PRELIMINARY SHIELDING CALCULATIONS (PHASE 1) FOR THE MIRACLES INSTRUMENT

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Introduction

This report describes shielding calculations performed for the instrument MIRACLES. All the calculations aimed to provide, outside the instrument (beamline and cave) a safe environment with dose limits corresponding to a ESS Supervised Area (*H* < 3 μSv/h) [ESS-0001786].

Calculations were carried out analytically (for a first approach) and using Monte Carlo (MCNPx). The first approach to estimate the thickness of the shielding for gamma photons in every case is to consider the flux of gamma photons just outside of the shield, given by [Sullivan, Lamarsh]:

$$\varphi = \sum \frac{\varphi_{0i} B_i e^{-\mu t}}{4\pi r_i^2} dr_i$$

where φ_0 is the produced flux of the source (supermirror coating, sample,…) prior to shielding, *B* is the buildup factor (estimated using [Lamarsh]), μ is the attenuation coefficient (obtained using [NIST] database), *t* is the thickness of the shield, and *r* is the distance source-detector point. From here, the estimated dose is obtained applying the flux to dose conversion factors (*C*) applied for γ-ray photons [ESS-0019931]. After the analytical estimations, a more complex analysis to obtain a detail overview of the shielding and dose map using Monte Carlo calculations in extensive areas is achieved.

This report, such as the official documents to be submitted during Tollgate 2, is a working document, and ongoing development is envisaged. Several areas were selected for preliminary calculations: the curved guide section of the beamline, the cave, and the beam stop. Further extension of the calculations, and more complex scenarios will be developed in the following months.

1. Primary Spectrometer: curved section of the beamline

1.1. Preliminary Shielding Design Curve for Neutrons

MIRACLES, like any other instrument, features a neutron guide that is essentially a hole through the bunker. The presence of such a feature will cause a large number of neutrons to escape said barrier, to an area that can be potentially accessed to the general public. It is necessary to shield the guides throughout their path, in order to ensure that the public will not be subject to doses exceeding limits.

Because the guide must transport the low-energy neutrons to the instrument while shielding as many as possible from those of higher energy, it features a curved section with a very large radius. This, combined with the reflecting coating of the guide, allows a large number of thermal neutrons to travel down the guide while making higher energy neutrons be scattered. However, said neutrons need to be shielded effectively.

In this document, a MonteCarlo study of the neutron transport throughout the guide is presented. MCNP6 was used, with ENDF VII/B libraries. For the generation of the geometry, SuperMC 3.1 was used, with some manual modifications. Neutron source used is taken from the calculations of our colleagues in ESS for MMX as a provisional source. All the calculations were performed in the ESS DMSC cluster.

