sections of the ITER model used for the MCsen sensitivity/uncertainty analyses. Note that both HCLL and HCPB TBMs have been integrated in the test blanket port.

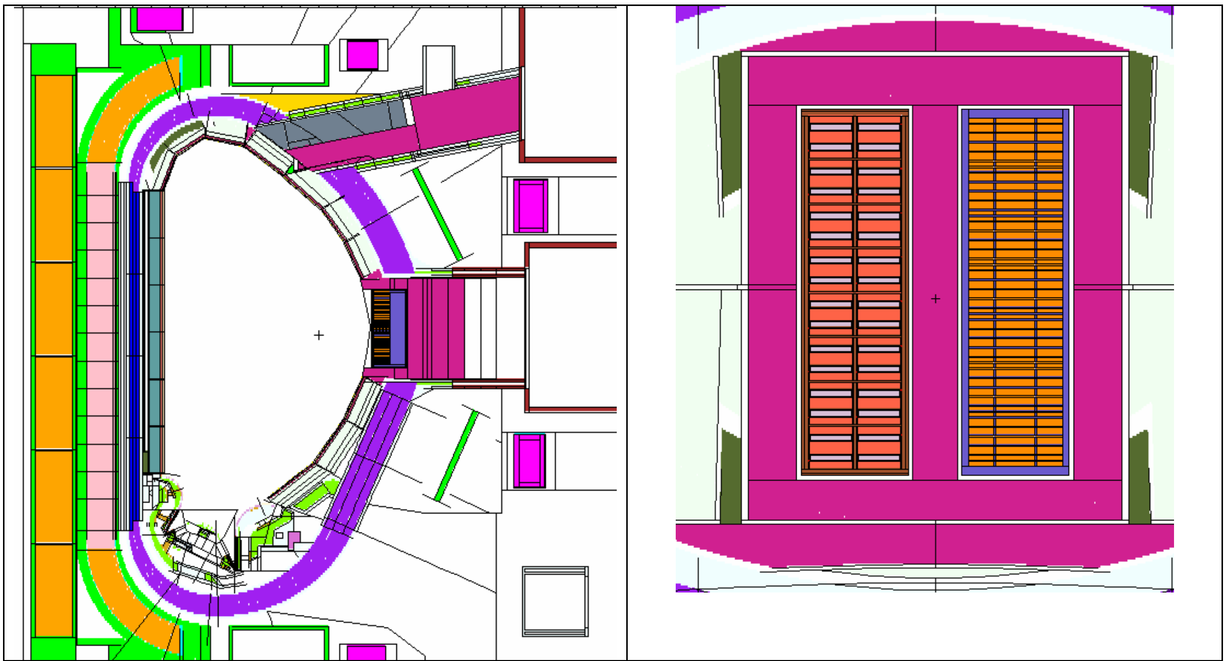

FIG 6a: Radial-poloidal cross-section	*FIG. 6b: Toroida-ploidal cut through blanket port with HCLL (right) and HCPB (left) TBM.*

FIG. 6 a, b: MCNP model of ITER used for the Monte Carlo sensitivity calculation with MCsen

Sensitivity profiles and integrated sensitivities were calculated for the total tritium production and the neutron flux densities in the HCLL TBM by using the track length estimator approach of MCsen. The associated uncertainties of the tritium production due to nuclear data uncertainties were assessed by making use of available co-variance data from different sources. The tritium production was shown to be most sensitive to Pb, Fe and Li^6. The associated nuclear data related uncertainties, however, are comparatively small. In general, they are below 2 % for most of the isotopes and individual contributions. The resulting computational uncertainty margin (1σ) of the tritium production rates in the HCLL TBM in ITER amounts to 2 % to 4 %, based on available covariance data and takin into account the statistical inaccuracy of the Monte Carlo calculation. The uncertainties assessed for the total neutron flux densities in the TBM are in the range of 2 % to 3 %.

5. Neutronics breeder blanket benchmark experiment

Testing and validation are essential in the process of assuring the quality of the computational tools and the nuclear data for design application calculations. This is achieved through integral benchmark experiments and their computational analyses. The recent European efforts were devoted to experiments on a neutronics mock-up of the HCLL TBM [21]. The related experiments were conducted at the Fascati Neutron Generator (FNG) [22, 23]and the neutron laboratory of the Technical University of Dresden (TUD) [24] including measurements of the tritium production applying different techniques, measurements of dedicated reaction rates using the activation foil technique, and measurements of fast neutron/ photon flux spectra and of time-of-arrival spectra of slow neutrons.

