Advanced Computational Tools and Methods for Nuclear Analyses of Fusion Technology Systems

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Abstract. An overview is presented of advanced computational tools and methods developed recently for nuclear analyses of Fusion Technology systems such as the experimental device ITER ("International Thermonuclear Experimental Reactor") and the intense neutron source IFMIF ("International Fusion Material Irradiation Facility"). These include Monte Carlo based computational schemes for the calculation of three-dimensional shut-down dose rate distributions, methods, codes and interfaces for the use of CAD geometry models in Monte Carlo transport calculations, algorithms for Monte Carlo based sensitivity/uncertainty calculations, as well as computational techniques and data for IFMIF neutronics and activation calculations.

1. Introduction

The worldwide efforts in fusion technology aim at developing, in the long-term, power reactors which can contribute substantially to the supply of electricity. The construction and operation of the experimental fusion device ITER ("International Thermonuclear Experimental Reactor") and the intense neutron source IFMIF ("International Fusion Material Irradiation Facility") are considered as essential next steps towards this long-term goal. The availability of qualified computational tools and nuclear data for the neutron transport simulation and the calculation of relevant nuclear responses is a pre-requisite to enable reliable design calculations for these facilities.

Significant effort has been spent over the past few years to provide suitable neutronics tools and nuclear data for nuclear analyses of Fusion Technology systems. The focus of this paper is on the computational methods and tools developed recently for nuclear analyses of ITER and other like fusion devices as well as the IFMIF neutron source facility. These include Monte Carlo based computational schemes for the calculation of three-dimensional shut-down dose rate distributions, methods, codes and interfaces for the use of CAD geometry models in Monte Carlo transport calculations, algorithms for Monte Carlo based sensitivity/uncertainty calculations, as well as computational techniques and data for IFMIF neutronics and activation calculations. In the following an overview of the recent achievements in the respective fields is presented.

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2. Monte Carlo based 3D shut-down dose rate calculations

For safe operation and maintenance of nuclear fusion devices it is important to be able to predict the induced activation and the resulting shut-down dose rate distributions. This requires a suitable system of codes, data and interfaces which is capable of simulating both the neutron induced material activation during operation and the decay photon transport after shut-down in the proper 3D geometry. Two different computational schemes have been developed recently, both of them relying on the Monte Carlo technique for the transport simulation. The rigorous 2-step (R2S) method [1] makes uses of the Monte Carlo code MCNP [2] for the transport calculations (neutron and decay photons) and the FISPACT inventory code [3] for the activation calculations with a suitable coupling scheme for the automated routing of decay photon source distributions and neutron flux spectra. The direct 1-step (D1S) method [4] is based on the assumption that a radioactive nuclide generated during irradiation spontaneously emits the associated decay photons. Neutron and decay photon transport then can be treated in one single Monte Carlo calculation run. When calculating the dose rate, correction factors are applied to account for the proper decay rate of a radioactive nuclide. The D1S approach uses a modified version of the MCNP code together with special, ad hoc generated nuclear cross-section data.

The two approaches have been successfully applied to dose rate analyses of ITER and the JET (Joint European Torus) tokamak revealing, however, some inherent discrepancies. Good agreement was found for a benchmark experiment performed on a ITER shield blanket mock-up at the Frascati 14 MeV neutron generator (FNG) . Fig. 1 shows the graphical comparison of calculated (C) and experimental (E) shut-down dose rates following the irradiation of the shield mock-up assembly with $1.95 \cdot 10^{15}$ 14 MeV neutrons.

Further benchmarking was considered necessary by utilizing, as much as possible, a real fusion device with a plasma volume source such as the JET tokamak. First benchmark tests on JET were made by means of comparison calculations employing a 3D torus sector model of the device. The shut-down dose rates were calculated for different positions specified inside and outside the vessel and in the torus hall assuming a representative irradiation scenario. The R2S and D1S results of this calculational benchmark showed agreement within ± 25 % [5]. This was considered satisfactory taking into account the very different approaches.

