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Advanced Neutronics Simulation Tools and Data for Fusion Applications

U. Fischer[1], J-Ch. Jaboulay[2], A. Konobeev[1], D. Leichtle[1,2], L. Lu[1], E. Nunnenmann[1], P. Pereslavtsev[1], Y. Qiu[1]

[1]Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

[2]CEA-Saclay, DEN, DM2S, SERMA, LPEC, 91191 Gif-sur-Yvette, France

[3]Fusion for Energy (F4E), Josep Pla 2, Barcelona 08019, Spain

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

Abstract. This paper reports on development works conducted at the Karlsruhe Institute of Technology (KIT) in the field of computational tools and data for fusion neutronics applications. The related R&D activities are conducted in the frame of the Power Plant Physics and Technology (PPPT) programme of EUROfusion and specific grant agreements with F4E with the objective to make available the tools and data as required for a sufficient prediction capability of the neutronic simulations performed for fusion power reactors.

1. Introduction

Neutronics simulations play an important role for the design and optimisation of the nuclear components of a fusion reactor and the related performance analyses. Suitable computational approaches, tools and data need to be available to provide the required nuclear responses 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, eventually, a simulation model which replicates the real 3D geometry without severe restrictions. Such requirements are satisfied with the Monte Carlo (MC) particle transport technique which, on one hand, can easily handle any complex 3D geometry, and second, employ the nuclear cross-section data in the continuous energy representation without any severe approximation. The simulations will thus provide results which are limited only by the uncertainty of the nuclear cross-section data, the statistical uncertainty of the Monte Carlo calculation and the accuracy of the applied geometry model.

Key issues for reliable neutronics simulations of future power reactors are thus related to (i) the reliability of the employed MC particle transport code, (ii) the quality of the nuclear cross-section data evaluations for fusion applications, and (iii) the capability to describe in the simulation the real reactor geometry with high fidelity and sufficient detail. All of these key issues are addressed in R&D activities embedded in the European fusion 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.

The focus of this paper is on the computational tools developed for the high fidelity geometry representation in MC particle simulations and the provision of high quality nuclear cross-section data with uncertainty assessments. Related activities, conducted by KIT in the frame of the Power Plant Physics and Technology (PPPT) programme of EUROfusion and specific grant agreements with F4E, Barcelona, are presented including recent achievements and applications. Complementary activities conducted in these areas are also addressed.

2. Computational tools for fusion neutronics simulations

The MC particle transport technique is the most suitable method for fusion neutronics simulations since it is capable of handling complex 3D geometries like tokamaks or stellarators and employing the nuclear cross-section data in the continuous energy representation without any severe approximation. With the high performance computers available nowadays, it is even possible to provide high resolution 3D maps of nuclear responses with sufficient statistical accuracy throughout the entire geometry. MC codes suitable for fusion neutronics applications are briefly addressed in section 2.1

A key issue of faithful neutronics simulations is the capability to describe in the MC simulation the real reactor geometry with high fidelity and sufficient detail. This can be achieved with a modelling approach which ensures a true one-to-one translation of the CAD geometry, as produced for the engineering design of the reactor, into the MC geometry representation. Such an approach is enabled, among others, with the McCad conversion software tool [1,2] presented in section 2.2.

2.1 Monte Carlo codes for fusion neutronics applications

The Monte Carlo code MCNP with the current versions 5 and 6 [3, 4], developed by the Los Alamos National Laboratory (LANL), USA, is the standard code for fusion neutronics applications including nuclear analyses for ITER and DEMO within the PPPT programme. MCNP is very powerful in its capabilities, well validated and benchmarked, and most suitable for fusion applications. MCNP, however, is subject to US export control regulations and thus not freely available, in particular with regard to the source code which is required for adaptation to many applications. Several alternative MC codes have been considered for application to DEMO within the PPPT programme [5]. The TRIPOLI-4 code [6], developed by CEA Saclay, France, was selected as most promising candidate and was accepted as analysis code for PPPT neutronics. TRIPOLI-4 is a mature code, well advanced in its functionalities, successfully validated for fusion neutronics and benchmarked against MCNP for the application to DEMO [7,8]. It is thus required to provide interfaces for the TRPOLI-4 MC code which enable access to the CAD geometry data and the coupling to nuclide inventory calculations. The latter issue is addressed by CEA’s development work while the former one is provided by KIT through the McCad software development presented in section 2.2. Both activities are conducted within the PPPT programme of EUROfusion.