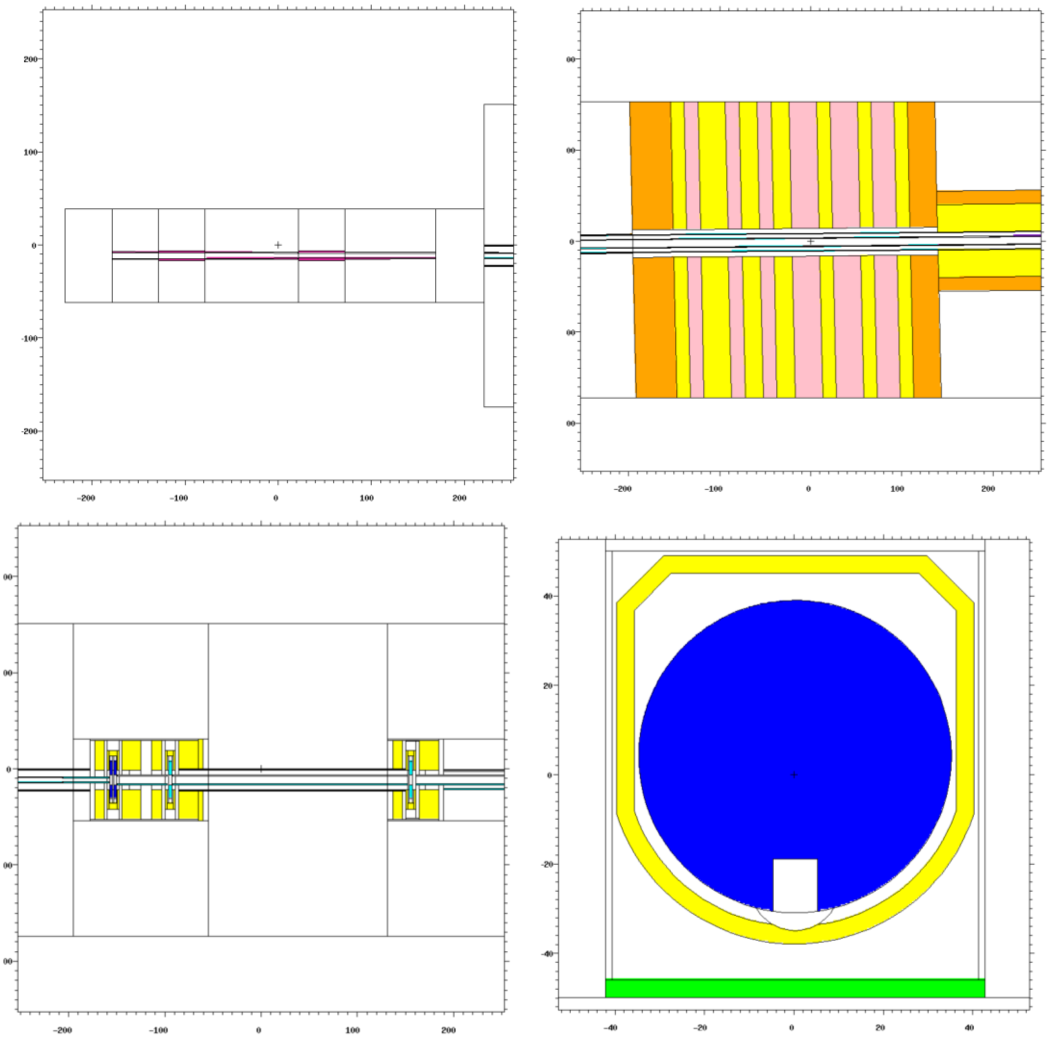

Fig. 1: (above) Geometry of the NBOA and bunker-wall feedthrough; (below) Geometry of the choppers (1 to 4).

The origin of coordinates correspond to the beginning of the MIRACLES beamline at the exit of the monolith wall and light shutter (L=6 m → X=0 m):

- NBOA, consisting of 3.5m of copper, with a 5x6 cm rectangular section. (X from -4 to -0.5m).
- Light shutter gap which is actually a void part in operation. (X from -0.5 to 0 m).

- 1st chopper area, a 4.8m straight area, with the guide sustratum made of Aluminum where the choppers are featured. Said choppers have been implemented in MCNP using SuperMC for geometry conversion. For the purposes of this simulations, all choppers are statically set at their 'open' position. Later calculations to study other scenarios can set them to closed simply changing the composition of a cell. (X=0 to 4.8m).
- Curved section. This is a 2025 m radius, 36 m length section that is used to lose direct line of sight from moderator. This part goes through the bunker wall feedthrough. The bunker has been represented using the layered shielding given in "Wall feedthru block-set location outline" (ESS-0062215). A 5 cm gap is assumed between the guide casing and the bunker walls. No doglegs or similar measures to minimize streaming have been considered, but notice that the shielding in the ex-bunker part of the guide does minimize streaming on its own.
- Ex-Bunker straight section This is the final section in the analysis (though not in the guide itself), and is simply a straight section leading up to X=70m.

As a tentative design, a simple shielding design has been modeled, in order to get an insight of the biological dose rates. This shielding can be improved later, both in terms of costs and efficiency, when more detailed analysis, with greater information, are performed. The shielding design features the following elements:

- Guide housing: Inside the bunker, all the guide is encased in a 1 cm thick aluminium tube.
- Ex-bunker steel shielding: The ex-bunker curved section is encased in a further 30 cm steel shielding in the curved section, aiming at further shielding in the nearest area, where the doses are expected to be higher. Moreover, the beginning of the straight part is encased in 9 cm of steel up to the current end of the model.
- Curved section B-HDPE shielding: In the outer part of the guide, in the same section as the steel shielding, a 15 cm thick HDPE layer is used to slow down and capture neutrons.
- Final straight section HDPE shielding: In the Ex-bunker straight section, a 6 cm thick HDPE layer is used to stop the remaining neutrons. While this area is, in principle, subjetc to a much lower neutron flux compared to the previous one, some measure of neutron shielding is still advisable

1.2. <u>Variance Reduction and Results</u>

Due to the nature of this problem, there will be a factor of many orders of magnitude between the flux in different parts of the guide. Thus, an analog solution is unfeasable, and techniques to get more tracks in the lower flux sections are needed. A MAGIC-like Global Variance Reduction (GVR) method is used to generate many low-weight particles along the guide.