The outcome of the calculational benchmark suggested a more realistic benchmark exercise on JET. The real irradiation history of D-T and D-D campaigns conducted at JET during the years 1997-98 were used to calculate the shut-down doses at four different locations (positions 1-4, inside the machine, on the torus hall floor , in contact with the upper coil, in contact with the machine structure) and three different irradiation histories (labelled #1, 9 and 15) with different decay times. The two computational procedures gave results that in general agree with the available measurements within a factor 2 to 3 as shown in Figs. 1b-d. The comparison between calculational and experimental JET dose rate results was constrained, however, by the rather high uncertainties associated with the available measurements. These data were recorded by the JET Health Physics team as part of the regular monitoring programme under not well defined conditions and were judged to be not accurate enough to validate computational results. It was therefore concluded that a dedicated experiment on JET need to be conducted for the benchmarking of R2S and D1S shut-down dose rate calculations. This is planned as part of the 2005 experimental programme during D-D operation of JET.

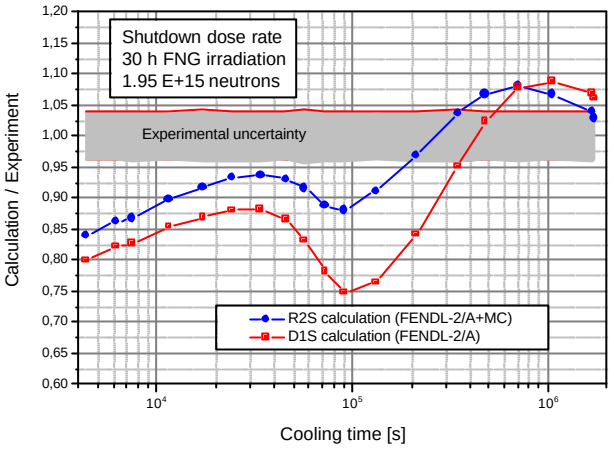

Fig. 1 a: FNG irradiation experiment

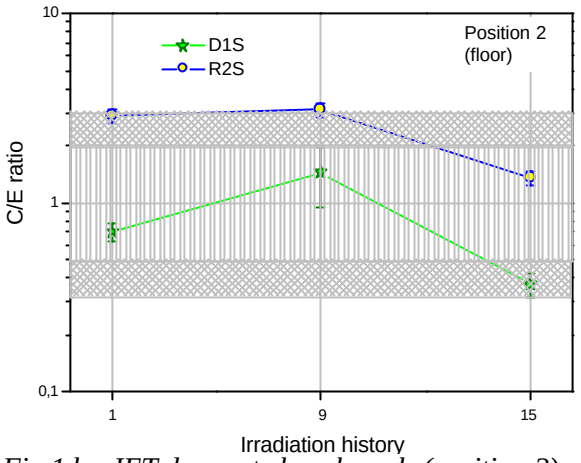

Fig.1 b : JET dose rate benchmark (position 2)

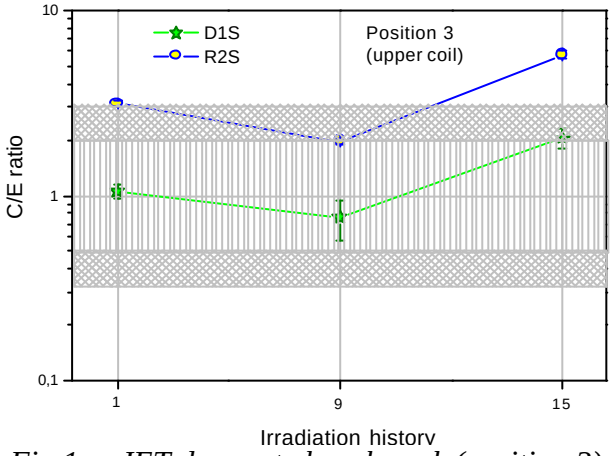

Fig.1c : JET dose rate benchmark (position 3)

