

KIT Fusion Neutronics R&D Activities and Related Design Applications

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Abstract. Various efforts are being conducted worldwide to develop and extend the capabilities of neutronics simulation tools for reliable nuclear design and performance analyses of future fusion devices including the capabilities to model the problem geometry in true 3D representation and taking advantage of the high performance parallel computing resources available nowadays. This paper presents the development efforts of the Karlsruhe Institute of Technology (KIT) on the development of such computational tools. The efforts focus on the development of various computational schemes based on the Monte Carlo technique for the particle transport simulation, by adapting and coupling available codes, and extending their capabilities to specific application requirements. The recent progress is presented and the suitability of the tools developed for fusion neutronics design calculations is demonstrated on specific application examples for the ITER device and the IFMIF neutron source facility.

1. Introduction

The availability of suitable computational methods, tools, models and data, qualified for design applications, is a pre-requisite to enable reliable nuclear design and performance analyses of future fusion devices. Various efforts are being conducted worldwide to develop and extend the capabilities of the neutronics simulation tools including the capabilities to model the problem geometry in true 3D representation and taking advantage of the high performance parallel computing resources available nowadays.

At the Karlsruhe Institute of Technology (KIT), Institute for Neutron Physics and Reactor Technology (INR), the efforts focus on the development of various computational schemes based on the Monte Carlo technique for the particle transport simulation, by adapting and coupling available codes, and extending their capabilities to specific application requirements. This includes, among others, a coupled programme system for the Monte Carlo based calculation of shut-down dose rate distributions in full 3D geometry, and an enhanced version of the MCNP code, called McDeLicious, with the ability to sample in the transport calculation the generation of d-Li source neutrons on the basis of tabulated cross-section data. A dedicated effort is being conducted on the development of the in-house geometry conversion software tool McCad to enable the automatic generation of MCNP models from available CAD geometry data.

In the following the progress achieved recently in the development of the mentioned computational tools is presented and their suitability for fusion neutronics design calculations is demonstrated on the example of specific applications to design and performance analyses of the ITER device and the IFMIF neutron source facility.

2. R2Smesh approach for the calculation of high resolution shutdown dose rate distributions

A computational scheme for the rigorous calculation of shutdown dose rates in full 3D geometry has been previously developed at the former Research Centre of Karlsruhe, now KIT. The scheme, called Rigorous-2-step (R2S) method [1], is based on the use of MCNP [2] for the transport calculations (neutron and decay gammas) and FISPACT [3] for the inventory calculation (decay gamma source). A suitable coupling scheme has been devised to enable the automated routing of the MCNP neutron flux spectrum distributions to FISPACT and the FISPACT decay gamma source distributions to MCNP. The decay gamma source distribution is sampled in a source routine linked to MCNP according to the distribution provided by the preceding MCNP neutron transport and FISPACT inventory calculations. This procedure allows applying the procedure for any complex geometry without principal restrictions.

The R2S approach has been recently extended to enable calculations of high resolution shutdown dose rate distributions by utilizing MCNP's mesh tally capabilities [4]. With this technique, called R2Smesh, the neutron fluxes and the decay gamma sources are provided on a fine spatial mesh grid superimposed to the real geometry. In this way proper account is taken of the spatial variations of the flux and the decay gamma source distribution without the need to modify the MCNP geometry model.

The R2Smesh technique utilizes two types of mesh grids, a coarse one for providing the neutron spectra which vary only weakly over spatial distances within the average neutron mean free pathway, and a fine one for providing the map of the total neutron flux density. The coarse mesh neutron flux spectra are re-normalised to match the fine mesh neutron flux densities. This approach is essential for providing statistically reliable results for the neutron flux spectra. The present R2Smesh version allows for any rectangular mesh tally, in particular with non-uniform spacing. Thus high resolution maps can be limited to regions of particular importance.