Furthermore, as the guide provides a direct, path without collisions downstream the guide, a Deterministic Transport Sphere (DXTRAN) is used in the curved section of the guide. This achieves a double goal: It creates more tracks arriving to the location, and eliminates very high weight, uncollided tracks that can single-handedly destroy the result of even a multi-billion source particle simulation. Source biasing has not been used in these simulations

The source term has been taken from NMX as an approximation. The total intensity of the source is 1.65E13 n/s.

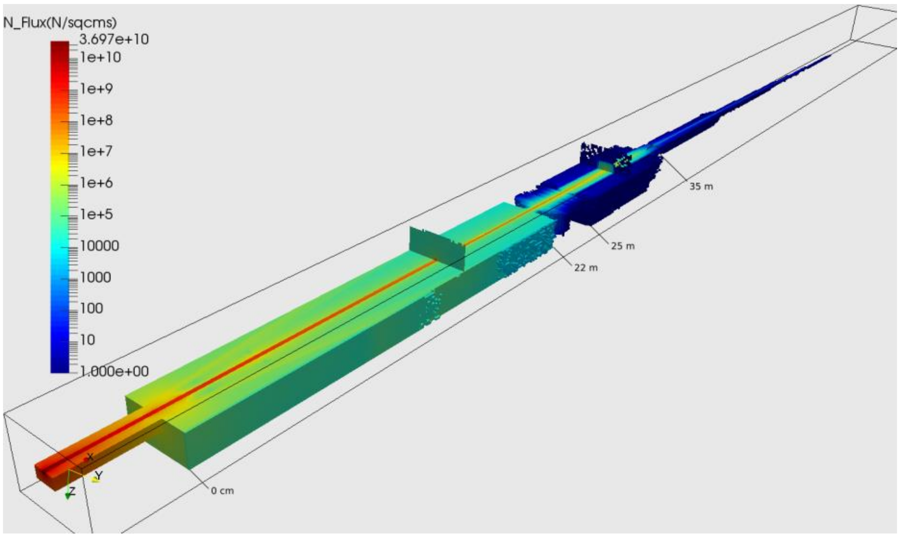

Fig. 2: Neutron flux, overall view, cut at Y=10 cm and 2 slides, 1st slide in-bunker 2nd slide ex-bunker

- The first shielding sections in the choppers does a first reduction of neutron flux, to the point that the neutron flux at the beginning of the bunker wall (outside the guide) is around 1E5-1E6n/s·cm^2. Notice, however, that the simulations only consider the neutron flux coming from the entrance of the guide, so the actual flux at the entrance of the wall may be much higher. Inside the guide, neutron flux is around 1E8, so even before losing line of sight there is a 4 orders of magnitude difference.
- The bunker wall attenuates the flux by around 3 orders of magnitude, even taking into account the 2 mm streaming gap. The shape of the flux at that area is detailed in Figure 3, and makes it obvious that much of the flux is coming from the guide itself, and not going through the wall. Thus, the bunker wall is perfectly acceptable in this context.

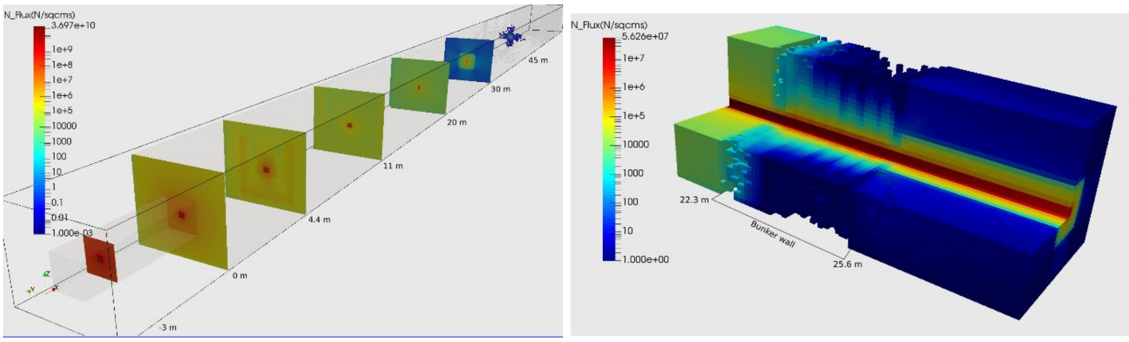

Fig. 3: Neutron flux at several distances along the X axis(left) in the bunker and (right) at the bunker wall.