For the measurements of the tritium production using Li_2CO_3 pellets, both natural and enriched lithium samples were employed. This allowed to differentiate between the tritium producing reactions $^{6}Li(n, \alpha)$ t and $^{7}Li(n,n'\alpha)t$. Stacks of three pellets, the first two with natural lithium and the third one with 95at% enriched lithium, were placed at seven different depths in symmetric rows with respect to the mock-up axis. Independent measurements have been performed in a collaborative effort by ENEA, KIT/TUD and JAEA. The tritium activity measurements were carried out by ENEA and KIT/TUD employing the β-counting technique after dissolving the irradiated pellets in a solution with acids, distilled water and a liquid scintillator. Four pellets were analysed by JAEA in a third independent measurement.

The tritium production in the ^{6}Li enriched Li_2CO_3 pellets is well reproduced by the MCNP based calculations using both JEFF-3.1 and FENDL-2.1 nuclear cross-section data, see Fig. 7. As for the pellets with natural lithium, good agreement is found for the pellets in the front positions showing that both $^{6}Li(n,t)\alpha$ and $^{7}Li(n,n't)\alpha$ reaction channels are well predicted. The pellets placed adjacent to the lithium enriched pellets, however, suffered from a contamination of tritons produced in the enriched pellets close to the surface in contact with the natural pellets. This resulted in lower C/E values for the central pellets with natural lithium by about 6% on average.

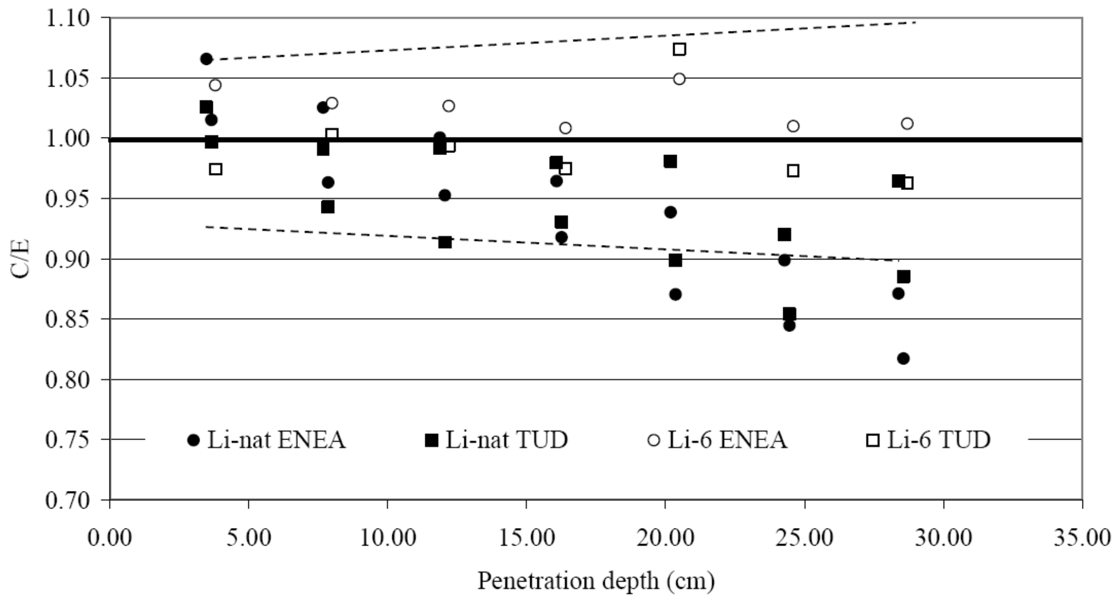

FIG. 7: Calculation/Experiment (C/E) comparison of the tritium production rate measurements using Li_2CO_3 pellets and the JEFF-3.1 nuclear cross-section data.

In addition to the tritium production measurements employing Li_2CO_3 pellets, two methods involving LiF TLD were used in independent measurements. In one case, the dose deposited by the charged particle emissions from the tritium breeding reaction was used to obtain the local tritium production. The other method utilized the thermoluminescence signal from the decay of tritium bred in the LiF TLD.