The open source MC codes SERPENT [9] and GEANT [10], both freely available, are also considered as long-term alternatives which still require substantial development and qualification effort for fusion neutronics applications including the adaptation to DEMO analysis needs. Related development work on these codes is not conducted within the EUROfusion programme. The McCad software, however, has been already extended to process CAD geometry data for use with GEANT, see section 2.2.

2.2 The CAD to MC geometry conversion tool McCad

The McCad conversion software has been developed at KIT to enable the automatic conversion of CAD models into the semi-algebraic geometry representation as utilized in MC particle transport simulations. McCad is entirely based on open-source software and libraries, which utilizes Open Cascade (OCC) as CAD kernel and the Qt4 and OpenGL libraries for the graphical user interface (GUI). CAD geometry data can be imported via neutral files (STEP/IGES), visualized with McCad's GUI, converted into Monte Carlo geometry representation and output in the syntax of the MC codes including MCNP and TRIPOLI.

The current development work on McCad is conducted within the PPPT programme of EUROfusion. The latest enhancements include improved algorithms for the decomposition of solids with the addition of splitting surfaces, a collision detecting technique based on mesh triangles, and an algorithm for the sorting of the splitting surfaces. These improvements were verified with several test models derived from the DEMO model and were shown to result in a more efficient conversion process with a better, less complex, geometry representation. Fig. 1 illustrates the decomposition process, as enabled with McCad's new decomposition algorithm, on the example of DEMO model components.

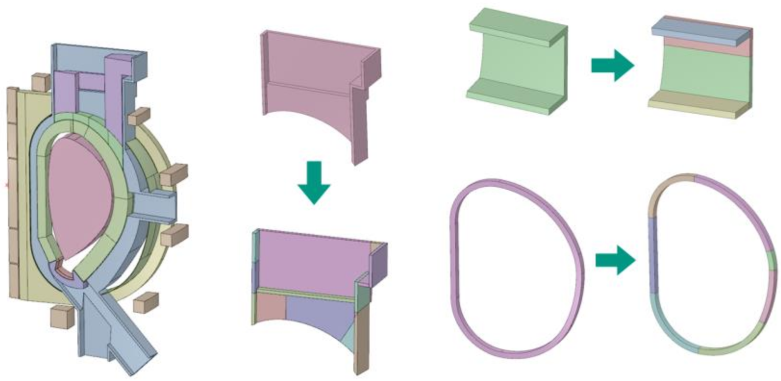

FIG. 1: Automated decomposition of DEMO model components with McCad's new decomposition algorithm

2.2.1 McCad interface for TRIPOLI-4

The McCad interface for TRIPOLI-4 has been developed only recently on the basis of the already existing conversion functionalities developed for MCNP. TRIPOLI utilizes a similar geometry description as MCNP, namely the constructive solid geometry (CSG) representation, though with different syntaxes. In MCNP, a combination of convex solids can be described directly with a variety of symbols while TRIPOLI defines each decomposed convex solid as virtual cell and then defines the combination geometry with these virtual cells. After the conversion of material solids, McCad creates void spaces. In TRIPOLI, those parts of material solids colliding with void boxes also have to be defined first as virtual cell, afterwards the void spaces are defined by combination of these virtual cells. Some new classes have been thus added to McCad for the TRIPOLI file generation.

Successful verification tests have been performed for the conversion of various DEMO models. These tests included, among others, detailed comparisons of MCNP and TRIPOLI models derived from the same underlying CAD model. Recent applications of McCad's TRIPOLI interface within the PPPT programme include the generation of a detailed TRIPOLI analysis model of DEMO as shown below in section 2.2.5.

2.2.2 McCad implementation on the SALOME simulation platform

The McCad software, originally developed under the Linux operation system, has been ported to the Windows platform. This has been achieved through its implementation on the SALOME simulation platform [11]. A new Graphical User Interface (GUI), as shown in Fig.2, was developed to this end on SALOME under Windows. The SALOME platform builds on the same graphic kernel as McCad and provides a convenient and flexible interactive graphic environment. To make McCad available on the SALOME platform, new conversion function modules including the decomposition, the void filling and the material editing have been integrated. The CAD to MC geometry conversion is thus enable just by calling the McCad conversion functions in SALOME. Fig. 2 shows a screenshot of the SALOME GUI for McCad with a torus sector model and the parameter setting window.