- Further downstream, neutron flux drops sharply as the line of sight is lost. At the end of the simulated part (which is not the end of the guide) neutron flux is around 10 n/s·cm^2 inside the guide, and zero in practical terms (1E-3) outside it. Notice that the simulations still give numbers and the errors are in the orders of 0.2 to 0.3, so, even if the results have significant uncertainty, the flux can safely be considered negligible.

Overall, the neutron flux distribution shows that the design achieves strong shielding of neutrons, with no significant streaming or issues. It also shows that, downstream the guide, neutron flux will be irrelevant compared to that reflected throughout the guide, and thus, can safely be ignored for activation purposes in the sample cave. The above does not mean that there are not possible enhancements to the design. The thickness of the shielding layers has not been optimized, so it is possible that similar or better shielding with lower costs is achievable. Future work shall explore possible enhancements and costs reductions.

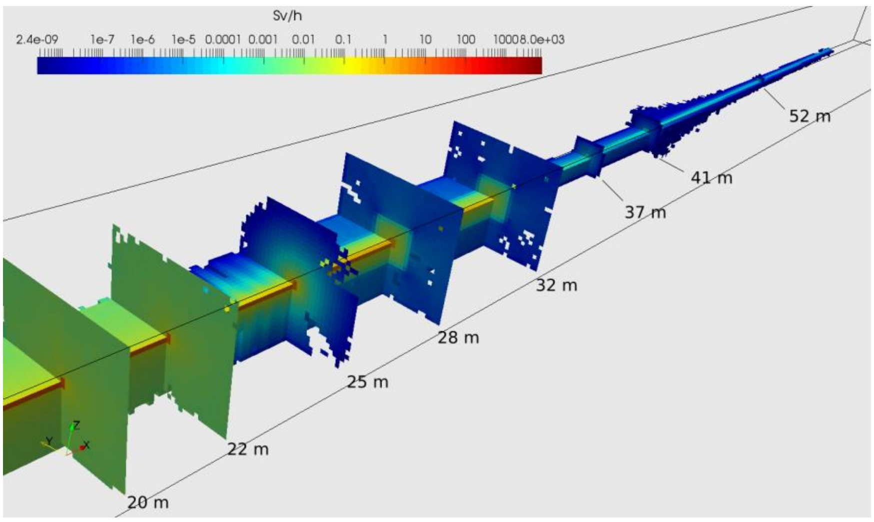

Fig. 4: Neutron dose rate, overall view along the X axis.

Given the above results, it seems reasonable to expect neutron dose rate outside the guide to be well within acceptable limits. In particular, in this document we have made a temptative assessment of the dose outside the bunker wall, in areas that can be assumed as accessible to general public. In particular, in this document, we have tested the dose rate over the surface of B-HDPE shielding, at X=35, 45 and 55 meters. This is very close to the outer surface of the guide, even if it is not exactly a contact dose, so it should be representative of the maximum dose that a person can get staying at those points.

Table I: Dose rates at several point

Position X (m)	Neutron dose (μSv/h)	Photon dose (μSv/h)	Total dose (μSv/h)
35	0.014	6.17E-3	0.020
45	0.046	<0.001	0.046
55	0.010	<0.001	0.010

1.3. Analytical Approach for Gamma Photon Flux

Previous analytical calculations were performed to provide first hints on the shielding required for the gamma dose produced by thermal neutron capture by the supermirror coating (the source here).