To retrieve the materials of the problem geometry a dedicated MCNP run using the PTRAC feature is required. PTRAC counts hits of uniformly distributed source particles. From the specific output the materials and their abundances in each coarse mesh element are obtained. The decay gamma sources are calculated by FISPACT for each neutron spectrum from the coarse mesh and pure material combination. This leads to a rather moderate number of FISPACT calculations. The effective gamma source map is constructed from the FISPACT sources by properly weighting of the material composition and normalizing to the neutron flux in each fine mesh element. When sampling the decay gamma source distribution given in the source file, R2Smesh takes into account void and non-activated parts of the problem geometry at each distinct location. This sampling scheme is fully working with repeated structures as available with MCNP, in particular universes which are frequently used in complex MCNP geometry models.

The further enhanced R2Smesh-2.0 technique [5] adds another useful novelty to the R2Smesh approach by determining the materials and their volume fractions in a mesh cell in a dedicated sampling subroutine. Thus the material distribution of the mesh can be provided as part of a regular MCNP calculation without the need to perform an additional PTRAC calculation which is very expensive in terms of computing times and very demanding in terms of disk space required to store the large amount of PTRAC data. The new interface scans the MCNP input deck and prepares a master file for the subsequent FISPACT calculations. No

additional data or MCNP input file modifications are required at this step. The interface then prepares and submits tasks for parallel FISPACT calculations controlling each process. At the final step, the spatial decay gamma source file is prepared for the subsequent MCNP decay gamma transport calculations.

For validation purposes, the R2Smesh approach has been benchmarked against dose rate measurements performed on the JET device during shut-down in 2010. The measurements were performed by the experimental team of ENEA, Frascati, and the JET health physics group [6] for several positions along the mid port horizontal axis of JET Octant 1 as shown in Fig. 1. Two Geiger Müller type detectors, an Automess Teletector 6112D and a Mini Rad series 1000R, were used for the measurements along the port while an Eberline R02-W ionization chamber was used for the measurement inside the plasma chamber.

The R2S benchmark calculations were performed making use of the 3D MCNP geometrical model of Octant 1 (Fig. 1) developed and optimised by ENEA, Frascati, for the specific purpose of shut-down dose rate analyses of the experiment. The assumed irradiation history took into account the entire DD and DT operation periods from 1983 until shut-down in 2009 as provided with the measured neutron yield data.

