Analysis of the ITER Computational Shielding Benchmark with the Monte Carlo TRIPOLI-4 Neutron Gamma Coupled Calculations

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Commissariat à l'Energie Atomique et aux Energies Alternatives,
CEA-Saclay, DEN/DANS/DM2S/SERMA, 91191 Gif-sur-Yvette, France

With the growing interest in using the continuous-energy TRIPOLI-4® Monte Carlo radiation transport code for ITER applications, a key issue that arises is whether or not the released TRIPOLI-4 code and its associated nuclear data libraries are verified and validated for the D-T fusion neutronics calculations. Previous published benchmark results of TRIPOLI-4 code on the ITER related activities have concentrated on the first wall loading, the reactor dosimetry, the nuclear heating, and the tritium breeding ratio. To enhance the TRIPOLI-4 verification and validation on neutron-gamma coupled calculations for fusion device application, the computational ITER shielding benchmark of M. E. Sawan was performed in this work by using the 2013 released TRIPOLI-4.9S code and the associated CEA-V5.1.1 data library. First wall, blanket, vacuum vessel and toroidal field magnet of the inboard and outboard components were fully modelled in this 1-D toroidal cylindrical benchmark. The 14.1 MeV source neutrons were sampled from a uniform isotropic distribution in the plasma zone. Nuclear responses including neutron and gamma fluxes, nuclear heating, and material damage indicator were benchmarked against previous published results. The capabilities of the TRIPOLI-4 code on the evaluation of above physics parameters were presented. The nuclear data library from the new FENDL-3.0 evaluation was also benchmarked against the CEA-V5.1.1 results for the neutron transport calculations. In general, relevant benchmark results were obtained. Both data libraries can thus be run with TRIPOLI-4 for the fusion neutronics study. This work also demonstrates that the "safety factors" concept is necessary in the nuclear analyses of ITER.

Keywords: ITER, neutronics, TRIPOLI-4® Monte Carlo code, Shielding calculation, JEFF-3.1.1, and FENDL-3.0

1. Introduction

The International Thermonuclear Experimental Reactor (ITER) is currently under construction at Cadarache in southern France. The Tokamak Complex foundations of this large scientific facility are already in place. Manufacturing of components for ITER Tokamak is underway in ITER members' industries all over the world. Major technical challenges associated with the design, fabrication, assembly, and integration of the ITER Tokamak components have to be compromised between ITER staffs in order to follow the cost and schedule targets for the project [1].

ITER nuclear analyses are highly complex activities. Nuclear responses including neutron and gamma fluxes, nuclear heating, gases production, radiation dose and material damage estimation are essential physics parameters to be evaluated. The conduction of ITER nuclear analyses is currently scattered and iterated between ITER Central Teams, ITER Domestic Agency teams, and contractors of both. Because the results of nuclear analyses affect many ITER systems at once, accurate, detailed and extensive calculation models are required to obtain reliable solutions [2].

The priority issues on current ITER nuclear analysis are the TF (toroidal field) coil heating and the shut-down dose rates in the cryostat. The verification of the nuclear analyses by experimental benchmarks, the verification of nuclear data by computational benchmarks, and the advanced benchmark study by using a wider range of nuclear analysis codes are also important [3].

Continuous-energy Monte Carlo radiation transport calculations are regularly performed by the engineers and scientists on ITER nuclear analyses. TRIPOLI-4® is the fourth generation of the TRIPOLI® family of Monte Carlo codes developed by CEA [4]. With the growing interest in using the continuous-energy TRIPOLI-4 Monte Carlo transport code on ITER applications, a key point is to make sure that the released code and its associated nuclear data libraries are verified and validated for the D-T fusion neutronics calculations.

Accordingly, to enhance the TRIPOLI-4 verification and validation on neutron, gamma, and neutron-gamma coupled calculations for ITER application, many experimental and computational benchmarks have been performed on the related physics parameters, including the 3-D first wall loading, the reactor dosimetry, the nuclear heating, and the tritium production from the Test Blanket Module (TBM) mock-ups.

The capabilities of the TRIPOLI-4 code on the evaluation of nuclear heating, gases production, and material damage estimation have been renewed in the 2013 released TRIPOLI-4.9S version. The associated

Corresponding author: yi-kang.lee@cea.fr

CEA-V5.1.1 nuclear data library, mainly based on the JEFF-3.1.1 evaluation, is available with the code package. The purposes of this study are firstly to extend the validation database of the TRIPOLI-4 code on ITER neutronics related physics parameters and secondly to test the CEA-V5.1.1 data library for nuclear fusion applications. The new released FENDL-3.0 evaluation is also tested to verify its compatibility with the code.

