Neutron Deep Penetration Calculations in Light Water with Monte Carlo TRIPOLI-4® Variance Reduction Techniques

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Abstract

Nuclear decommissioning takes place in several stages due to the radioactivity in the reactor structure materials. A good estimation of the neutron activation products distributed in the reactor structure materials impacts obviously on the decommissioning planning and the low-level radioactive waste management. Continuous energy Monte-Carlo radiation transport code TRIPOLI-4 has been applied on radiation protection and shielding analyses. To enhance the TRIPOLI-4 application in nuclear decommissioning activities, both experimental and computational benchmarks are being performed. To calculate the neutron activation of the shielding and structure materials of nuclear facilities, the knowledge of 3D neutron flux map and energy spectra must be first investigated. To perform this type of neutron deep penetration calculations with the Monte Carlo transport code, variance reduction techniques are necessary in order to reduce the uncertainty of the neutron activation estimation. In this study, variance reduction options of the TRIPOLI-4 code were used on the NAIADE 1 light water shielding benchmark. This benchmark document is available from the OECD/NEA SINBAD shielding benchmark database. From this benchmark database, a simplified NAIADE 1 water shielding model was first proposed in this work in order to make the code validation easier. Determination of the fission neutron transport was performed in light water for penetration up to 50 cm for fast neutrons and up to about 180 cm for thermal neutrons. Measurement and calculation results were benchmarked. Variance reduction options and their performance were discussed and compared.

KEYWORDS: TRIPOLI-4 Monte Carlo Code, Light water shielding, Neutron transport, Variance reduction

I. Introduction

Nuclear decommissioning is one of the most important activities in current nuclear industry. Generally it takes place in several stages due to the radioactivity in the nuclear facilities. The decontamination work can be actively performed to reduce the removable radioactive materials from the contaminated zones. The radioactivity caused by the neutron activation of shielding and structure materials can be actively removed or passively treated with the cooling time. A good estimation of the neutron activation products distributed in the shielding and structure materials impacts obviously 1) the decommissioning techniques, planning, and costs, 2) the radiation protection implementation, and 3) the low-level radioactive waste management [1, 2].

The continuous-energy Monte-Carlo radiation transport code TRIPOLI-4 has been used for radiation protection and shielding analyses [3]. To develop its application on nuclear decommissioning activities, both experimental and computational benchmarks are being developed and performed. For the neutron activation calculation of shielding and structure materials of nuclear facilities, the knowledge of 3D neutron flux map and the energy spectra must be first investigated. In this kind of neutron deep penetration calculation in shielding, variance reduction techniques are necessary in order to reduce the uncertainty of the Monte-Carlo calculations [3, 4].

Different water shielding benchmarks are available from the OECD/NEA SINBAD database. The NAIADE 1 water benchmark was essential because of its important water thickness [5, 6]. In this study, the fission neutron deep penetration in water shielding was investigated with TRIPOLI-4 code for NAIADE 1 water benchmark. In order to make the code validation easier, a simplified shielding model of the NAIADE 1 water experiment was first developed in this work from the 2007 published fixed-source sub-criticality model [6]. Calculations were performed in water for penetration up to 50 cm for fast neutrons and up to 180 cm for thermal neutrons. Measurement and calculation results for equivalent fast and thermal neutron flux of ^{31}P(n,p), ^{32}S(n,p), and ^{10}B(n,α) were benchmarked. Different variance reduction techniques based on the INIPOND module of TRIPOLI-4 code were investigated. Their performances were compared and discussed.

II. NAÏADE 1 light water benchmark

NAÏADE 1 shielding experiments were realized at Fontenay -aux-Roses (France) during the 1960s and 1970s. These

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experiments were designed to study the fission and thermal neutron flux attenuation in various shielding materials including water, graphite, iron and concrete. The related calculation benchmarks were reassessed with TRIPOLI-4 Monte Carlo code by J.-C. Nimal [5-6]. Fig. 1 shows the configuration of the NAIADE 1 experiments. Neutron source in NAIADE 1 was produced from a natural uranium fission plate converter irradiated by a collimated thermal neutrons beam coming from the graphite reflector of the ZOE heavy water reactor. The thermal column of ZOE reactor is shown in the right side of Fig. 1. The fission plate and its Boral screen were installed in the central part. The removable shielding tank filled with light ordinary water is presented in the left side of Fig. 1.