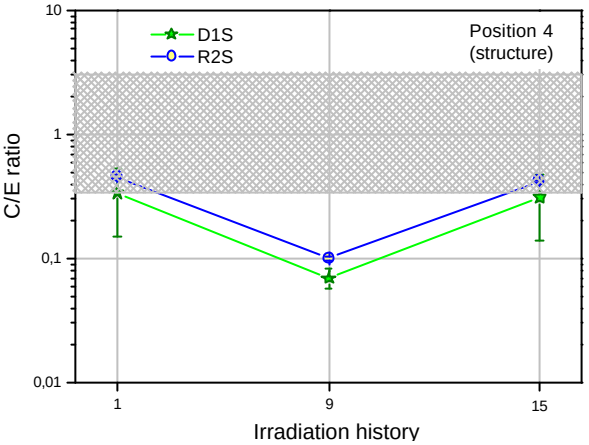

Fig.1d : JET dose rate benchmark (position 4)

FIG. 1 a-d: Comparison of calculated (C) and experimental (E) dose rates obtained for the ITER shut down dose rate experiment at FNG and different positions and irradiation histories at JET.

3. CAD geometry data for Monte Carlo calculations

The Monte Carlo technique enables the use of full and detailed 3D geometry models in neutronics calculations. The modelling of a complex geometry with a Monte Carlo code such as MCNP is, however, an extensive and time-consuming task. Different approaches have been recently developed to make available CAD data for Monte Carlo calculations.

3.1. CAD Interface for the Monte Carlo code MCNP.

The geometry needed for the MC particle transport simulation is a decomposition of the problem space into a finite collection of disjoint regions (cells) whose union is the problem space. It is usually represented as a Boolean form of primitive solids or algebraic half-spaces. Most commercial CAD systems use the boundary representation (B-rep) method to store geometric models of solids. A solid is assumed to be a compact and regular point set, whose boundary is composed of closed oriented manifolds. The difference in the representation schemes makes a conversion necessary. In this approach, the geometric and topological data of a B-rep solid from a CAD system is used to construct its semi-algebraic representation as employed in MC codes. The two main steps involved in this approach are the access to the data of the CAD system and the conversion process itself. Access to the data of a CAD system can be provided

through export of the data in neutral format. Given a solid in boundary representation, it can be shown that its semi-algebraic representation is computable. The algorithm which solves this problem is described elsewhere [6].The conversion proceeds in two steps. After the traversal of the B-rep data structure of a solid and extraction of the boundary supports, the first step is to determine the definability of the solid by the available boundary support set. If this is not the case the set is enlarged until definability is achieved. In the second step, a cell construction is performed by a sign constant decomposition of the solid by the boundary supports.

The interface programme developed for the conversion of the CAD data into the semi-algebraic surface representation is based on a software design integrating a CAD kernel, which is a C++ class library, a graphical user interface (GUI) and the conversion algorithm. It relies on open CAD and graphics software (Open Cascade/Open GL) and has been programmed on the Unix/Linux platform. The C++ based GUI is used for the 3D visualization with the capability of manipulating the geometry model. Standard CAD interface files (IGES and STEP format) can be imported and converted to the MCNP geometry representation. The conversion algorithm relies on the CAD kernel for its geometric and related computations. The implementation of the interface program is realized in a framework like library. The automatic generation of the MCNP geometry representation is treated as data exchange operation.

A first successful test application has been recently performed for a full octant model of the JET tokamak. Starting from available design models, a suitable CAD model of JET octant 3 was generated at the JET drawing office using CATIA V5. Several iteration steps were required to optimise the CAD model for the conversion programme and the use with MCNP [7]. In particular many free form surfaces had to be replaced by algebraic surfaces. Figs. 2 a and b show the final CAD and the converted MCNP models. Validation of the converted model was achieved by comparing the volumes of the components as calculated by CATIA and MCNP.