Fast neutron and γ-ray flux spectra were measured at the TUD neutron laboratory using a slightly modified mock-up assembly as compared to the tritium production rate measurements performed at FNG. The central channel, which accommodated the tritium detectors, was replaced by solid Pb-Li bricks. A dedicated channel with a square cross section of 5x5 cm^2 was prepared to accommodate the NE-213 detector and the ^3He proportional counter.

Fast neutron and γ-ray flux spectra were obtained by means of the cylindrical NE-213 scintillator with 3.25 cm diameter and thickness. The pulse height spectra obtained where unfolded with the MAXED code and response matrices experimentally obtained for this detector. Fig. 8 and b show the resulting experimental spectra in comparison with those calculated by MCNP using JEFF-3.1 nuclear cross-section data.

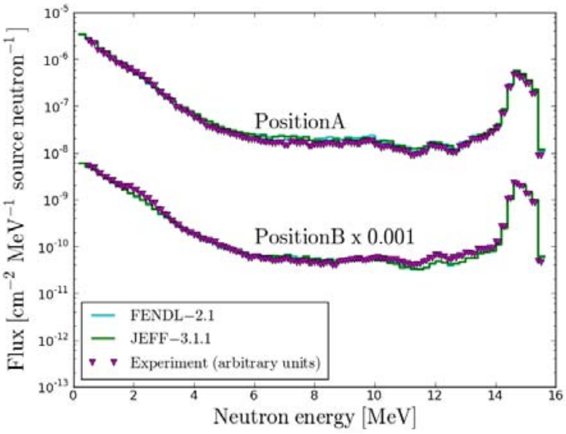

FIG. 8a: Fast neutron spectra

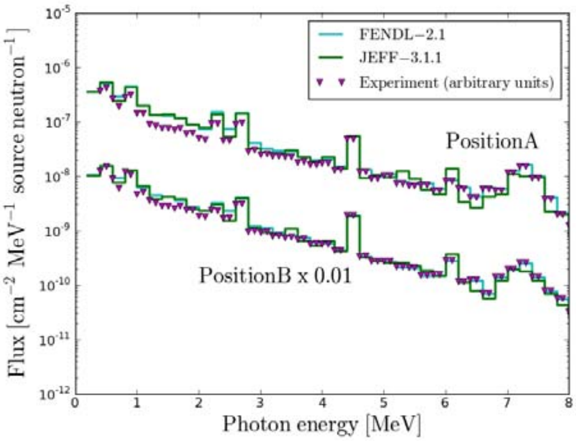

FIG. 8b: Photon spectra

FIG.8 a,b: Spectra measured with the NE-213 spectrometer in positions A and B of the HCLL TBM mock-up in comparison with spectra calculated with MCNP.

6. Conclusions

Significant progress was achieved over the past two years in the European R&D programme on neutronics and nuclear data by providing consistent high quality nuclear data evaluations including co-variance data, in developing advanced computational tools such as the McCad conversion software for the generation of Monte Carlo analysis models from CAD geometry data, and the MCsen code for efficient Monte Carlo based calculations of sensitivities/uncertainties of nuclear responses in arbitrary geometry. In the experimental field, a major progress was achieved with the conduction of a neutronic benchmark experiment on Pb-Li breeder blanket mock-up employing various techniques for the measurement of the tritium production. The good agreement obtained for the measurements and the MCNP based calculations confirmed the high reliability of neutronics design calculations for Pb-Li breeder blankets.

Acknowledgement

This work was partly supported by Fusion for Energy under the grant contract No. F4E-2008-GRT-14. The views and opinions expressed herein reflect only the author's views. Fusion for Energy is not liable for any use that may be made of the information contained therein.

References:

[1] FISCHER, U., et al, "The European effort on the evaluation and validation of nuclear data for Fusion Technology Applications", Int. Conf. Nuclear Data for Science and Technology, Jeju Island, Korea, April 26-30, 2010 (ND-2010)

[2] KONING, A., et al, "Status of the JEFF nuclear data library", ND-2010 conference.

[3] PERESLAVTSEV, P., et al, "Evaluation of n+Cr-52 cross section data up to 150 MeV neutron energy ", ND-2010 conference, Jeju Island, Korea, April 26-30, 2010.

[4] KONING, A., HILAIRE, S., DUIJVESTIHN, M.C., "TALYS-1.0", Int. Conf. Nuclear Data fot Science and Technology, Nice, France, April 22-27. 2007.