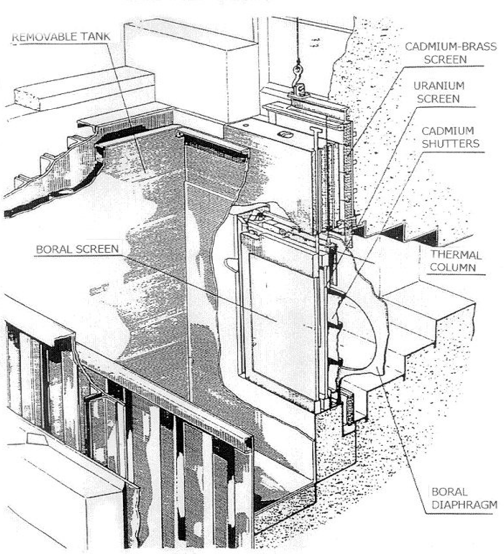

Figure 1: **NAIADE 1 shielding experiment facility (Right - Thermal neutron column from ZOE reactor core, Middle - Natural Uranium fission plate and Boral screen, Left – Removable shielding tank for light water) [5, 6]**

The water along the fission plate axis was 250 cm deep. The square section of the tank was 300 cm x 300 cm. The tank was surrounded laterally by an ordinary concrete shield of thickness 50 - 80 cm. This sub-critical system was first evaluated with the TRIPOLI-4 sub-critical option [6]. The following detectors were used in experiments: ^{31}P(n,p), ^{103}Rh(n,n'), and ^{32}S(n,p) dosimeters for fast neutron flux measurements, ^{115}In(n,γ), ^{55}Mn(n,γ), and ^{197}Au(n,γ) foil covered by cadmium for epithermal neutron, and bare ^{55}Mn(n,γ) and BF_3 chamber for thermal neutron measurements.

III. TRIPOLI-4 modeling of NAÏADE 1 water shielding benchmark

Fig. 2 shows the TRIPOLI-4 modeling of the NAÏADE 1 light water shielding experiment. The fission plate converter was modelled in the left side in red color. The 250 cm-thick light water in blue color was modelled in the center of the gray concrete wall. Using this shielding experiment to validate different options of TRIPOLI-4, two calculation models were developed. As shown in Figure 3, these two models presented different geometry representations of the experiment structure and tally. Table 1 presents different details in modeling and calculation of these two models.

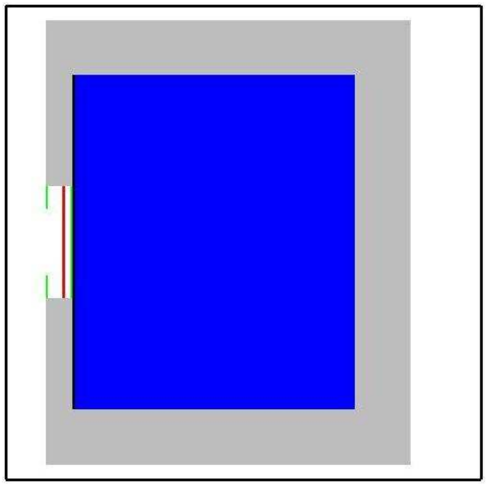

Figure 2: **TRIPOLI-4 modeling of NAIADE 1 light water shielding experiment (Red – natural uranium fission plate, Blue – light water shielding 250 cm x 300 cm x 300 cm, and Gray – ordinary concrete shielding wall) [5, 6]**

The earlier 2006 model simulated the collimated thermal neutron source and the fission neutron attenuation in water via a fixed-source sub-criticality mode. This mode calculates both the neutron multiplication effect of the central fission plate and the neutron transport in water shielding. However in this study, a simplified shielding model of the NAIADE 1 water experiment was developed in order to make the validation work easier on variance reduction techniques and recent options of the code. That means, the present calculations concentrate on the neutron transport from the fission plate to the water by taking into account different TRIPOLI-4 variance reduction options.