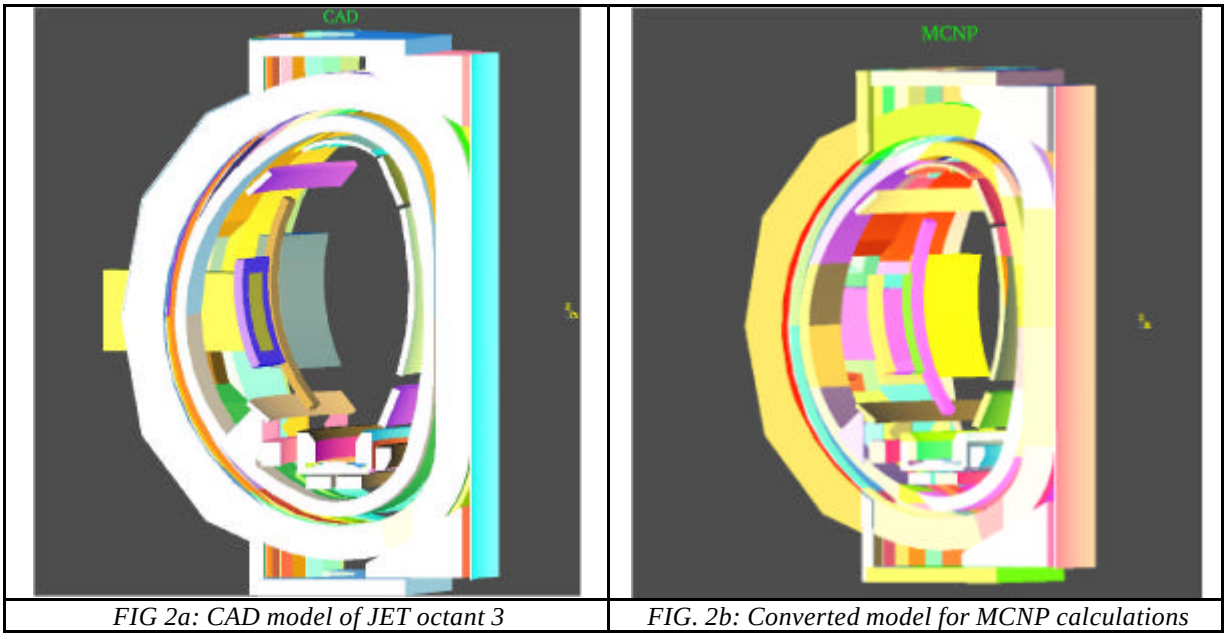

FIG 2a: CAD model of JET octant 3 | *FIG. 2b: Converted model for MCNP calculations*

FIG. 2 a, b: Comparison of CAD and MCNP models converted by the CAD-MCNP interface programme

3.2.Direct CAD-MCNPX Coupling Using The Common Geometry Module (CGM)

As an alternative, the CGM geometry engine [8] is being integrated directly in the MCNPX code to replace the internal representation of the geometry. The advantages of this approach over translation-based approaches described above are i) the ability to model free-form surfaces and other geometry (e.g. voxel-based, subdivision surface-based) handled in CGM but not the MC code, and ii) a faster turnaround time after CAD-based design changes. The primary disadvantage is that the expense of direct CAD-based evaluation results in the CAD-based MC code 10-20 times slower than the original MC code. Specific information on the integration and verification effort of this approach is given elsewhere [9].

In a first real application, the MCNPX/CGM code was used to calculate the neutron wall loading distribution in the ARIES compact stellarator design [9]. A fully accurate CAD model of the plasma surface is shown in Fig. 3a, with horizontal decompositions made to facilitate tallying at different azimuthal angles. A custom neutron source, depending on the magnetic center and a radial distribution between there and the plasma surface, was also implemented. Results of this calculation are shown in Fig. 3b. This problem required 5 days of CPU time on a 2.4GHz Linux workstation, for a relative error of 9-10%. Even at these long run-times, this is a useful result, which would not be possible to model using MCNPX alone.