To eliminate any geometry model uncertainty, the early 1-D computational ITER shielding benchmark of M. E. Sawan [5] was addressed in this work. Since the FENDL-2.1 is cited as the reference nuclear data library for current ITER neutronics calculations, the published results based on FENDL-2.1 were also used to compare with the TRIPOLI-4 (CEA-V5.1.1) results [6-8].

2. Computational ITER shielding benchmark

The 1-D computational ITER shielding benchmark was initially prepared to test FENDL-1.0 multi-group data with ONEDANT discrete ordinates radiation transport code [5]. Fig. 1 shows the ITER 1-D shield benchmark model and the associated dimensions and materials. This benchmark was then applied by A. Serikov to check FENDL-1 and FENDL-2 pointwise data with MCNP transport code [6]. Recently, it was routinely used to verify the FENDL-3 libraries [7-10].

This simplified ITER benchmark was designed to represent the reference steel/water shielding blanket model in the early reacor outline design. The basic components including first wall (FW), blanket, vacuum vessel (VV) and toroidal field (TF) magnet of the inboard (IB) and outboard (OB) regions were completely included in the benchmark model. The initial purpose of this 1-D toroidal cylindrical benchmark model was mainly to clarify the discrepancies found in the nuclear data for fusion neutronics calculations. With the central D-T neutron sources, this benchmark can also be applied to verify and validate modern neutron transport codes and to test improved evaluations of nuclear data.

According to the model in Fig. 1, the FW is 1.4 cm thick, consisting of 0.8 cm thick Be coating and 0.5 cm copper attached to 0.1 cm thick SS316 steel. The shielding blanket is 52.6 cm thick with alternating layers of SS316 and water. A double wall Inconel-625 VV is used with single size water cooled SS316 balls. The VV walls are 5 cm thick. A back shield zone made of lead and boron carbide is used at the back of the vessel. The total VV thickness is 45.5 cm in inboard region and 61.9 cm in outboard region.

A uniform 14.1 MeV neutron source is set in the plasma zone. The angular distribution of the neutron source is isotropic. The source strength in the plasma zone is normalized to 6.1E17 n/cm.s yielding IB and OB neutron wall loadings of 1 and 1.5 MW/m^2, respectively.

The material composition of the Fig. 1 is well defined in the reference [5]. The FW copper zone is a mixture of Cu, Be, and Ni. The TF coil insulator is composed of R-glass epoxy. The magnet zones are a volume mixture of SS316 (47%), Cu (12%), liquid helium (17.2%), R-glass epoxy (13.3%), Nb3Sn (3%), and bronze (7.5%). The benchmark physics parameters include neutron and gamma fluxes in the FW layers (Be, Cu, SS316), peak neutron and gamma fluxes in VV and magnet, peak nuclear heating in selected zones, and peak dpa per full power year (FPY) of irradiation in zones with SS316 steel.

3. TRIPOLI-4 neutron and gamma calculations

The TRIPOLI-4 Monte Carlo radiation transport code has been widely used in radiation shielding, criticality safety and fission reactor physics fields to support French nuclear energy research and industrial applications [4]. Based on the international benchmarks and the CEA internal measurements, extensive validation studies of TRIPOLI-4 on nuclear heating of research reactors, radiation damage of reactor grade steels, neutron dosimeter activation analysis, shielding materials optimization, time-of-flight D-T neutron experiments, and reactor radiation skyshine calculations have been performed [11-17].

Basically, the TRIPOLI-4 transport code is a neutron and gamma particle fluxes solver. The production and transport secondary gamma, produced from neutron inelastic scattering (n,n'), radiative capture (n,γ), and other reactions such as (n,p), (n,α), and (n,T) etc. are simulated in the neutron and γ coupled run as far as the gamma production data are available in the nuclear data library. Nuclear heating and Fe radiation damage results were evaluated by using related tally options.

Nuclear heating calculation

The magnets surrounding the ITER Tokamak will be cooled to very low temperatures, approximately minus 269°C, in order to keep the superconductor coils working. The knowledge of nuclear heating levels in the different ITER Tokamak components is essential for an accurate design analysis. Continuous energy Monte Carlo neutron-γ coupled transport calculation enables not only to analyse the neutron and γ fluxes in the ITER Tokamak, but also to know "how many fusion neutrons, inelastic gammas, and capture gammas etc. will reach the TF coils, how much they will heat them" [3].

