

VALIDATION OF THE MCSTAS-MCNPX INTERFACE FEATURES IN CALCULATION OF SHIELDING AND GAMMA/NEUTRON BACKGROUNDS

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Abstract: The interfacing McStas and MCNPX (Virtual_mcnpx_ss_Guide component) have been developed since 2012 for overcoming the limitations of the gap between McStas and MCNPX such as complex moderator geometries, backgrounds, and interference between beam-lines as well as shielding requirements along with the neutron guides. In the present, there is no study about the validation of this feature. The aim of this study is to validate the McStas-MCNPX interface by comparison between the calculated results of the McStas-MCNPX interface with the other codes (VITNESS, PHITS) and experiments. Based on the validation, the calculation of the shielding and gamma/neutron background along the neutron instruments can be easy by using the interfaces.

Keywords: *McStas-MCNPX interface, CONAS, HANARO, Neutron instrument, Simulation.*

PHÊ CHUẨN GIAO THỨC MCSTAS-MCNPX TRONG TÍNH TOÁN CHE CHẮN VÀ PHÒNG NỀN GAMMA VÀ NƠTRON

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Tóm tắt: Giao thức McStas và MCNPX (*Virtual_mcnpx_ss_Guide*) được phát triển từ năm 2012 nhằm giải quyết những hạn chế khi kết nối hai chương trình mô phỏng là McStas và MCNPX trong việc tính toán các hình học phức tạp, phòng nền bức xạ và ảnh hưởng qua lại giữa các chùm tia và thiết bị che chắn dọc theo ống dẫn chùm nơtron. Hiện nay chưa có một nghiên cứu nào về việc chuẩn hóa giao thức này vì vậy mục tiêu của nghiên cứu này là để phê chuẩn giao thức này thông qua việc so sánh giữa kết quả tính toán bằng chương trình MCNPX với thực nghiệm. Dựa vào việc phê chuẩn này, việc tính toán che chắn và phòng nền gamma/nơtron xung quanh các thiết bị nơtron được thực hiện trong nghiên cứu này.

Keywords: *McStas-MCNPX, CONAS, HANARO, Thiết bị nơtron, Mô phỏng.*

1. INTRODUCTION

In the recent years, a cold neutron research facility that utilizing cold neutrons with a characteristic wavelength larger than 4.0 \AA (energy less than 5.0 meV) would be a powerful national resource due to the increase of the studies in the condensed matter physics. A cold neutron source at the HANARO Research Reactor had been constructed in the framework of a five-year project and ended in 2009 [1, 2]. Cold Neutron Activation Station (CONAS), which utilizes a cold neutron source of HANARO, is a complex facility including several radioanalytical instruments utilizing neutron capture reaction to analyze elements in a sample. It was intended to include three instruments like a CN-PGAA (Cold Neutron - Prompt Gamma Activation Analysis), a CN-NIPS (Cold Neutron - Neutron Induced Pair Spectrometer), and a CN-NDP (Cold Neutron - Neutron-induced prompt charged particle Depth Profiling). For this station, we constructed two cold neutron guides called CG1 and CG2B guides from the CNS. Ni/Ti super mirrors with $m = 2$ grade for the neutron guide were domestically fabricated by using a sputtering machine of the KAERI neutron guide system. Fig. 2 shows the conceptual configuration of the CONAS concrete bio-shield and the instruments. The average neutron wavelength is calculated from the wavelength distribution to be 4.01 \AA corresponding to 59.0K at the end of the CG1 guide and 4.68 \AA corresponding to 43.3K at the end of the CG2B guide, respectively. After installation, we determined the neutron flux by using a gold activation method. For the CG1 guide, the thermal eq. flux is $7.16 \times 10^8 \text{ n.cm}^{-2}.\text{s}^{-1}$ and the real flux is $3.21 \times 10^8 \text{ n.cm}^{-2}.\text{s}^{-1}$, and for the CG2B guide, the thermal eq. flux is $1.59 \times 10^9 \text{ n.cm}^{-2}.\text{s}^{-1}$ and the real flux is $6.13 \times 10^8 \text{ n.cm}^{-2}.\text{s}^{-1}$.

To protect users from radiation exposure, a concrete bio-shield was constructed around the cold neutron guides and experimental instruments, as shown in Fig. 1. This concrete bio-shield is called CONAS bunker, which has three sections for neutron guide room, CN-NDP experimental room, and prompt gamma experimental room. CG1 guide was allocated for CN-NDP, and CG2B guide was allocated for two prompt gamma instruments.