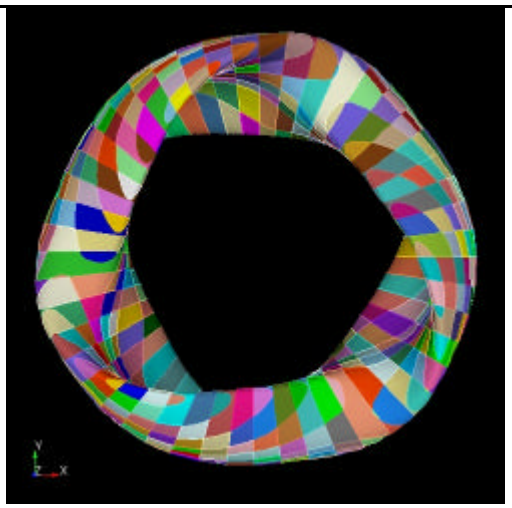

FIG 3a: CAD model of ARIES-CS (with tally surfaces).

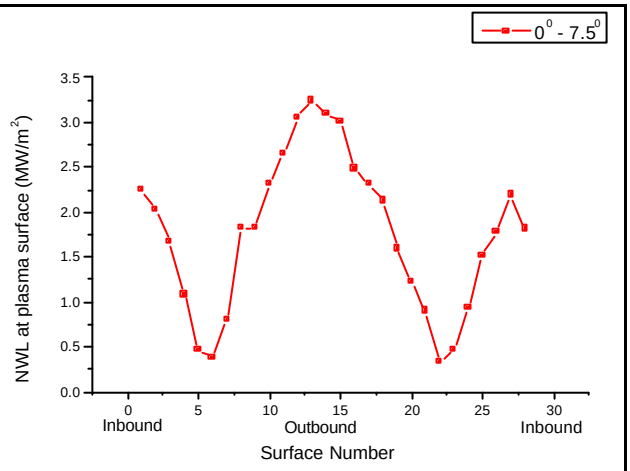

FIG. 3b: Neutron wall loading between 0 and 7.5 degree toroidal angle.

FIG. 3 a, b: CAD model of ARIES-CS plasma, and preliminary MC analysis results using MCNPX-CGM.

Several approaches for speeding up MCNPX/CGM will be investigated. Preliminary analyses show that the horizontal decompositions made in the model have no influence on the run-time. It was thus concluded that ray-tracing in the CAD engine is not taking advantage of surface-based bounding box accelerations, at least on the trimmed CAD surfaces. Testing ray intersections against such bounding boxes should substantially improve run-times for this model. Other well-known ray-tracing acceleration techniques applied to this problem, possibly including Oriented Bounding Box (OBB) and hierarchical subdivision of the domain, will also be investigated. Finally, it is planned to investigate limiting the ray-tracing distance to the maximum distance to interaction as determined by the MC analysis. This may be especially useful for charged particle transport, where flight distances are typically quite short.

4. IFMIF neutronics tools and data

The IFMIF neutron source uses the d-Li stripping reaction to produce neutrons for high fluence irradiations of fusion power reactor candidate materials. A flowing liquid lithium target is bombarded by a high current deuteron beam accelerated up to 40 MeV energy. The resultant neutron spectrum is fusion-relevant but includes a high-energy tail that extends up to 55 MeV (Fig. 4). Dedicated computational tools and nuclear data have been developed over the past years for IFMIF neutronics and activation calculations [10,11].

The Monte Carlo code McDeLicious [12] was developed as enhancement to MCNP 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 set of evaluated cross-sections was prepared to this end for the d + ^{6,7}Li the reaction system up to 50 MeV deuteron energy. The McDeLicious approach was extensively tested against available experimental thick lithium target neutron yield data. As an example, Fig. 5 shows a comparison of measured and calculated forward neutron yields as a function of the deuteron incidence energy. It was concluded that McDeLicious can predict the D-Li neutron generation with the best achievable accuracy.