IV. TRIPOLI-4 variance reduction techniques

Basically, the TRIPOLI-4 built-in variance reduction techniques such as implicit capture (survival biasing) and Russian roulette, are involved by default in the shielding mode calculation but they are not sufficient for neutron deep penetration transport calculations.

The importance map generator INIPOND module of TRIPOLI-4 can also be used to improve the variance reduction performance and to reduce the user involvement, especially for the neutron deep penetration cases [3-8]. The generated important map is then used by TRIPOLI-4 in the same run to perform importance sampling through the exponential transform method, quota sampling, splitting and Russian roulette, and source biasing.

Different options under INIPOND module were investigated in this study. Generally the importance function from INIPOND is assumed to be factorized in space, energy, and angle variables, with a coupling between space and energy variables. A space mesh and an energy grid were separately defined by the author for the initialization of the importance map by the code.

Benchmark models	SINBAD [6] (2006)	This work (2016)
Mode	Fixed-source sub-criticality	Fixed-source shielding
Simulation	Neutron transport only	Coupled Neutron-photon transport
Neutron source	Thermal neutron from graphite (Mono –directional)	Fission neutron from U plate (Isotropic)
Source distribution	R - θ - Z based on Mn-55 (n,γ) measurements	X-Y-Z based on P-31 (n,p) measurement
Geometry	Analytical surfaces	Combinatorial volume cells
Tally	Surface	Mesh & thin volume
Variance reduction (INIPOND)	Point attractor	Spherical surface attractor
Data library	ENDF/B-VI.r4 & IRDF 1990	JEFF3.2 (CEAV6) & IRDF 2002

Table 1: **NAIADE 1 Water shielding benchmark and TRIPOLI-4 calculation models**

In this initialization step of the TRIPOLI-4 shielding calculation with the INIPOND module, the simulation of the first batches of neutron histories is specific. Case-dependent information is first collected and subsequently used to improve the multi-group and 3D mesh-based important map. As each case may have different geometry volume cells, materials distributions, neutron source energy and space zones, tally energy and space zones, so the particle transport information of the sampled neutrons need to be collected in order to know the visited volume cells and the neutron energy slowing-down in space. The purposes of this batch-based iteration procedure are to regulate and improve the neutron population distribution in geometry and energy space. At the end of this initialization step, the importance map from this learning-by-simulation procedure helps guiding the neutron transport in all next sets of neutron histories.

The "monitoring" option was used by default in the TRIPOLI-4 variance reduction run. The adjustments of the importance map were performed from energy group to energy group by taking advantage of statistics on discrepancies between particle weights and reference weights given by the importance map, when particles slowing down in energy from group to group. Of course the performance of the associated variance reduction depends importantly on the input data dedicated to the INIPOND module.

The options for displaying of collision points and iso-importance curves were helpful to understand the particle propagation in water and useful to improve the importance map calculation. Considering the measurement positions in water, fictitious detector(s) can be placed in deep water of the calculation model so as to act as ''attractor(s)'' for simulated particles.

The β and K parameters of the INIPOND module were usually set in order to adjust the global strength of the "biasing" by the exponential transform techniques [4, 7]. When using the INIPOND AUTO option, the values K were calculated in the code according to the β input by solving the Placzeck equation, after collapsing the pointwise cross-sections in each composition and each energy group. As each mesh can contain different compositions, the initialization of importance map may be built using graph theory with the user-estimated or code-generated K values. Generally the shorter paths in the 3D graph between the neutron source and the "attractor" were also the guiding ways in neutron transport simulation. The optional energy factor α (with a set of parameter values given for each energy group) was also useful to adjust neutron population for high energy neutrons in this work as the uranium thermal fission spectrum has a peak zone around 2 MeV.

Due to the mesh-based variance reduction method used in INIPOND point(s) attractor, a file per thread calculation line is generated to store the importance map data. The size of this file depends on the meshes dimensions in space and energy. To reduce the memory requirement for the importance map calculations of INIPOND, the spherical analytical surface attractor was also chosen for the spatial importance calculation. This option is useful in massively parallel calculations.