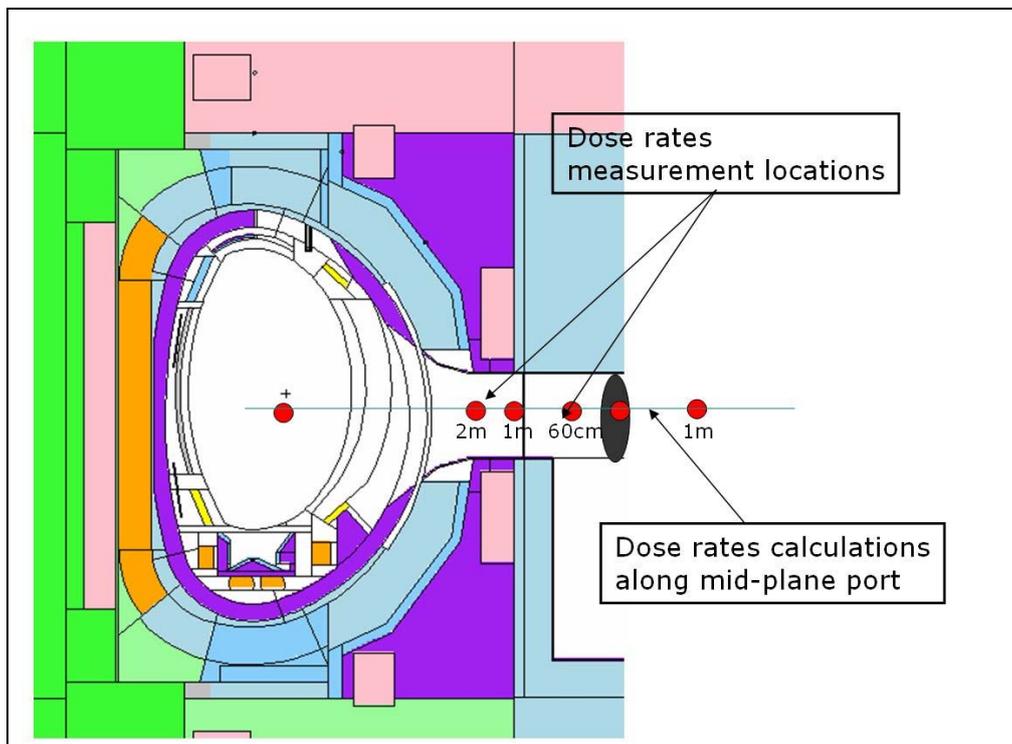


FIG.1: MCNP model of JET Octant 1 with dose rate measurement locations indicated

The entire JET octant was overlaid with a fine spatial (rectangular) grid of 3 cm mesh size for the neutron fluxes and a coarse grid with 15 cm mesh size for the neutron spectra. The R2Smesh shut-down dose rate calculations were performed for 81, 109, 137 and 263 days after shut-down. Fig. 2 compares the R2Smesh results for the shutdown dose rates at 81 and 137 days after shutdown with the measurements which refer to the designated positions in the mid-plane port where the dose measurements were performed with the Teletector and the Mini rad detectors. There are also included the shut-down dose rate results obtained with the original cell based R2S approach which employs the material cells of the MCNP model with-

out any modification in the activation calculations[1]. An overall good agreement of the calculated and the measured dose rates is obtained with C/E (calculation/experiment) ratios in the range between 0.7 and 1.3, i. e. within the experimental $\pm 30\%$. It is noted, however, that there is a trend for underestimating the measurements at short cooling times and for overestimating at longer cooling times.

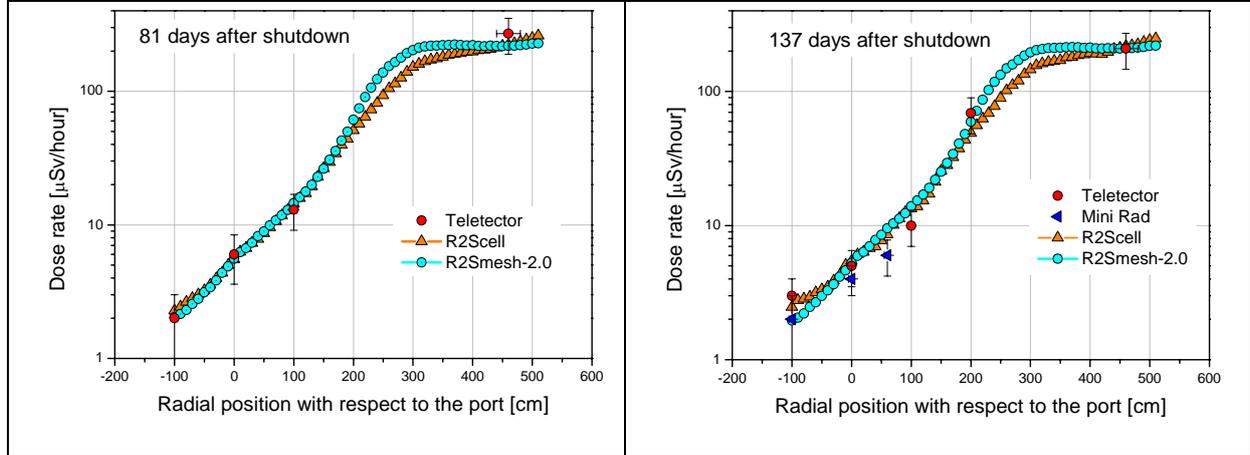


FIG.2: Calculated shut-down dose rate profiles along the JET Octant 1 mid-plane port compared with experimental results available at the designated positions.

Recent R2mesh applications include shutdown dose rate analyses of the NBI (Neutral Beam Injection) cell in the Upper Port of ITER [7], the European Test Blanket System in the equatorial port with HCLL and HCPB Test Blanket Modules integrated [8], and the Diagnostic Equatorial Port Plug (EPP) [8,9].