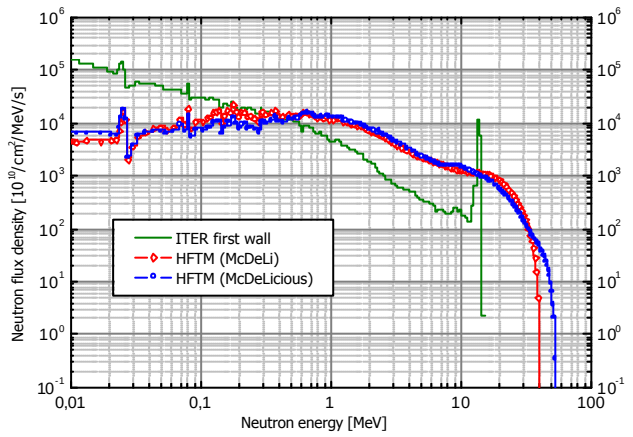

FIG. 4 Neutron flux spectra in the High Flux Test Module (HFTM) of IFMIF compared to a typical fusion reactor spectrum (ITER first wall)

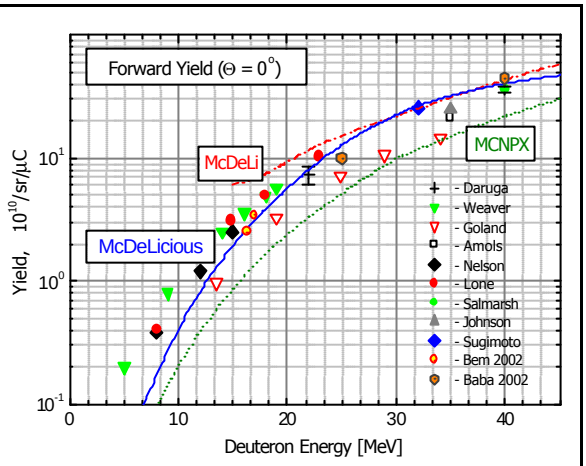

FIG. 5: Thick Lithium target forward yield data: comparison of calculated and measured data as a function deuteron energy

The Intermediate Energy Activation File IEAF-2001 [13] has been developed for IFMIF activation and transmutation calculations. IEAF-2001 contains neutron-induced activation cross sections for 679 target nuclides from Z=1 (hydrogen) to 84 (polonium) up to 150 MeV. Two different working libraries with 256 group data in different data formats have been derived for application calculations [14]. One of them, the G-IEAF-2001/XS-256 group library, can be used by activation codes capable of handling an arbitrary number of reaction channels such as ALARA (Analytical and Laplacian Adaptive Radioactivity Analysis) of the University of Wisconsin-Madison [15]. ALARA implements new modelling and mathematical techniques for exact simulation of fusion activation, particularly in pulsed systems, with direct calculation of many engineering responses (e.g. waste disposal rating, contact dose, total heating and biological dose). ALARA has the ability to handle the IEAF-2001 activation cross section data in a straightforward way since the reactions are defined entirely by the library, requiring only a list of resultant isotopes and cross-sections for the production of each. The other IEAF-2001 working library, denoted as G-IEAF-2001/PY-256, uses pseudo fission product yields to

describe the generation of transmutation products [14] and can be used with standard activations codes such as FISPACT of UKAEA Culham [3]. A series of benchmark analyses has been performed to validate the different computational approaches [14,16], see Fig. 6. for the results of a computational benchmark and Fig. 7 for the results of an experimental benchmark [17]. As a result, it can be stated that both the ALARA/G-IEAF-2001/XS-256 and the FISPACT/G-IEAF-2001/PY-256 approach are qualified for activation and transmutation calculations of intermediate energy systems.