V. Results

TRIPOLI-4 calculation results are divided in three parts. The first part shows the intermediate graphic results. These results are helpful to understand the variance reduction effects on fission neutron transport in water, to adjust the variance reduction parameters, and to improve the calculation performance. The second part presents the numerical calculation results of the NAIADE 1 water benchmark including the fast neutron and thermal neutron equivalent flux as a function of water shielding thickness. The third part shows the variance reduction performance results.

The graphic intermediate results including the collision sites maps and the importance maps generated in this study are presented in Fig. 4 and 5. Two different input data sets for the INIPOND variance reduction module, one with discrete attractors and the other with the spherical attractor surface [7], were applied to qualitatively demonstrate the variance reduction effects.

The direction of interest of simulated particles is calculated with the gradient of the importance lines/surfaces and it is perpendicular to the iso-importance surfaces (see Fig. 5). According to the position of the measurement, the neutrons were guided from the fission source plate and the collision sites to the pre-defined attractor(s). For the INIPOND variance reduction, the space mesh dimensions were 7.5 x 7.5 x 7.5 cm and three energy groups were set for fast, intermediate, and slow neutrons. Using the point attractor, initial computational resources are necessary. They depend on the mesh size and the number of energy groups. Several point attractors can be assigned to guide the neutron transport. Using the spherical attractor surface in INIPOND module, the importance map calculation time was shorter and very limited computer memory was necessary. But only one spherical attractor surface can be set.

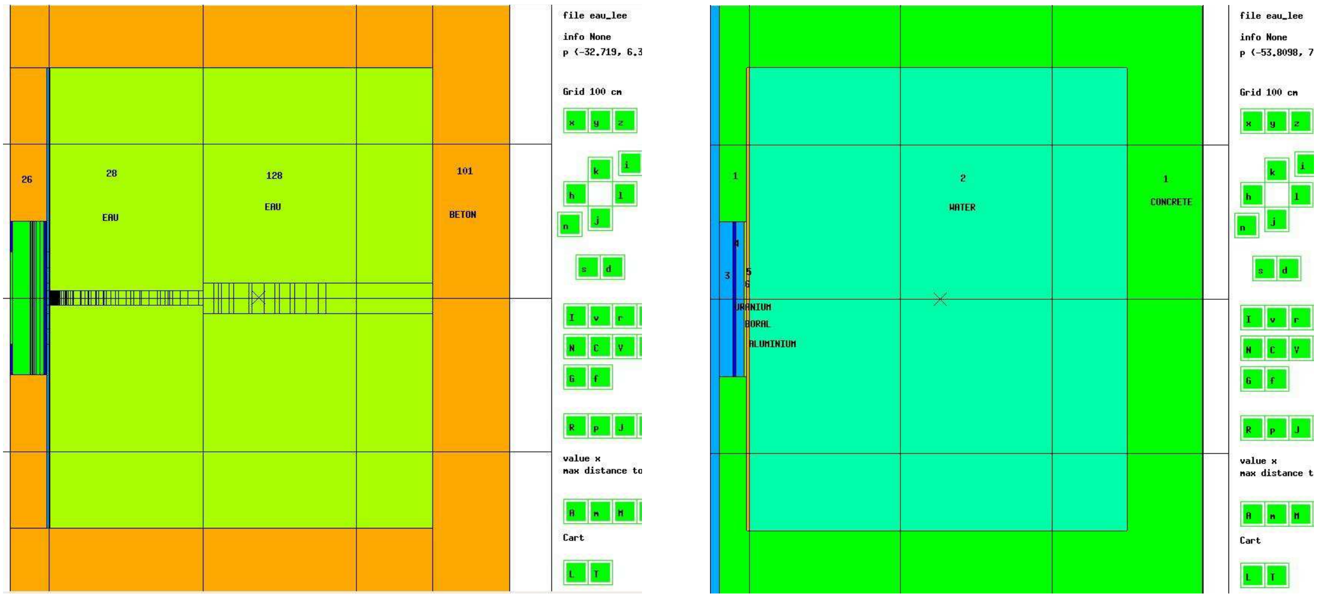

Figure 3: **TRIPOLI-4 modeling of NAIADE 1 light water shielding experiment**
Left: fixed-source sub-criticality model from SINBAD ([6], 2006), Right: related simplified shielding model (2016)