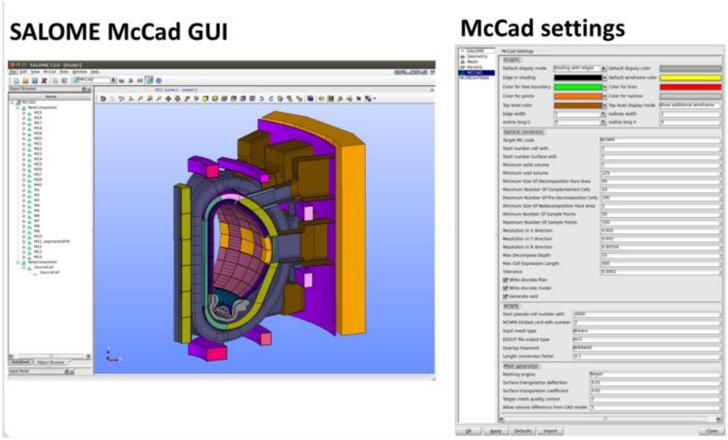

FIG. 2: McCad GUI on the SALOME simulation platform (left) and window with Mcad settings (right)

2.2.3 Advanced McCad features

As a further advanced feature, the support of the hybrid geometry modelling technique has been implemented in McCad. This technique enables to combine geometry models prepared in the standard CSG representation and models composed of tessellated solids or unstructured meshes. The converted hybrid models can be used only with MCNP6 since no other MC code has currently the capability to track particles on unstructured meshes. Fig. 3 shows an example of such a hybrid model developed for an HCPB blanket module.

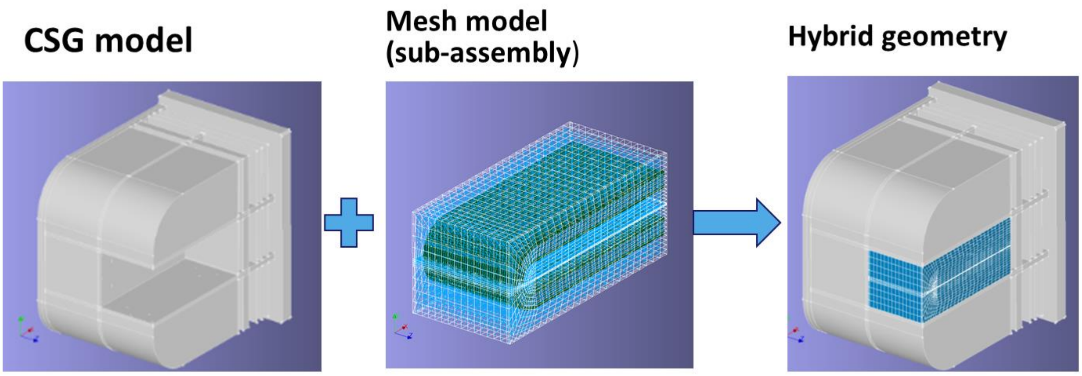

FIG. 3: Generation of hybrid geometry model for MCNP6 with McCad.

In addition, a dedicated hybrid CSG and tessellated solid interface has been developed for the Open Source MC code GEANT4. GEANT4 uses primitive CSG solids like boxes, spheres, and cylinder sections which cannot be directly provided by McCad. Hence a half-space based CSG solid approach was developed for GEANT4 to enable the CAD geometry conversion. The Geometry Description Markup Language (GDML) was extended to store this solid type, and the Geant4 GDML parser was enabled to process these solids. A GDML interface was developed for the SALOME version of McCad to export the converted CAD solids. Complex CAD solids which cannot be converted are tessellated into facets and exported to GDML as tessellated solids. Successful test verifications have been performed for simple geometry set-ups. Extensive testing is underway for a full 3D tokamak torus model based on the ITER benchmark.

2.2.4 McCad availability and multi-physics capabilities

McCad is conceived as open source software and is thus available to the internal scientific community without restrictions. The McCad code package, including the source code and pre-compiled binaries, is available on the GitHub software development platform, see https://github.com/inr-kit/McCad. Additional tools were developed, and also made available, which allow to process high resolution mesh tally data and visualize them on the CAD geometry on the SALOME platform. For coupled multi-physics analyses, involving e. g. CFD and FEM calculations, such data can be also exchanged with other codes, integrated as SALOME modules or linked via external interfaces [12,13].