In order to benchmark against the published peak nuclear heating for selected positions of the benchmark model, the unit of power density results is represented by W/cm^3. Two ways can be used to calculate the nuclear heating with TRIPOLI-4, the first applies the KERMA response functions from the elaborated data library on the calculated neutron and γ fluxes, the second one, used in this study, computes directly the deposited energy, in MeV, of neutrons and γ for all collision events in a specific volume cell. Considering the neutron source intensity per unit time, the volume of the target cell or mesh, and the conversion of energy units, the sum of neutron heating and γ heating is our benchmark item.

Fe radiation damage calculation

The energetic fusion neutrons interacted with ITER structure materials will produce charged particles and recoil nuclei. These interaction products can cause damage to the crystalline structure of the materials that they pass through. And these radiation damages in metal produced during the D-T neutron irradiation can cause the embrittlement of steels present in the reactor FW, blanket, and VV. Therefore, the radiation damage is one of the key limiting factors for reactor lifetime and its evaluation is important in ITER nuclear analyses.

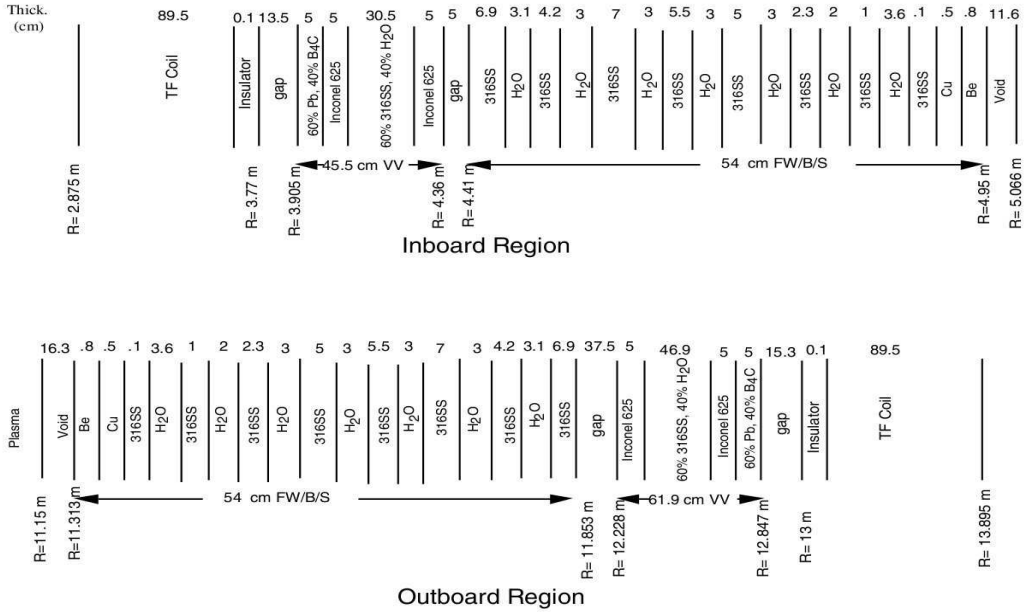

Fig.1 Radial configuration of the ITER 1-D toroidal cylindrical model with inboard and outboard regions [5].

A major source of neutron radiation damage in metals is the displacement of atoms from their normal lattice sites. The number of displacements per atom (dpa) associated with neutron irradiation depends on the amount of energy deposited in the material by the neutrons. In order to benchmark against the published peak Fe radiation damage in SS316 steel for selected positions of the ITER benchmark model, the results are represented by dpa/FPY, where the dpa is calculated with TRIPOLI-4 and normalized to the neutron source (6.1E17 n/cm.s), and the FPY means the full power year irradiation time (3.154E7 s).

Two ways were used in this study to calculate the dpa with TRIPOLI-4. The first one applies the dpa response function from the International Reactor Dosimetry File (IRDF-2002) on the calculated neutron flux. The second and most recent one computes the number of displaced atoms per unit time, in agreement with the specifications in the HEATR module of the NJOY code. The results depend on the displacement energy, Ed, provided by the user [4].

The 640-groups IRDF-2002 dpa response function was taken from the ASTM-E693 standard for characterizing neutron exposures in iron and low alloy steels in terms of dpa. HEATR computes the damage-production energy, which can be correlated to macroscopic damage, such as tensile strength, ductility, or resistivity, through phenomenological factor dpa.