As a starting point, the photon flux produced by the source is calculated from the intensity of the neutrons at the end of the curve (at the entrance of the expander, at L=48 m, where the direct line of sight of the moderator and other secondary sources like the bunker choppers is lost). We used an expression similar to that of C-SPEC to estimate the collision length of neutrons in the guide wall, defined as $h/\tan\theta_c$,[CSPEC] where h is the height of the guide and θ_c is the critical angle (assuming m=2.5 for exterior wall):

$$\varphi_0\left[\frac{\gamma}{s\cdot cm}\right] = Flux\left[\frac{n}{s}\right]\frac{\tan\theta_c}{h[cm]}Conv\left[\frac{\gamma}{n}\right]$$

In this expression, we assume a conversion of captured neutrons to gammas of 100% ($Conv\left[\frac{\gamma}{n}\right]$=1). This might be likely a conservative value (overestimated photon flux), but it is useful as a starting point. We obtain φ_0=1.3×10^8 photons/(s·cm).

An estimation of the photon energy is done by averaging the gamma yield production of Ni and Ti, the elements that form the supermirror coating. Using the NDS database [Prompt], we use a photon energy of E_γ=4.4 MeV as input for the calculations. With this energy, the flux to dose conversion factor is C=1.25×10^{-5} μSv·cm^2.

Preliminary calculations were done for steel and concrete. The attenuation factors [NIST] are μ/ρ^{steel}=3.22×10^{-2} cm^2/g (the one for iron) and $\mu/\rho^{concrete}$=3.05×10^{-2} cm^2/g, respectively. The buildup factor for steel is obtained using [Lamarsh] at about ~10 MFP at these photon energies (~40 cm for steel, 1 m for concrete), thus B^{steel}=7.1 and $B^{concrete}$=5.0.

As above mentioned, since the final exposure must be $H < 3$ μSv/h, the thickness for steel estimated is t^{steel}=30.6 cm. For concrete, the value estimated is $t^{concrete}$=60.5 cm.

2. Secondary Spectrometer: cave and beamstop

2.1. First Approach Cave (analytical)

To estimate a starting point for the thickness of the cave walls, we use the expression for the radiation dose outside of a wall (analogous to what we have done with the beamline):

$$H = \varphi \times C \times 3600 s/h$$

where φ is the flux and C is the conversion factor. Here, we established that the source is a sample (located at the sample position) in which all the neutrons are absorbed and every neutron is converted into a gamma photon of E_γ=2 MeV.

The same equations apply:

$$\varphi = \sum \frac{\varphi_{0i} B_i e^{-\mu t}}{4\pi r_i^2} dr_i$$

where, in the case of a sample with a width of w:

$$\varphi_0 \left[\frac{\gamma}{s \cdot cm}\right] = Flux \left[\frac{n}{s \cdot cm^2}\right] w[cm] Conv \left[\frac{\gamma}{n}\right]$$

We assume the flux arriving to the sample estimated by our McStas calculations (n=3.0×10^{10} n/s) confined to 1 cm (the conservative case of all neutrons arriving to a small sample with an assumed upgrade of the focusing guide). Also, we assume a full conversion of neutrons into gamma photons (i.e. φ_0=3.0×10^{10} n/(s·cm^2)).

The dose conversion for photons with E_γ=2 MeV is C=7.47×10^{-6} μSv·cm^2. Also, first calculations were carried out using concrete as the shielding material for the cave. The attenuation factor at this energy is then [NIST]e $\mu/\rho^{concrete}$=4.577×10^{-2} cm^2/g. The buildup factor is estimated as B=10.4.

The dose estimation was obtained assuming an internal, isotropic point source inside a shield structure and considering 2 detector points at the exterior of the cave: a lateral point at the rear part of the cave (within the E01 corridor, being r=3.5 m) and a point at the roof of the cave (r=2.5 m).

Results (dose of $H < 3$ μSv/h in this supervised area) give a preliminary value for the roof wall thickness of t=77.1 cm and for the lateral of t=70.8 cm.

2.2. First Approach Beam Stop (analytical)

The beam stop located after the sample to absorb all the transmitted neutrons minimizing scattering processes (thus, the background ratio) consists of a B_4C canister (5-10 cm thick) surrounded by shielding material that shield the gamma photons produced by neutron capture (typically lead, steel and/or concrete). Boron emits gamma photons of E_γ=0.477 MeV through neutron capture processes.