Fig. 3 shows a comparison of shut-down dose rate distributions calculated for a local model of the EPP port [9] with the original cell based R2S approach and the R2Smesh technique. As indicated in the figures, the resulting average dose rate values in the port extension agree very well. Note that no meshes are applied in the neutron transport calculations with the cell based R2S approach, i. e. neutron flux spectra and decay photon sources are averaged over the material cells as described in the MCNP calculations. Meshes are applied, however, in the standard way for the decay photon transport calculation. Thus high resolution shut-down dose rate distributions are also obtained with the cell based R2S approach as shown in Fig. 3. The averaging, however, results in some inherent inaccuracy of the spatial decay gamma source distribution which affects the shut-down dose rates.

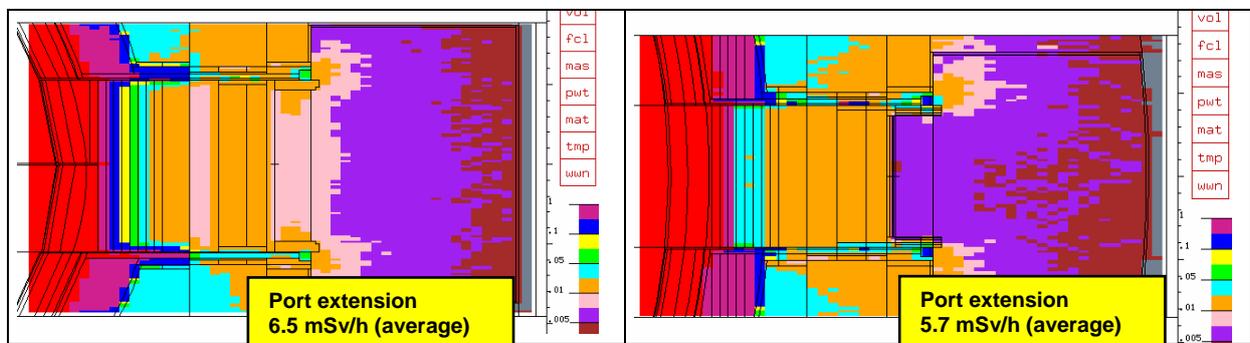


FIG.3: Applications of the R2S approach, cell based (left) and mesh based (right), to shut-down rate analyses of the ITER Diagnostic Equatorial Port Plug (EPP) using a local EPP model [9].

Another illustrative example of R2Smesh based calculation of shut-down rate distribution is shown in Fig. 4 for the European TBMs integrated in the equatorial Test Blanket Port in ITER. For these analyses, an MCNP model of the test blanket port plug with HCLL and HCPB TBM assemblies was integrated into the A-lite model of ITER. With the R2Smesh technique and the McCad approach, described in Section 3 below, high resolution maps of both the neutron flux density (first transport calculation step in the R2Smesh approach) and the shut-down dose rate (second transport calculation step) are obtained and overlaid to the port plug geometry.

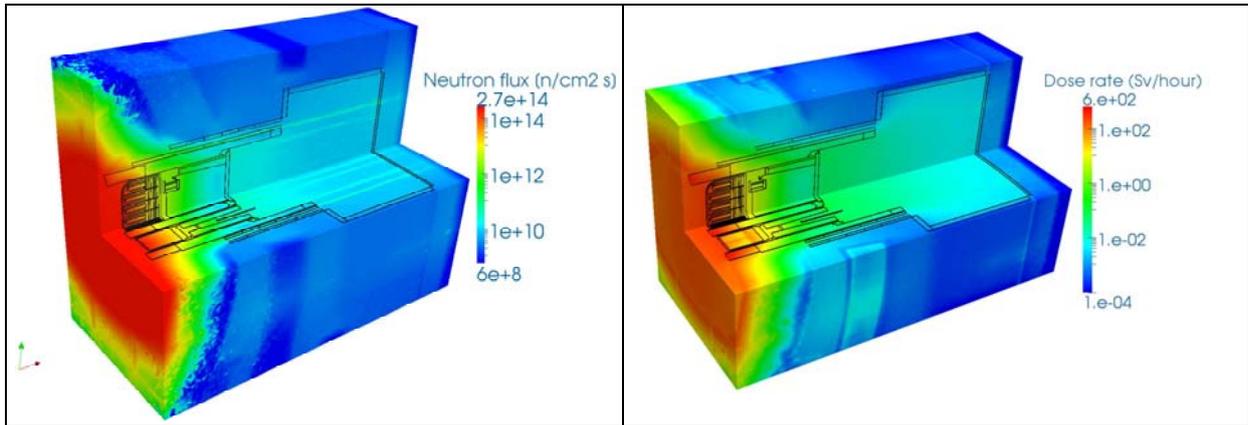


FIG.4: Maps of the neutron flux density (left) and the shut-down dose rate (right) calculated with R2Smesh technique for the test blanket port region in ITER (overlaid to the CAD geometry).