2.2.5 McCad applications

McCad is predominantly used for generating the DEMO simulations models for the various nuclear analyses performed within PPPT. The general modelling approach is to generate first a generic CAD neutronics model from the CAD Configuration Management Model (CMM) of DEMO. This model includes the Toroidal Field Coil (TFC), vacuum vessel (VV), divertor, blanket segment box, vessel ports, and plasma chamber, represented in a single torus sector with envelopes. All components are thus described by their bounding surfaces (“envelopes”) without any internal structure specified. This model is converted to analysis models for the MC simulation codes with McCad and serves as basis for the adaptation to specific tasks.

Such specific tasks are, among others, design analyses for the development of different breeder blanket concepts for DEMO. Accordingly, specific models are derived from the generic DEMO model by integrating blanket modules of the different breeder blanket concepts. To this end the engineering CAD model of a single blanket module is processed and converted into an MC analysis model. It is then repeatedly filled into the empty blanket segment envelope of the generic DEMO model. Thus specific DEMO breeder blanket models are generated which are consistent with the DEMO baseline configuration and the specific engineering blanket design with the internal structures of the blanket modules. Figs. 3 and 4 illustrate this process on the example of DEMO variants with a Helium-Cooled Pebble Bed (HCPB) and a Helium-Cooled Lithium Lead (HCLL) breeder blanket, prepared for the MCNP and TRIPOLI 4 MC codes, respectively.

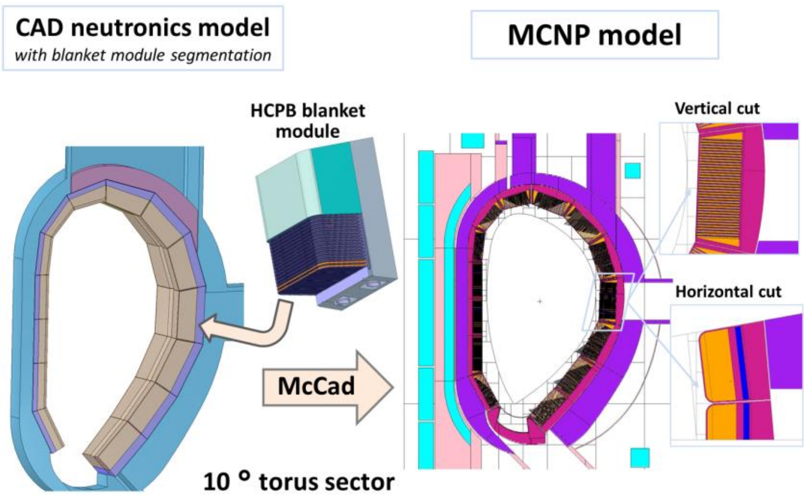

FIG. 4: Generation of an MCNP simulation model of DEMO with integrated HCPB blanket modules using the McCad conversion software.

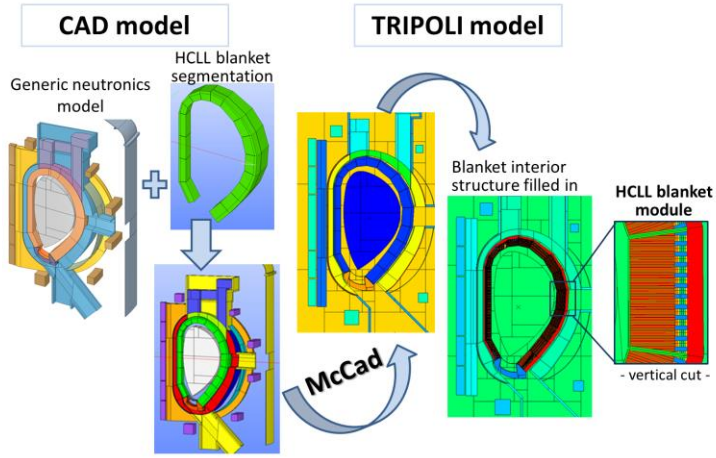

FIG. 5: Generation of a TRIPOLI-4 analysis model of DEMO with integrated HCLL blanket using McCad's windows version on the SALOME platform

3. Nuclear data for fusion applications

To satisfy the needs for high quality nuclear data, a dedicated programme on Nuclear Data Development (NDD) is conducted with the support of F4E. The related activities include the evaluation and validation of relevant nuclear cross-sections, the development/extension of codes and software tools which are required for nuclear model calculations and sensitivity/uncertainty assessments. After passing a thorough benchmarking and validation process, the cross-section data evaluations are eventually fed into the Joint Evaluated Fusion File (JEFF), maintained by the NEA Data Bank, Paris, France. Special data libraries are developed for activation/transmutation, gas production and displacement damage calculations.