[5] KONOBEEV, A.., et al. "Implementation of the geometry dependent hybrid model in TALYS", ND-2010 conference, Jeju Island, Korea, April 26-30, 2010.

[6] SMITH, D.L., "A Unified Monte Carlo Approach to Fast Neutron Cross Section Data Evaluation," ANL/NDM-166, Argonne National Laboratory (2008).

[7] KONOBEEV, A.., et al, "Computational approach for the evaluation of nuclear data including covariance information", ND-2010 conference, Jeju Island, Korea, April 26-30, 2010.

[8] GROSSE, D., TSIGE-TAMIRAT, H., "Current Status of the CAD Interface Program for MC Particle Transport Codes McCad, Int. Conf. on Advances in Mathematics, Computational Methods, and Reactor Physics, Saratoga Springs, May 3-7, 2009.

[9] X-5 Monte Carlo Tean, "MCNP – A general Monte Carlo N-particle Transport Code, Version 5," LA-UR-03-1987, Los Alamos National Laboratory (April, 24, 2003).

[10] BOTH, J. P. et al, "User Manual for version 4.3 of the TRIPOLI-4 Monte Carlo method particle transport computer code", CEA-Report : CEA-R-6044, DTI, CEA/Saclay, France, 2003

[11] SERIKOV, A, et al, " Use of McCad for the generation of MCNP models in fusion neutronics", Int. Conf. Adv. in Math., Comp. Methods, and Reactor Phys., Saratoga Springs, May 3-7, 2009.

[12] FISCHER, U., et al, "Design optimisation and measuring techniques for the neutronics experiment on a HCLL-TBM mock-up", Fusion Engineering and Design 84 (2009) 323–32.

[13] FISCHER, U., et al, "Integral approach for neutronics analyses of the European test blanket modules in ITER", 26th Symp. Fusion Technology, Sept. 27 – October 1, 2010, Porto, Portugal.

[14] SERIKOV, A, et al, "Overview of recent nuclear analyses for the Upper ECH launcher in ITER", 9th Int. Symp. Fusion Nuclear Technology, October 11-16, 2010, Dalian, China.

[15] FISCHER, U., et al, "State-of-the-art of Computational Tools and Data for IFMIF Neutronics and Activation Analyses", 14th Int. Conf. Fus. Reactor Mat., Sapporo, Japan, September 7-12, 2009.

[16] PEREL, R. L:, WAGSCHAL, J. J., YEIVIN, Y., "Monte Carlo Calculation of Point-Detector Sensitivities to Material Parameters," Nucl. Sci. Eng. 124, 197-209 (1996).

[17] LEICHTLE, D., FISCHER, U., KODELI, I., PEREL, R. L. et al, "Sensitivity and Uncertainty Analyses of the HCPB Blanket Mock-up Experiment", Fus. Eng. Des. 82 (2007), 2406–2412.

[18] FISCHER, U., LEICHTLE, D., PEREL, R. L., "Monte Carlo based sensitivity and uncertainty analysis of the HCPB Test Blanket Module in ITER", Fus. Eng. Des. 83 (2008), 1222–1226.

[19] LEICHTLE, D., et al., "Sensitivity and Uncertainty Analyses of the HCLL Mock-up Experiment", 9th Int. Symp. Fusion Nuclear Technology, October 11-16, 2010, Dalian, China.

[20] LEICHTLE, D., et al., "Sensitivity and uncertainty analysis of nuclear responses in the EU HCLL TBM of ITER",26th Symp. Fusion Technology, Sept. 27 – October 1, 2010, Porto, Portugal.

[21] BATISTONI, P., et al., "Design optimisation and measuring techniques for the neutronics experiment on a HCLL mock-up", 25th Symp. Fus. Techn., Sept. 15-19, 2008, Rostock, Germany

[22] BATISTONI, P., et al., "Neutronics experiments on HCPB and HCLL TBM mock-ups in preparation of nuclear measurements in ITER",ISFNT-9, October 11-16, 2010, Dalian, China."

[23] BATISTONI, P., et al.," Neutronics experiment on a HCLL tritium breeder blanket mock-up", 26th Symp. Fusion Technology, Sept. 27 – October 1, 2010, Porto, Portugal.

[24] KLIX, A, et al, "Measurement and Analysis of Neutron and Gamma-ray Flux Spectra in a Neutronics Mock-up of the HCLL Test Blanket Module", ISFNT-9, Oct. 11-16, 2010, Dalian, China.