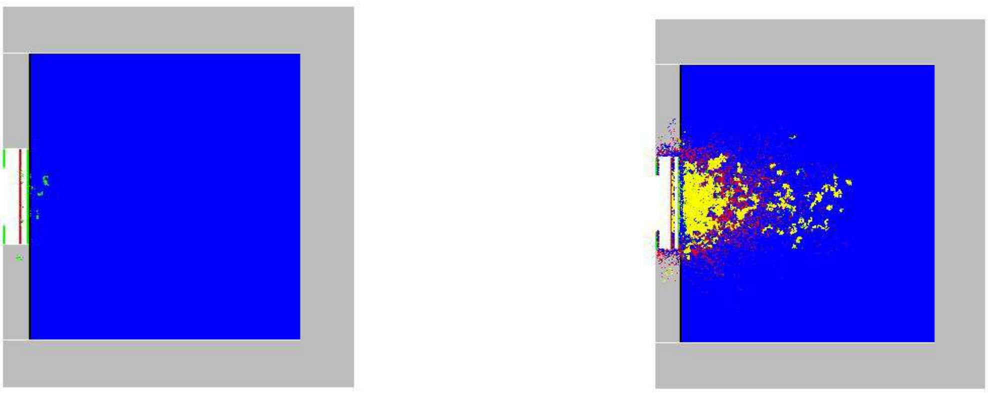

Figure 4: **TRIPOLI-4 calculated projection maps of neutron collision sites for NAIADE 1, 250 cm x 300 cm x 300 cm, light water shielding surrounded by an ordinary concrete and irradiated by fission neutrons from a fission plate**
Left: INIPOND option not used, Right: Variance reduction with INIPOND - Yellow points show the collision sites of slow neutrons.

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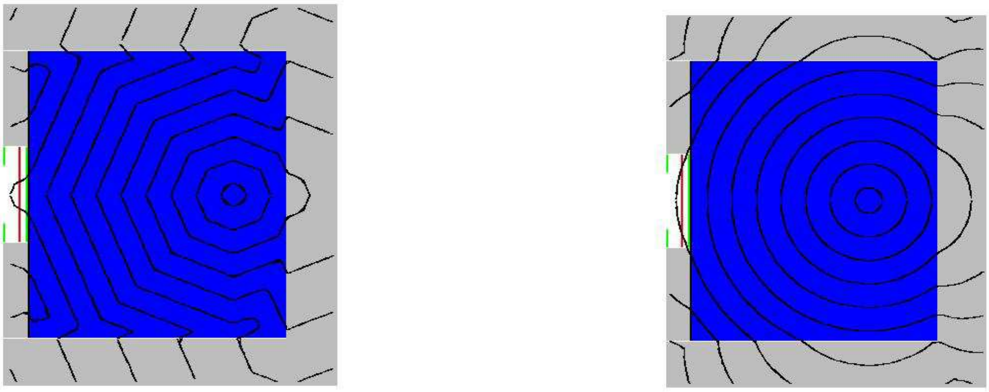

Figures 5: **TRIPOLI-4 calculated iso-importance maps for NAIADE 1, 250 cm x 300 cm x 300 cm, light water shielding surrounded by an ordinary concrete and irradiated by fission neutrons from a fission plate**
Left: Variance reduction with discrete attractor, Right: Variance reduction with a spherical attractor surface

The numerical calculation results are presented in Figures 6 to 9. Figure 6 shows the TRIPOLI-4 calculated and measured equivalent fast neutron flux based on ^{31}P(n,p) dosimeters. The calculation results of this work are generally in good agreement with the previous calculations of 2006 and the measurements of 1965 [6].

It should be noted that the average cross section of ^{31}P(n,p) based on the ^{235}U thermal fission spectrum was used to get the equivalent neutron flux from the calculated reaction rates. A 25% difference of this ^{31}P(n,p) average cross section has been found between 2.858e-2 barns from IRDF-1990 and 3.586e-2 barns from the recent evaluation of IAEA-NDS-0668.