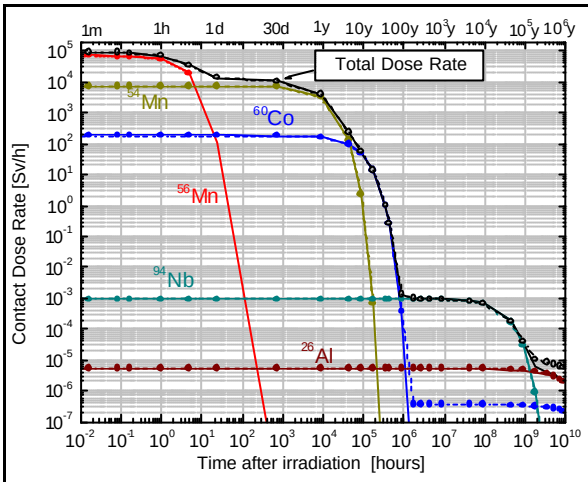

FIG.6: Irradiation simulation of Eurofer steel in a fusion reactor spectrum ALARA (straight lines) vs. FISPACT(symbols with dashed lines):

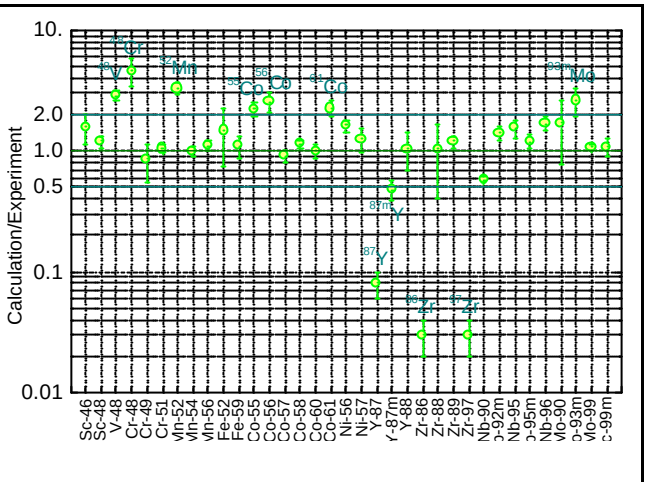

FIG.7: Comparison of calculated (ALARA/IEAF-2001) and measured [19] radio-activities induced by irradiating SS-316 in an IFMIF-like white neutron field.

5. Monte Carlo based sensitivity/uncertainty calculations

Sensitivity and uncertainty analysis is a powerful means to assess uncertainties of nuclear responses and track down these uncertainties to specific nuclides, reaction cross-sections and energy ranges. A method to calculate sensitivities of Monte Carlo point detector responses has been previously developed [18] and implemented in a local version of MCNP4C, called MCSEN. The method has been extended to include sensitivities to secondary angular distributions [19]. The point detector method for sensitivity calculations has been extensively benchmarked against deterministic sensitivity/uncertainty calculations [20]. It is well suited for the analysis of integral experiments, enables the assessment of the calculational accuracy and provides information for improving the cross-section data. Recent applications include sensitivity- and uncertainty analyses of integral fusion benchmark experiments on SiC and W assemblies. The Monte Carlo based calculation of uncertainties of nuclear responses such as the Tritium production in the Test Blanket Modules of ITER requires the capability to calculate sensitivities for responses by the track length estimator. Suitable algorithms are being implemented for the efficient calculation of cross-section sensitivities in 3D geometry.

6. Conclusions

Significant progress has been achieved over the past few years in developing advanced computational methods and tools for nuclear analyses of Fusion Technology systems. This development was partly driven by the needs of the Fusion Programme with focus on "next step" facilities such as ITER and the IFMIF neutron source. Accordingly, Monte Carlo based com-

putational schemes for the calculation of three-dimensional shut-down dose rate distributions, methods, codes and interfaces for the use of CAD geometry models in Monte Carlo calculations, algorithms for Monte Carlo based sensitivity/uncertainty calculations, as well as computational tools and data for IFMIF neutronics and activation calculations have been developed. Further development work is though required in the areas reviewed in this paper, in particular with regard to the use of CAD geometry data in Monte Carlo calculations.