3. McCad geometry conversion tool and visualization of spatial distributions

The McCad geometry conversion tool [10] has been developed at KIT to enable the automatic conversion of CAD models into the semi-algebraic geometry representation as utilized in Monte Carlo particle transport simulations like MCNP [2] or TRIPOLI [11]. With the McCad approach, the input geometry is converted in two steps into a geometry description suitable for MC particle transport codes. In the first step the input geometry is decomposed into volumes that can be described by the Boolean combination of algebraic half-spaces. The overall geometry is not affected by the decomposition, i.e. the total volume content and the shape before and after the conversion are identical. In the second step McCad generates the void space which is not available in the CAD system but mandatory for the particle transport simulation codes.

McCad is coded in C++ based on object-oriented design patterns. It integrates the open source CAD kernel from Open CASCADE (OCC) for all geometry related computations and CAD related file exchange. The build system makes use of the cross-platform makefile generator CMake. Its graphical user interface (GUI) is based on the cross-platform application and user interface framework Qt4. In its current version (0.3) McCad is available exclusively for Unix-like operating systems. Crucial for its operation is the integrated CAD kernel. Since end of 2011 the user community of Open CASCADE Technology (OCCT) decided to branch the official release of OCC for a better usability and shorter bug fixing cycles. The branch implements fixes for bugs discovered by the user community which will officially be fixed in the next public release of OCCT and provide a more comfortable installation procedure. McCad supports OCCT as well as the community edition (OCE).

Latest development efforts were dedicated to improve the robustness of the code and increase the performance in terms of precision and speed. Furthermore, capabilities for the visualization of results were enabled by coupling McCad with the ParaView software [12]. This allows, among others, to overlay mesh tally distributions provided by a preceding MCNP calculation, to the CAD geometry. The interface programme mt2vtk, developed to this end, converts MCNP's mesh tally data into a file format based on the Visualization Toolkit (VTK) as depicted in Fig. 5. The CAD geometry must be available in STEP format to this end. When starting with an MCNP model (i.e. no CAD geometry available), the MCNP geometry needs to be converted into CAD representation. Such a re-conversion is also provided with the McCad software although not all geometry options are currently supported.