In Figure 6 the calculated fast neutron flux attenuation in water was also shown as a function of penetration thickness. Both the above 1 MeV and the above 0.1 MeV fast neutron flux were included. Generally, they were lower than the equivalent fast neutron flux based on ^{31}P(n,p) dosimeters.

Using the ^{32}S(n,p) dosimeter measurement results, a similar benchmark trend was found in Figure 7. The fission neutron transport in light water for penetration up to 50 cm for fast neutrons was benchmarked. For water thicknesses larger than 30 cm, the calculated fast neutron flux and the equivalent fast neutron flux diverged because of the degradation of the fission neutron spectrum in water and the constant average cross-section of the dosimeter.

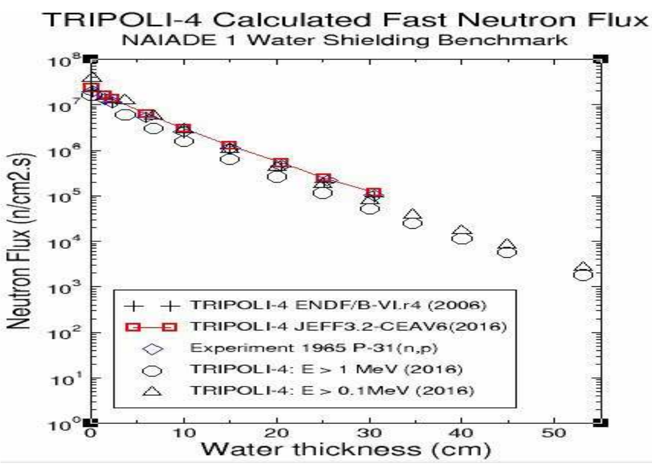

Figure 6: **TRIPOLI-4 calculated fast neutron flux and equivalent fast neutron flux based on ^{31}P(n,p) measurements**

In Figure 8, the calculated equivalent thermal neutron flux attenuation in water was shown as a function of the penetration thickness up to 180 cm. The equivalent thermal neutron flux was obtained from the calculated ^{10}B(n,α) reaction rate. The ^{10}B(n,α) average cross-section based on the 2200 m/s thermal neutron was 3840 barns [6].

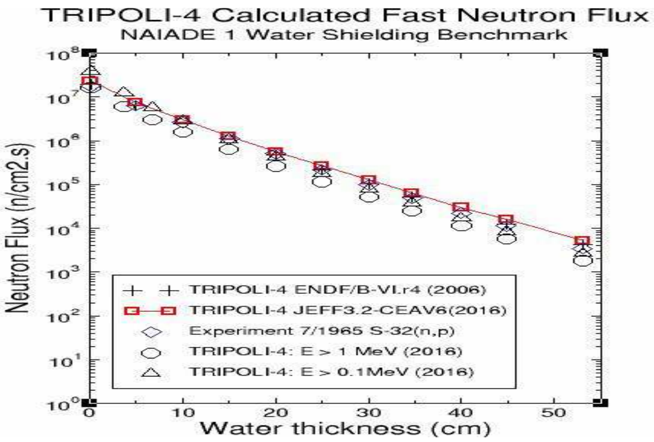

Figure 7: **TRIPOLI-4 calculated fast neutron flux and equivalent fast neutron flux based on ^{32}S(n,p) measurements**

The typical build-up of thermal neutron flux in the first water zone was observed for water thicknesses from 0 to 5 cm in Figure 8. The thermal neutron flux attenuation factor of 180 cm light water was about ten decades. The TRIPOLI-4 INIPOND variance reduction module was really helpful. The calculation results of this work are in good agreement with the previous calculations of 2006 and the measurements of 1957-1960 [6].