Acknowledgement

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References:

[1] CHEN, Y., FISCHER, U., "MCNP based shutdown dose rate calculations: Computational scheme, verification calculations and applications", Fus. Eng. Des. 63-64 (2002), 107-114.
[2] BRIESMEISTER, J. F. (ed.), "MCNP - A General Monte Carlo N-Particle Transport Code, Version 4C", Los Alamos National Laboratory, Report LA-13709-M, April 2000.
[3] FORREST, R., SUBLET, J., "FISPACT 99: User Manual", Report UKAEA FUS 407 (1998)
[4] IIDA, H., VALENZA, D., PLENTEDA, R., SANTORO, R., "Radiation Shielding for ITER to allow for Hands-on Maintenance", J. Nucl. Sci. Techn,. Sup. 1 (March 2000) 235-242
[5] PETRIZZI, L., et al, "Benchmarking of Monte Carlo based shutdown dose rate calculations for applications to JET", ICRS-10, Madeira, Portugal, 9-14 May 2004
[6] TSIGE-TAMIRAT, H., "On the use of CAD geometry for Monte Carlo particle transport, Proc. of the Monte Carlo 2000 conference", Lisbon 23-26 October 2000, pp. 511-516
[7] TSIGE-TAMIRAT, H., et al, "Automatic Generation of a JET 3D Neutronics Model from CAD Geometry Data for Monte Carlo Calculations", SOFT-23, 20-24 September 2004, Venice, Italy
[8] TAUTGES, T. J., "CGM: a Geometry Interface for Mesh Generation, Analysis and Other Applications", Engineering with Computers, 17 (2001) 299-314.
[9] WANG, M., HENDERSON, D. L., TAUTGES, T. J, et al, "Three-Dimensional Modeling of Complex Fusion Devices Using CAD-MCNP Interface", 16th ANS Topical Meeting n the Technology of Fusion Energy, September 14-16, 2004, Madison, WI, USA.
[10] FISCHER, U., SIMAKOV, S. P., et al., "Neutronics and Nuclear Data for the IFMIF Neutron Source", Fus. Eng. Des. 63-64 (2002), 493-500
[11] FISCHER, U., et al., "Validated Computational Tools and Data for IFMIF Neutronic Calculations", AccApp'03 ANS Embedded Topical Meeting, San Diego, CA, June 1-5, 2003
[12] SIMAKOV, S. P., et al., "Advanced Monte Carlo Procedure for the D-Li Neutron Source Term Based on Evaluated Cross-Section Files", J. Nucl. Mat. 307-311 (2002), 1710-1714
[13] FISCHER, U., et al., "Intermediate Energy Activation File IEAF-2001", NEA data bank, Paris, NEA-1656/01 (2001), RSICC Oak Ridge, DLC-217/IEAF-2001 (2002)
[14] FISCHER, U, et al, "IEAF-2001 Cross Section Data Libraries for Activation and Transmutation Analyses", TRAMU Workshop, Darmstadt, September 2-5, 2003, http://www-wnt.gsi.de/tramu
[15] WILSON, P. P. H., HENDERSON, D. L., "ALARA: Analytical and Laplacian Adaptive Radioactivity Analysis", Volume I, Technical Manual, Report UWFDM 1080, January 1998
[16] SIMAKOV, S. P, et al., "Validation Analyses of IEAF-2001 Activation Cross-Section Data for Steels Irradiated in a white d-Li Neutron Field", ND2004, Santa Fe, Sept. 26 – Oct. 1, 2004
[17] VON MÖLLENDORFF, U., et al, "A Nuclear Simulation Experiment for the International Fusion Materials Irradiation Facility (IFMIF)", Report FZKA 6764, October 2002.
[18] PEREL, R.L., WAGSCHAL, J.J., YEIVIN, Y., "Monte Carlo Calculation of Point-Detector Sensitivities to Material Parameters," Nucl. Sci. Eng., 124 (1996),197-209.
[19] PEREL, R.L., "Monte Carlo Calculation of Sensitivities to Secondaries' Angular Distributions", Nucl. Sci. Eng. 143 (2003), 121-131.
[20] FISCHER, U., et al, "Sensitivity analysis for a 14 MeV neutron benchmark using Monte Carlo and deterministic computational methods", Fus. Eng. Des. 70 (2004), 221-232.