3.1 Neutron cross-section data for general purpose calculations

Such cross-section data evaluation are required for transport calculations and thus include all reactions cross-sections as function of the neutron energy energy (up to 200 MeV) as well as secondary angle and energy distributions. KIT's recent evaluation efforts, conducted in the frame of the NDD programme with F4E, were on the neutron cross-sections of ^{63,65}Cu and ^{90,91,92,94,96}Zr. The evaluations are based on nuclear model calculations with the TALYS code [14] including an improved description of the pre-equilibrium emission of particles with a modified version of the geometry depend hybrid (GDH) model, as implemented in an extended version of TALYS. This results in a better reproduction of the neutron emission spectra as shown in Fig. 5 for Cu and Zr. This is essential for an accurate simulation of the neutron transport through materials such as the CuCrZr alloy used as heat sink material for divertors. The evaluated data are processed into a standard ENDF data file and tested against available benchmark experiments such as the one on a Cu performed at the Frascati Neutron Generator [15]. Good agreement is obtained for most the measured reaction rates as shown in Fig. 7.

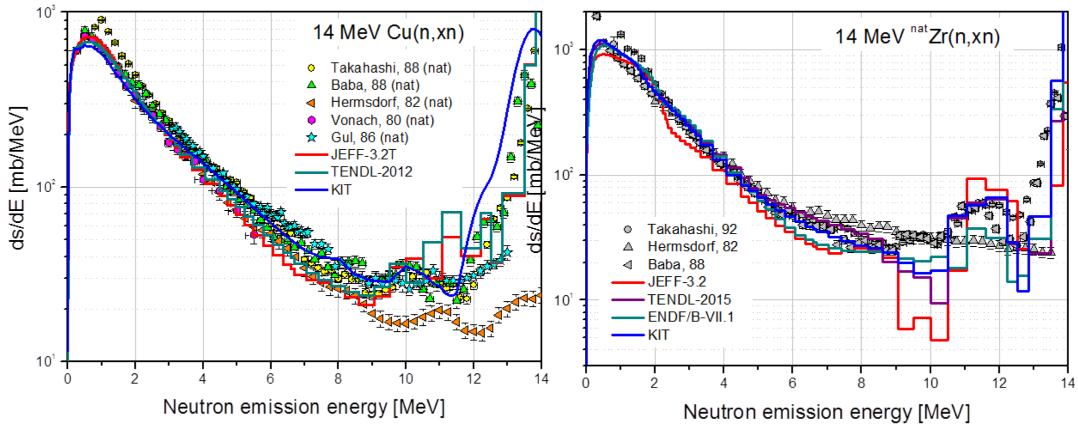

FIG. 6: Neutron emission spectra for natural Cu (left) and Zr (right) at 14 MeV neutron incidence energy.

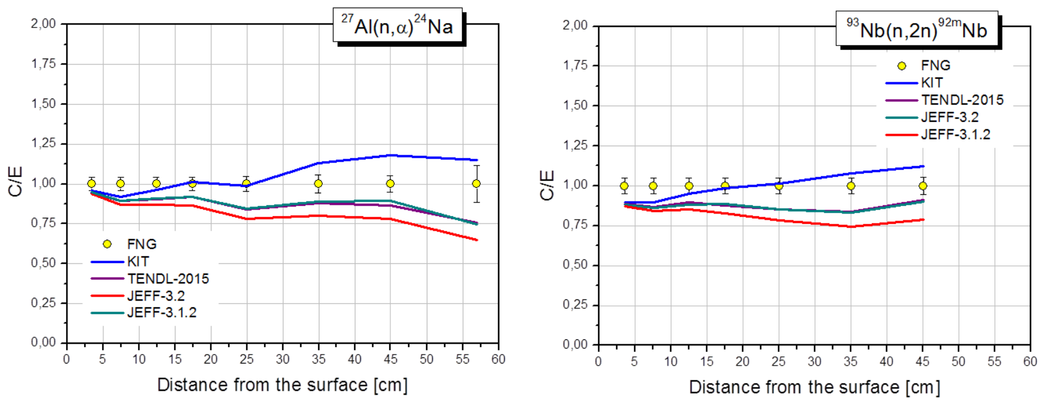

FIG. 7: C/E (calculation/experiment) ratios of the ^{27}Al(n,α)^{24}Na (left) and ^{93}Nb(n,2n)^{92m}Nb (right) reaction rates measured in the FNG copper benchmark [15].