The attenuation factor at this energy ($E_\gamma \approx 0.5$ MeV) is [NIST] $\mu/\rho^{concrete}=8.915\times10^{-2}$ cm^2/g for concrete, and $\mu/\rho^{steel}=8.414\times10^{-2}$ cm^2/g. The flux to dose conversion factor is $C=2.47\times10^{-6}$ μSv·cm^2. Finally, we assume that the gamma source (the B_4C canister) is at about 20 MFP (40 cm for steel, 1 m for concrete). The buildup factor for steel with all these parameters is estimated as $B^{steel}=59$ for steel and $B^{concrete}=5.4$ for concrete.

Preliminary results give an estimated thickness for the beam stop of $t^{steel}=15.4$ cm for steel and $t^{concrete}=34.8$ cm. These values will serve for the detailed calculations of the shielding and radiation dose outside the beamstop.

2.3. Shielding Design Cave and Beamstop

Considering that only a small fraction of the neutron beam striking the sample is absorbed, the unused neutrons need to be guided to the beam dump so as not to endanger the rest of the components at the experimental cave. The calculated neutron flux at high flux operation mode resulted to be 3×10^{10} particles/s. In this study, the beam is considered to be completely stopped by the dump or the sample resulting in the generation of one gamma ray per neutron. Consequently, the shielding of the experimental cave need to be tested for gamma radiation in order to assure that it efficiently shields the instrument hall and therefore, fulfils the safety regulation established by the European Spallation Source.

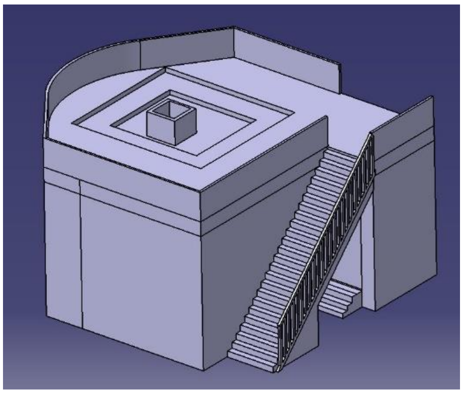

Fig. 5: CAD model of the MIRACLES cave.

The simulation code MCNP6 [Goorley] was used to quantify the equivalent dose measured at the point detector located outside the cave and due to the gamma radiation generated as a result of neutron interaction with matter. The geometry of the CAVE was converted from a CAD model to a MCNP input file using the Super Monte Carlo Program for Nuclear and Radiation Simulation (SuperMC).[Wu] A representation of the original CAD model can be seen in Figure 5 while its analog MCNP geometry has been presented in the following section.

The MCNP Data Library used was MCPLIB04 [3] and the gamma-ux-to-dose-conversion factors are taken from [ESS-0019931, Henss].

The layout of the cave is presented in Figure 2. The walls, ceiling and oor of the cave, as well as the stairs and the sample pedestal, are made of t=60 cm of Portland cement (ρ = 2.3 g/cm^3, yellow), only the central part of the ceiling has been reinforced with high density concrete (ρ = 3.6 g/cm^3, purple). The vessel consists of 5086 aluminum alloy (ρ = 2.66 g/cm^3, pink) with 5 cm outer coating walls of borated concreted (d = 2.1 g/cm3, blue) and 10 cm over-ceiling of borated polyethylene (B-HDPE, ρ = 1.0 g/cm^3, light-pink). The get-lost tube is made of Aluminum (ρ = 2.7 g/cm^3, orange) with 5 mm borated polyethylene inner coating. Finally, the Beam dump consists of four blocks: the first one is made of 10-cm-thick boron carbide (ρ = 2.52 g/cm^3, green), the second one is 20-cm-thick lead (d = 11.35 g/cm3, light-blue) and the third and fourth ones are made of Portland cement (35 and 40-cm-thick respectively).