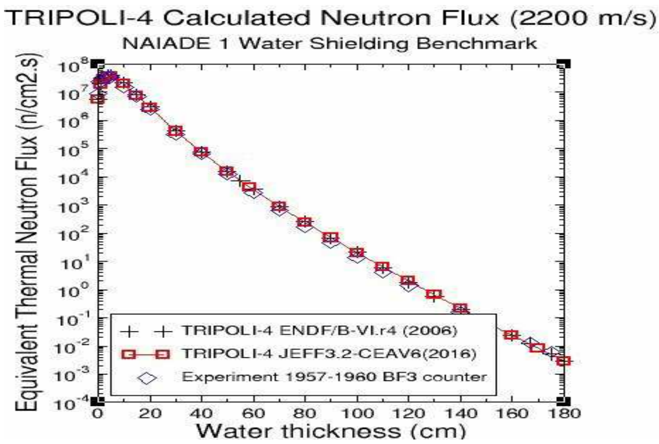

Figure 8: **TRIPOLI-4 calculated equivalent thermal neutron flux based on the ^{10}B(n,α) reaction rate of BF3 counter measurements**

The TRIPOLI-4 calculated equivalent dose rates in water as a function of the penetration thickness up to 90 cm was shown in Figure 9. For neutron dose rate, the calculation results of this work were in good agreement with the previous calculations of 2006 [6]. The dose rates from secondary gamma-ray contributions were also presented in this Figure. The main neutron absorption in water is based on the ^{1}H(n,γ) capture reaction. The 2.2 MeV secondary gamma dose was build-up in the first water zone and its domination in dose contribution appeared from 40 cm depth in water.

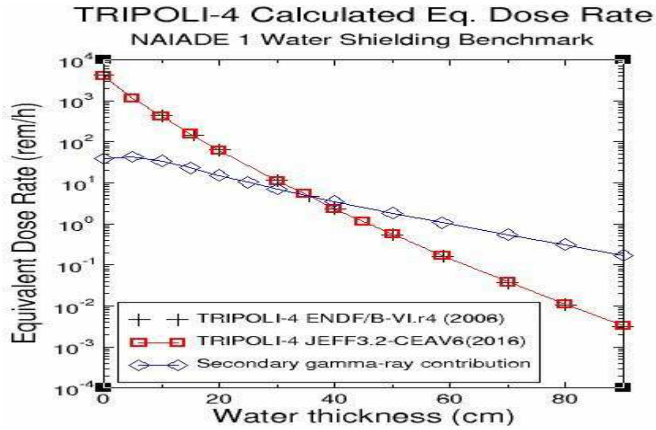

Figure 9: **TRIPOLI-4 calculated equivalent dose rates of neutron and secondary gamma-ray generated in water**

The performance study of the INIPOND variance reduction is presented in Table 2. Different options of the TRIPOLI-4 INIPOND variance reduction were used in this study to demonstrate and compare their performance on the fission neutron deep penetration calculation in water. Both the ^{31}P(n,p) equivalent fast neutron flux and the ^{10}B(n,α) equivalent 2200 m/s thermal neutron flux were taken into account to benchmark against the measurements. As the mean free path of slow neutrons is small and the neutron absorption in water based on the ^{1}H(n,γ) capture reaction is owing to the 1/v nature, the initial effort in adjusting the INIPOND variance reduction parameters was aimed at pushing fission neutron forward. In the same time, tally positions as a function of water thicknesses were assigned. An over push forward of fission neutron was not worthy. From fast to slow energy groups in runs (2) to (5) of Table 2, different K values of INIPOND module were adjusted according to the TRIPOLI-4 output of the initial runs.

FOM	**^{31}P(n,p) Eq. fast flux**	**^{10}B(n,α) - 2200 m/s Eq. thermal flux**
Eq. neutron flux in water depth	30 cm	50 cm
(1) TRIPOLI-4 Analog run	12	1
(2) INIPOND Point attractor	75	300
(3) (2) + Monitoring 0	3470	46
(4) INIPOND Surface attractor	100	137
(5) (4) + Monitoring 0	350	113
(6) (5) + INIPOND AUTO	3900	800

Table 2: **TRIPOLI-4 variance reduction performance for equivalent neutron flux calculation of NAIADE 1 Water shielding benchmark**

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The performance of the calculation with variance reduction was evaluated with the factor FOM (figure of merit). The FOM is defined as FOM = $1 / (\sigma^2 t)$, where the standard deviation σ and the run time t are available from the code output. The FOM values in Table 2 were calculated by the author and their uncertainties were estimated to be less than 5 %.