4. Calculation results and discussions

Tables 1 and 2 present the TRIPOLI-4 calculated peak neutron flux for selected positions of the benchmark model. Generally, CEA-V5.1.1 and FENDL-3.0 data libraries produced very close results. The slightly increase of neutron flux in VV wall (Inconel-625) by using FENDL-3.0 was also observed in previous studies when comparing to FENDL-2.1 results [8-9]. The results of Table 2 show that about 20% difference was obtained between TRIPOLI-4 and MCNP5 codes in magnet TF coil zone. This difference appears only at the deep penetrated magnet zone. It is mainly due to the different boron compositions of B_4C in the back shield of VV [5, 6]. The uncertainty of Monte Carlo calculations contributes slightly due to the statistical convergence.

Table 3 and 4 show the peak gamma flux and the nuclear heating benchmark results for selected positions of the benchmark model. Generally, a good agreement was obtained between the TRIPOLI-4 (CEA-V5.1.1) and the MCNP5 (FENDL-2.1) calculations when the boron compositions in VV back shield of reference [6] were used. The uncertainty of Monte Carlo calculations contributes mainly to the slight difference. Table 5 shows that the gamma heating dominates the total nuclear heating in most ITER parts. Behind the blanket steel/water shielding, the neutron energy spectrum becomes softer and the peak neutron heating of VV drops to less than 10% of the total nuclear heating.

Tables 6 and 7 show the radiation damage benchmark results. In the VV zone, the radiation damage indicator (dpa/FPY) reasonably decreases due to

the blanket shielding. Depending on the dpa calculation methods and the threshold displacement energies used in Fe [4, 18], the dpa results present a difference of 5-15%.

5. Conclusion

In this study, TRIPOLI-4® Monte Carlo calculations of the ITER 1-D toroidal cylindrical shielding benchmark were performed. Nuclear analyses including neutron and γ flux, nuclear heating, and material damage indicator were benchmarked and validated against previous published results. Two nuclear data libraries CEA-V5.1.1 and FENDL-3.0 were tested and verified. Generally, relevant benchmark results were obtained.

This work also demonstrates that the "safety factors" concept is necessary in the 3-D nuclear analyses of ITER [19]. With the present 1-D neutronics benchmark, the uncertainty already comes from the nuclear data, the boron compositions input data, and the dpa calculation methods and data. Future work will be reported on the He and H gases production, the gamma heating with FENDL-3.0, and the insulator dose for TF coil.

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Table 1: TRIPOLI-4 calculated peak neutron flux for selected positions of the ITER benchmark model

ITER structure component	TRIPOLI-4				
	CEA-V5.1.1		FENDL-3.0		% change
	Neutron flux	1σ %	Neutron flux	1σ %	
IB-FW					
Be	3.53E14	0.01	3.53E14	0.01	0.00
Cu	3.10E14	0.01	3.10E14	0.01	0.00
SS316	2.97E14	0.01	2.97E14	0.01	0.00
VV	8.52E11	0.09	8.73E11	0.06	2.46
Magnet (*)	2.91E09	2.00	2.91E09	1.31	0.00
TF coil			2.78E09	1.20	
OB-FW					
Be	4.38E14	0.01	4.38E14	0.01	0.00
Cu	3.96E14	0.01	3.96E14	0.01	0.00
SS316	3.81E14	0.01	3.81E14	0.01	0.00
VV	1.18E12	0.05	1.21E12	0.03	2.54
Magnet (*)	4.37E08	2.85	4.40E08	1.90	0.01
TF coil			4.18E08	1.67	

* Epoxy – Magnet insulator [5].

Table 2: Benchmark calculated peak neutron flux for selected positions of the ITER benchmark model

ITER structure component	TRIPOLI-4		MCNP5 [9]		T4/M5 ratio
	FENDL-3.0				
	Neutron flux	1σ %	Neutron flux	1σ %	
IB-FW					
Be	3.53E14	0.01	3.52E14	0.05	1.00
Cu	3.10E14	0.01	3.09E14	0.05	1.00
SS316	2.97E14	0.01	2.96E14	0.06	1.00
VV	8.73E11	0.06	8.66E11	0.19	1.01
Magnet					
TF coil	2.78E09	1.20	3.50E09	0.45	0.79*
OB-FW					
Be	4.38E14	0.01	4.37E14	0.03	0.00
Cu	3.96E14	0.01	3.94E14	0.03	0.00
SS316	3.81E14	0.01	3.80E14	0.03	0.00
VV	1.21E12	0.03	1.20E12	0.09	1.01
Magnet					
TF coil	4.18E08	1.67	5.12E08	0.41	0.82*

* TRIPOLI-4 boron compositions in VV back shield followed the benchmark dataset [5] but are different from those used in [6] and [9].