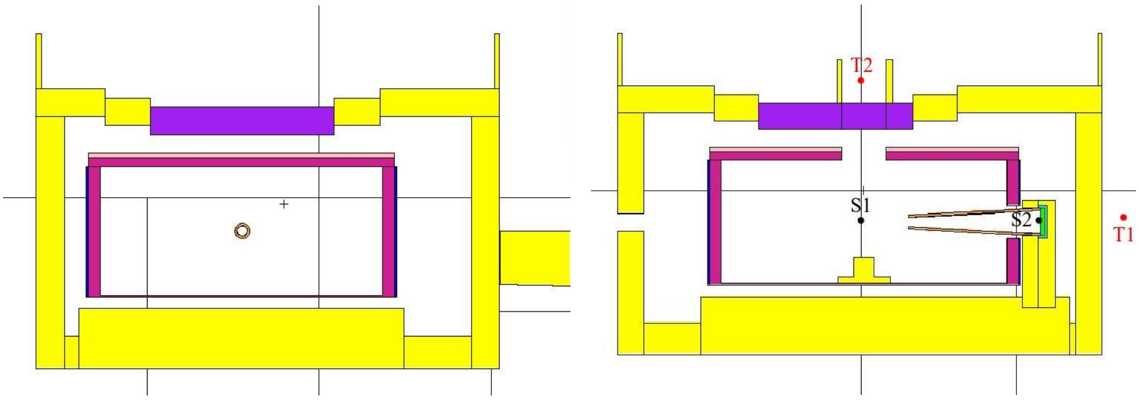

Fig. 6: (left) YZ cut view, and (right) XZ cut view of the MIRACLES cave. S1 (sample) and S2 (B_4C canister) are the gamma sources under study.

First, the reliability of the geometry was tested by using a mono-energetic photon cloud source around the whole block and running the model for 10^9 primaries. The output showed that not a single particle got lost and therefore, the trustworthiness of the geometry can be guaranteed. Afterwards, the cloud source was replaced by a 2 MeV photon point isotropic source placed 1) at the sample position and 2) immediately before the first block of the beam dump. Besides, two point-detector tallies were located at a) 30 cm from the wall and, b) 30 cm above the ceiling. Both, source and tally positions, have been presented in Figure 2c. Finally, the simulation was run using 10^9 primaries.

2.4. Results

A graphical representation of the dose distribution can be seen in Figure 7 for both case studies: the source is placed at the sample position or on the dump surface. Considering a source term of 3×10^{10} particles/s, the final results have been calculated and presented in Table 1 below.

According to previous results, the equivalent dose rate would not be higher than 0.5 μSv/h at any point.

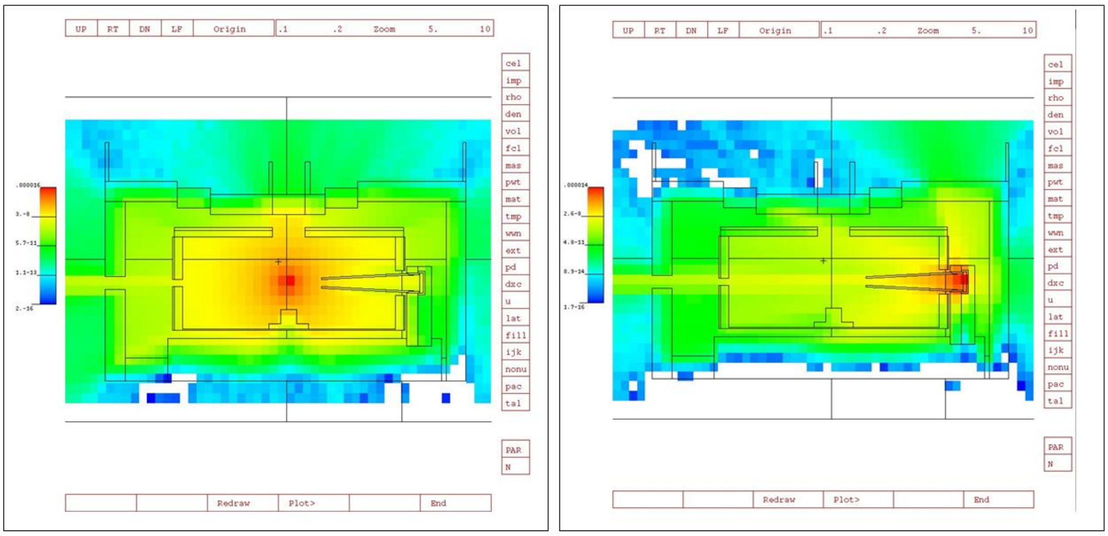

Fig. 7: Dose distribution inside and outside the experimental cave splitting two main gamma sources: (left) sample source, S1 and (right) beam stop source, S2.

Table II: Equivalent dose rates at several points outside the cave

Source	Tally	Eq. Dose (μSv/h/part/s)	Eq. dose (μSv/h)
S1	T1	5.22E-13 ± 4%	0.02
S1	T2	1.65E-11 ± 1%	0.50
S2	T1	5.55E-12 ± 2%	0.17

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