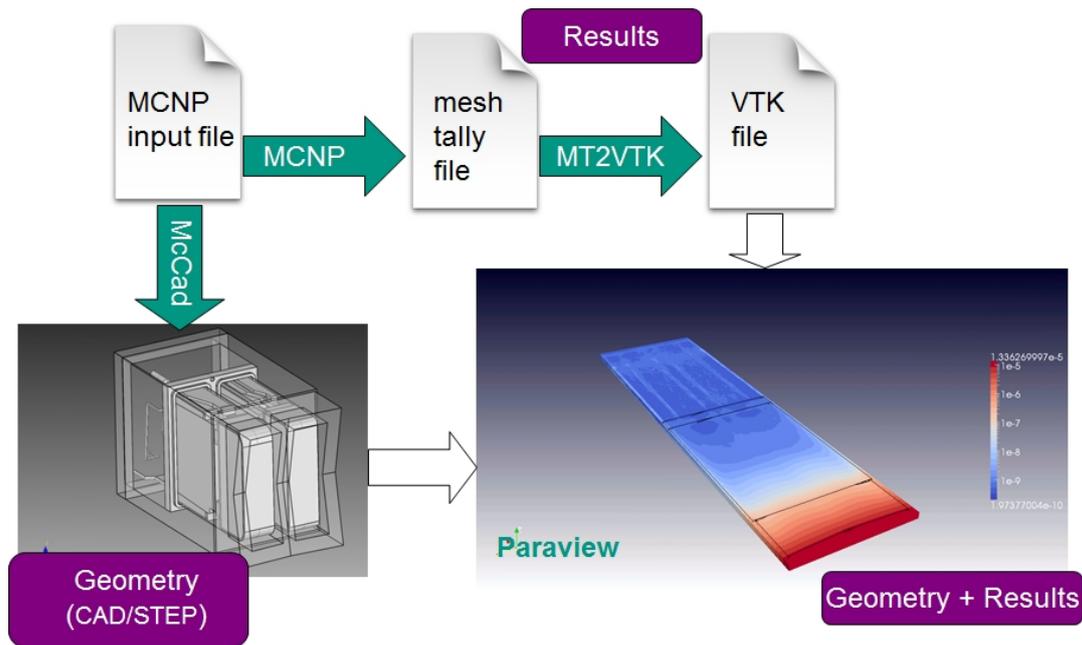


FIG.5: Scheme for visualizing mesh tally distributions on CAD geometry with the ParaView software.

McCAd is in routine use at KIT for the conversion of CAD geometry models for neutronics analyses with the MCNP code. Major recent applications include the generation of a detailed MCNP model of the European Test Blanket (TBM) System integrated into the ITER A-lite model, and the development of a very detailed and comprehensive MCNP model of the IF-MIF Target and Test Cell.

On the example of the TBM port plug, Fig. 6 illustrates the process for the generation of a full MCNP analysis model of ITER with integrated TBM system starting with the CAD model of the TBM port plug, its decomposition on the CAD platform, the conversion to the MCNP geometry, and, finally, the integration into the A-lite model. The use of this model for the calculation of shut-down dose rate distributions was shown in Section 1 above, see Fig. 4 for the maps of the neutron flux density and shut-down dose rates overlaid to the TBM CAD geometry.

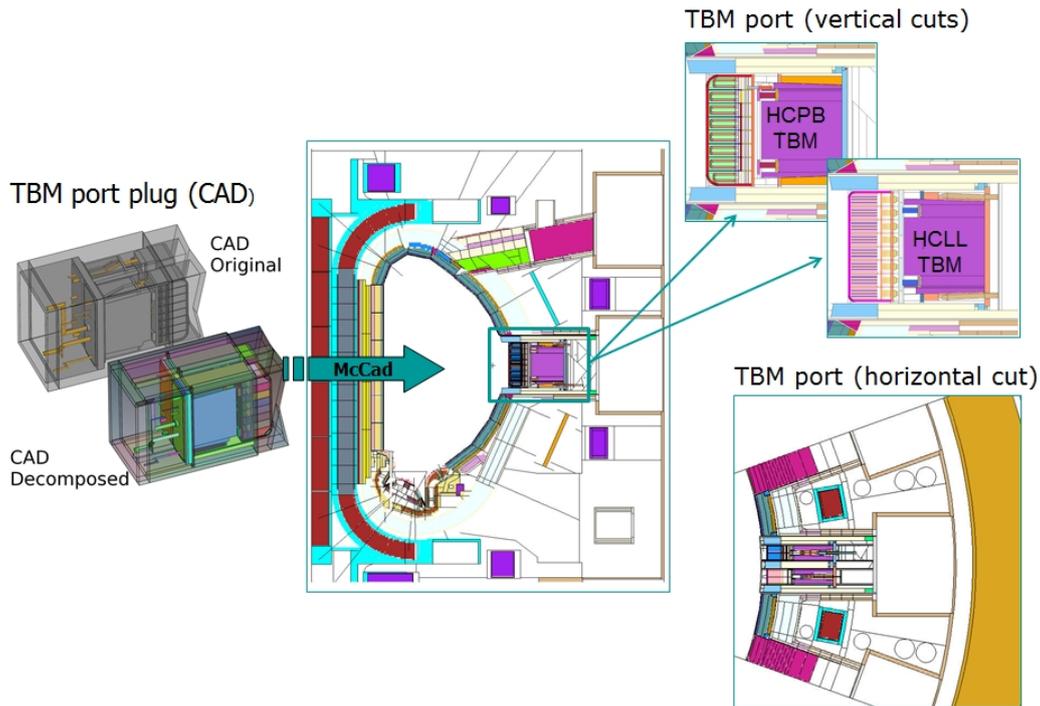


FIG. 6: Scheme for the processing of the TBM port plug model and its integration into ITER.