Table 3: Benchmark calculated peak gamma flux for selected positions of the ITER benchmark model

ITER structure component	TRIPOLI-4 *		MCNP5 [6]		T4/M5 ratio
	CEA-V5.1.1		FENDL-2.1		
	Gamma flux	1σ %	Gamma flux	1σ %	
IB-FW					
Be	2.96E14	0.01	2.97E14	0.05	1.00
Cu	2.87E14	0.01	2.88E14	0.05	1.00
SS316	2.86E14	0.01	2.87E14	0.06	1.00
VV	4.30E11	0.11	4.31E11	0.19	1.00
Magnet					
TF coil	8.01E08	2.29	8.30E08	0.45	0.96
OB-FW					
Be	3.36E14	0.01	3.37E14	0.03	1.00
Cu	3.36E14	0.01	3.37E14	0.03	1.00
SS316	3.41E14	0.01	3.42E14	0.03	1.00
VV	5.86E11	0.07	5.88E11	0.09	1.00
Magnet					
TF coil	1.19E08	3.10	1.23E08	0.41	0.97

* To eliminate the difference on boron compositions in the VV back shield, the boron compositions were taken from [6] instead of [5].

Table 4: Benchmark calculated peak nuclear heating (W/cm^3) for selected positions of the ITER benchmark model

ITER structure component	TRIPOLI-4 CEA-V5.1.1		MCNP5 [8] FENDL-2.1		T4/M5 ratio
	Power density	1σ %	Power density	1σ %	
IB-FW					
Be	1.03E01	0.03	1.01E01	0.05	1.02
Cu	2.03E01	0.07	2.02E01	0.06	1.00
SS316	1.77E01	0.20	1.78E01	0.08	0.99
VV	2.62E-2	0.72	2.62E-2	0.18	1.00
Magnet					
TF coil	3.67E-5	3.50	3.66E-5	0.45	1.00
OB-FW					
Be	1.42E01	0.02	1.39E01	0.03	1.02
Cu	2.49E01	0.04	2.47E01	0.04	1.01
SS316	2.21E01	0.10	2.23E01	0.05	0.99
VV	3.56E-2	0.38	3.57E-2	0.09	1.00
Magnet					
TF coil	5.37E-6	3.94	5.38E-6	0.43	1.00

Table 5: TRIPOLI-4 calculated peak nuclear heating (W/cm^3) for selected positions of the ITER benchmark model

ITER structure component	TRIPOLI-4 (CEA-V5.1.1) Gamma		Neutron		Gamma --------- Neutron
	Power density	1σ %	Power density	1σ %	
IB-FW					
Be	2.40E00	0.03	7.91E00	0.02	0.30
Cu	1.78E01	0.02	2.48E00	0.07	7.18
SS316	1.53E01	0.03	2.32E00	0.19	6.59
VV	2.41E-2	0.18	2.09E-3	0.69	11.5
OB-FW					
Be	2.80E00	0.02	1.14E01	0.01	0.25.
Cu	2.11E01	0.01	3.82E00	0.04	5.52
SS316	1.85E01	0.02	3.58E00	0.10	5.17
VV	3.28E-2	0.08	2.76E-3	0.36	11.9

Table 6: Benchmark calculated peak radiation damage in Fe for selected positions of the ITER benchmark model

ITER structure component	TRIPOLI-4 CEA-V5.1.1 & IRDF-2002*		MCNP5 [7] FENDL-2.1		T4/M5 ratio
	Fe dpa/FPY	1σ %	Fe dpa/FPY	1σ %	
IB					
FW	8.15E00	0.01	7.79E00	0.07	1.05
Blanket	4.65E00	0.01	4.43E00	0.07	1.05
VV	3.68E-3	0.20	3.35E-3	0.24	1.10
OB					
FW	1.24E01	0.01	1.18E01	0.03	1.05
Blanket	7.29E00	0.01	6.94E00	0.03	1.05
VV	5.51E-3	0.10	5.02E-3	0.12	1.10

* ASTM-E693 standard for dpa response function.

Table 7: TRIPOLI-4 calculated peak radiation damage in Fe for selected positions of the ITER benchmark model

ITER structure component	TRIPOLI-4 (a) CEA-V5.1.1 & IRDF-2002		TRIPOLI-4 (b) CEA-V5.1.1 & Ed = 44 eV *		T4 (b) -------- T4 (a)
	Fe dpa/FPY	1σ %	Fe dpa/FPY	1σ %	
IB					
FW	8.15E00	0.01	8.99E00	0.48	1.10
Blanket	4.65E00	0.01	5.12E00	0.21	1.10
OB					
FW	1.24E01	0.01	1.37E01	0.26	1.10
Blanket	7.29E00	0.01	8.05E00	0.11	1.10

* Displacement energy Ed of iron [4, 18]

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