The no monitoring feature "Monitoring 0" [7] in runs (3), (5), and (6) of Table 2 deactivated the monitor of importance and the regulation of neutron population between neutron energy groups as presented in section IV. That is why the FOM values of runs (3) and (5) show an improvement in equivalent ^{31}P(n,p) fast neutron flux, compared to runs (2) and (4) with the "monitoring" option. In the same time, the regulation of neutron population between energy groups was deactivated so the FOM values of equivalent thermal neutron flux in runs (3) and (5) decreased, compared to runs (2) and (4). When the option INIPOND AUTO in run (6) was activated with the spherical surface attractor option, the best FOM of this test was obtained for both fast and thermal neutron flux. In fact the attenuation of neutron flux in NAIADE 1 water benchmark was in important pure water. Neutron streaming was negligible. Different materials and void zones in attenuation way were absent. Under these conditions, the INIPOND AUTO option worked perfectly and produced converged results on both fast and thermal neutron flux.

```
VARIANCE_REDUCTION      NEUTRON        // Particle type

  GRID 4    20.   2.   0.005.   1.E-11      // Three groups in energy mesh

  ALFA        0.2    0.        0.           // Adjust group population size
  DETECT_RHO 1      1.      0.5             // Sphere surface attractor & β

 MESH      45        53        53          // VR geometry mesh no.
          7.247     7.551    7.551         //   Mesh dimension (cm)
            FRAME   CARTESIAN
        -25.9     -200.1    -200.1          // Mesh geometry origin (x, y, z)
     1.   0.   0.     0. 1. 0.    0. 0. 1.     //   vectors X Y Z
 END_MESH

 INIPOND   AUTO
   OMEGA SET_OMEGA SPHERE 50.    0.    0.   // Sphere center
 END_INIPOND

END_VARIANCE_REDUCTION
```

Table 3: **TRIPOLI-4 variance reduction (VR) input of run (6) for equivalent neutron flux calculation of NAIADE 1 Water shielding benchmark**

Table 3 shows the run (6) variance reduction input data. Three energy groups were set from 20 MeV to 1E-11 MeV to cover the fission neutron and the thermal neutron zones. A cartesian mesh geometry with 45 x 53 x 53 meshes in X, Y, and Z was set to cover the transport simulation geometry zone 326 x 400 x 400 cm^3 with a mesh size around 7.5 cm. The center of fission plate was placed at (-10, 0, 0) (see Fig. 2, red zone) and that of the spherical surface attractor was placed at (50, 0, 0) (Fig. 2, blue water zone) for this variance reduction performance study. The radius of the attractor sphere was set to 1 cm and the β value to 0.5. An α value was set only in the fast neutron group to improve the neutron population distribution above 2 MeV because only fast neutrons have a significant probability to penetrate into deep water.

VI. Conclusions

To support the nuclear decommissioning activities on reactor structure materials activation calculations, the TRIPOLI-4 Monte Carlo transport code capabilities on fission neutron shielding calculations were demonstrated by using the NAIADE 1 water benchmark experiments. Both the shielding mode and the fixed-source sub-criticality mode of the code were used. Collision sites projection maps were generated to show the neutron migration and the neutron energy slowing down along with the depth of the neutron transport routes. Iso-importance maps were generated to verify the direction dependent variance reduction effects and the shielding material dependent importance gradient. Neutron penetration in water up to 50 cm for fast neutrons and up to 180 cm for thermal neutrons was taken into account. Calculation results of equivalent fast neutron flux and thermal neutron flux were validated against the measurements. The variance reduction options of TRIPOLI-4 code were helpful to perform these calculations with the INIPOND point attractor and the INIPOND spherical surface attractor. A simplified NAIADE 1 water shielding model was proposed in this work. It allowed performing the code validation easier. New developed options for variance reduction in TRIPOLI-4 will be investigated with this simplified model in a future work.

Acknowledgment

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