4. McDeLicious Monte Carlo code for IFMIF neutronics calculations

McDeLicious [13] has been developed as enhancement to the MCNP Monte Carlo code with the new ability to simulate the generation of d-Li source neutrons and thus provide the computational tool for neutronics calculations of the IFMIF neutron source. The McDeLicious capabilities include the generation of source neutrons and photons based on evaluated $d + {}^{6,7}\text{Li}$ cross section data, and the sampling of the impinging deuteron beam intensity distribution using fitting functions or probability tables as prepared for the IFMIF EVEDA activities [14]. The McDeLicious software has been recently updated to comply with the standard of the state-of-the-art version 5 of the MCNP code. An MPI programme version enables to run McDeLicious in parallel mode on large computer clusters. In addition, the R2S methodology was extended with McDeLicious and high energy activation data to enable radiation dose assessments for IFMIF shut-down periods.

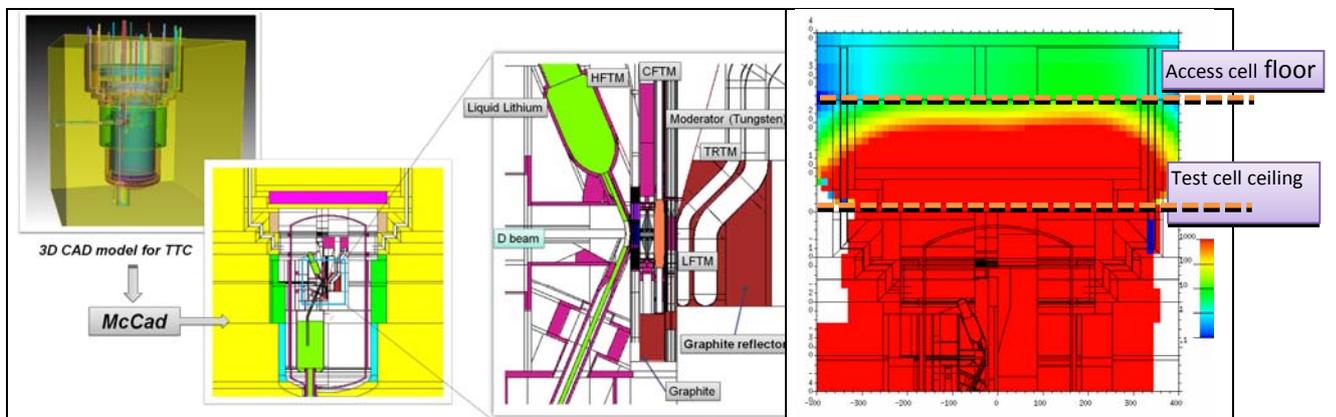


FIG. 7: IFMIF TTC model processing (left) and biological dose rate [$\mu\text{Sv/h}$] during operation (right).

McDeLicious is in routine use for IFMIF neutronics calculations in the frame of the EVEDA activities within the Broader Approach (BA) of Japan and Europe. Recent applications include the calculation of high resolution distributions of the nuclear responses across the IFMIF Target and Test Cell (TTC) making use of a detailed TTC model generated from CAD data with the McCad geometry conversion software (Fig. 7), as well as shielding and radiation dose assessments for the irradiated test modules and the test cell surrounding [15,16].

5. Conclusions

The recent progress achieved in KIT's development efforts on various computational schemes for fusion neutronics calculations has been presented. This includes the R2Smesh approach for Monte Carlo based shut-down dose rate calculations, the McDeLicious extension to the MCNP code for IFMIF neutronics calculations, and the McCad geometry conversion tool. The suitability of the tools developed for fusion neutronics design calculations was demonstrated on specific application examples for the ITER and the IFMIF neutron source facility.

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