3.2 Damage displacement and gas production data

Displacement damage cross-section data were evaluated for the Eurofer and SS-316 steels using advanced modelling approaches which take into account Binary Collison (BC) and Molecular Dynamics (MD) simulation results for the calculation of the number of lattice defects. This results in significantly lower dpa cross-sections as compared to the standard

NRT damage model approach, see Fig. 8 (left side). Related cross-section data files were prepared for the two steels, both using the NRT model and the advanced BC/MD modelling approach, and made available to the international community through the IAEA, Vienna.

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. To enable a reliable assessment of the gas production, 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. Fig. 8 (right side) shows, as example, the helium gas production cross-section evaluated for Cr compared to available experimental data. The evaluated gas production cross-sections are available as standard ENDF data files and can be used, after processing with the NJOY code, directly with MCNP in design calculations.

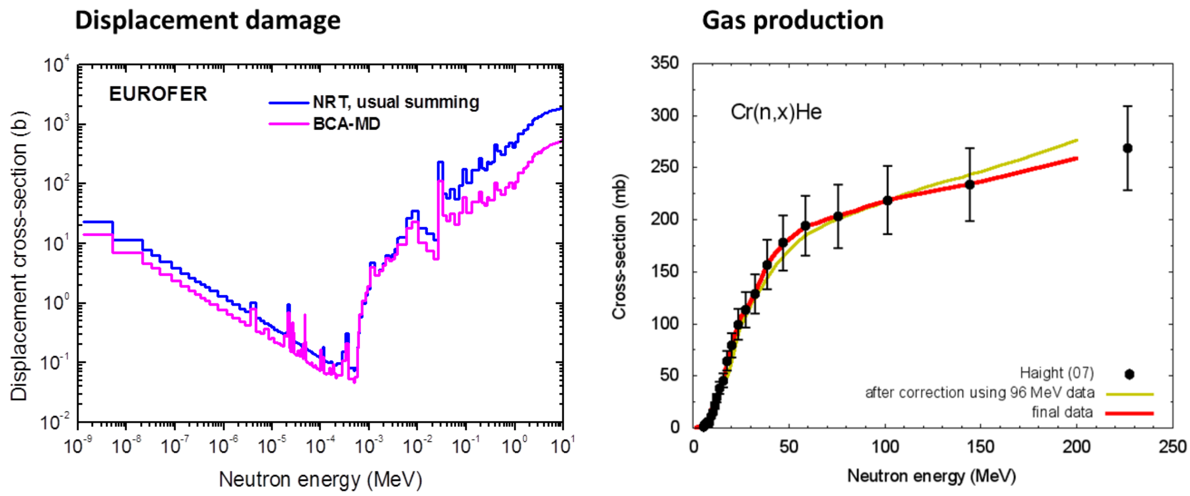

FIG. 7: Evaluated displacement damage and helium gas production cross-sections for Eurofer (left) and chromium (right), respectively.

3.3 TBR sensitivity/uncertainty analysis for DEMO

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. To this end the MCNP based sensitivity code MCSEN [16] has been developed. MCSEN is a local extension to MCNP with the capability to calculate sensitivities for responses by the point detector and the track length estimator based on the differential operator method. This enables the efficient calculation of sensitivities for nuclear responses in a geometry cell of an arbitrary 3D configuration. Thus the real 3D model of a fusion reactor, as routinely used for design analyses, can be employed in the sensitivity 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 the HCPB DEMO model developed within the PPPT programme.

The sensitivity and uncertainty of the tritium breeding ratio (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 pre-dominantly sensitive to the ^{16}O data, followed by ^{6,7}Li, ^{28}Si, ^{9}Be and ^{56}Fe. An overall uncertainty of ± 3.17% was obtained for the TBR when using JEFF-3.2 covariance data with the mentioned additions. The uncertainty is 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%.

4. Conclusions

Development works conducted at KIT in the field of computational tools and nuclear data for fusion neutronics were presented. Significant progress was achieved for the high fidelity geometry representation in Monte Carlo particle transport simulations through the translation of CAD geometry data for the MCNP, TRIPOLI and GEANT4 Monte Carlo codes with extended capabilities of the McCad conversion software. Application examples were shown on various DEMO models demonstrating the relevance of such capabilities for the European PPPT programme. Nuclear data evaluations relevant to fusion technology were provided for neutron transport applications, displacement and gas production calculations as well as uncertainty assessments.

Acknowledgments

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