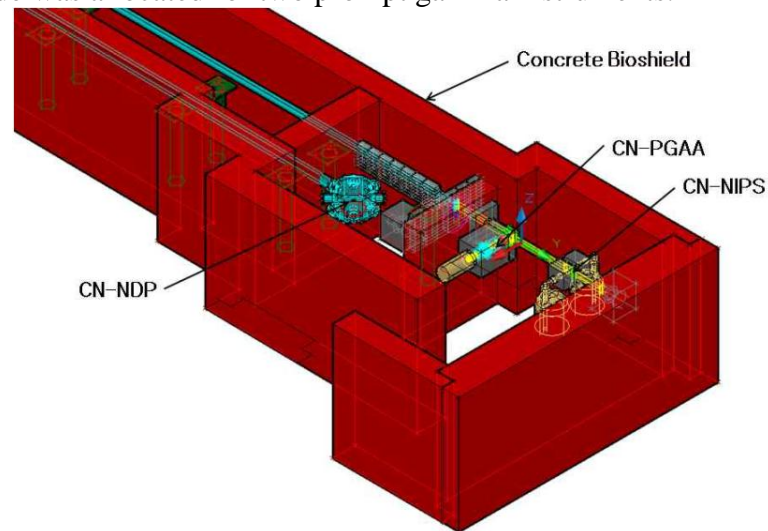


Fig. 1 CONAS includes three neutron activation analysis instruments like CN-PGAA, CN-NIPS and CN-NDP.

In this paper, the calculation of the radiation dose inside/outside the shield boundary of the CONAS bunker has been performed by using McStas [3] and MCNPX [4] simulation codes. The main objective is to reduce the biological dose to permit personnel to work outside the CNS guide hall during operation. The shield design was configured to reduce the biological dose to less than $5.0 \mu\text{Sv}.\text{hr}^{-1}$; this value is a factor of 5 less than the international standard of $25.0 \mu\text{Sv}.\text{hr}^{-1}$ for occupational limit, assuming 40 h work per week and 50 weeks per year. In addition,

this study was aimed to validate the McStas-MCNPX interface features when apply to calculate the radiation dose by comparing with the measured results.

2. METHODOLOGY AND RESULTS

2. 1. Methodology

In the family of particle transportation codes, no simulation code can readily model the gamma or neutron-background of neutron scattering instruments. The existing codes can be divided into two groups. The first group consists of programs (like MCNPX, FLUKA) designed to solve general particle transport problems, whereas the second group is intended to simulate neutron scattering instruments such as McStas and VITESS. It can be observed that none of these programs are capable of calculating the background of scattering instruments alone. We have chosen one from each group (MCNPX and McStas), and use the output of McStas to construct a realistic source term for MCNPX. We construct the model of the instrument with McStas and simulate the trajectories of neutrons from the HANARO cold source. The communication between McStas and MCNPX has been performed through the advantageous feature of McStas, as the *Virtual_mcnpx_ss_Guide* and *Virtual_mcnpx_output* components [5] that can allow for re-entry of neutrons into the MCNPX regime. The components of the CONAS were built-in MCNPX, which can simulate the neutron transport outside the instrument and simulate the particles produced by neutron collisions inside. In this way, both the neutron and gamma background of an instrument can be estimated with MCNPX. The direct coupling between McStas and MCNPX allows for more accurate simulation of, e.g., complex moderator geometry, backgrounds, interference between beam-lines as well as shielding requirements along with the neutron guides.

The shielding analyses require accurate characterization of the neutron and photon fluxes through the shield. The Monte Carlo computer code MCNPX was used with ENDF/B-VII [6] nuclear data libraries for performing the shielding analyses due to its updated capability for electron-, photon-, and neutron-coupled transport calculation. Given the fact that the neutron and gamma flux outside the shield boundary is very low to meet the working dose requirement, a direct analog MCNPX calculation is very time-consuming and not practical. Variance reduction techniques must be adopted to deal with the shielding problem with deep penetration. Three-dimensional mesh-based weight windows were used [7, 8], which could provide a space- and energy-dependent importance function for the calculation model; therefore, much more particles can be tracked outside the shield. Weight windows are generated to optimize a special tally. Considering the complicated geometry of the CONAS, multiple sets of weight windows, which are optimized for tallies at different locations of external shield boundary, are needed for an accurate neutron or gamma dose profile along the whole exterior boundary of the CONAS bunker.

A very high neutron and gamma radiation intensity exist during the irradiation and the analytical process. To reduce the intensity and protect those working around these systems, a bunker with the thick wall has been built to provide a necessary shielding. The CONAS bunker is a bio-shield of ordinary concrete that was built to meet the standard engineering requirements for massive concrete constructions, taking into consideration the load bearing characteristics of the site. Figure 2 presents a schematic top-view of the CONAS bunker, showing the surrounding concrete shielding structure and wall thickness. The wall 40 cm thickness with 1 cm iron shell was made of heavy concrete with high density ($d=3.7 \text{ g.cc}^{-1}$) and the components of heavy concrete were presented in Table 1. The CONAS bunker was covered by a 40 cm thickness heavy concrete roof with the same density and closed by 1 cm iron shell. This bunker has two roof parts with low part have a height from the roof to the floor as 190 cm and 220 cm for another part. The bunker length is 13.29 m and a width of 4.694 m. The dimension details of this bunker were also illustrated in Figures 2.16, and 2.17 is the actual picture of this bunker.

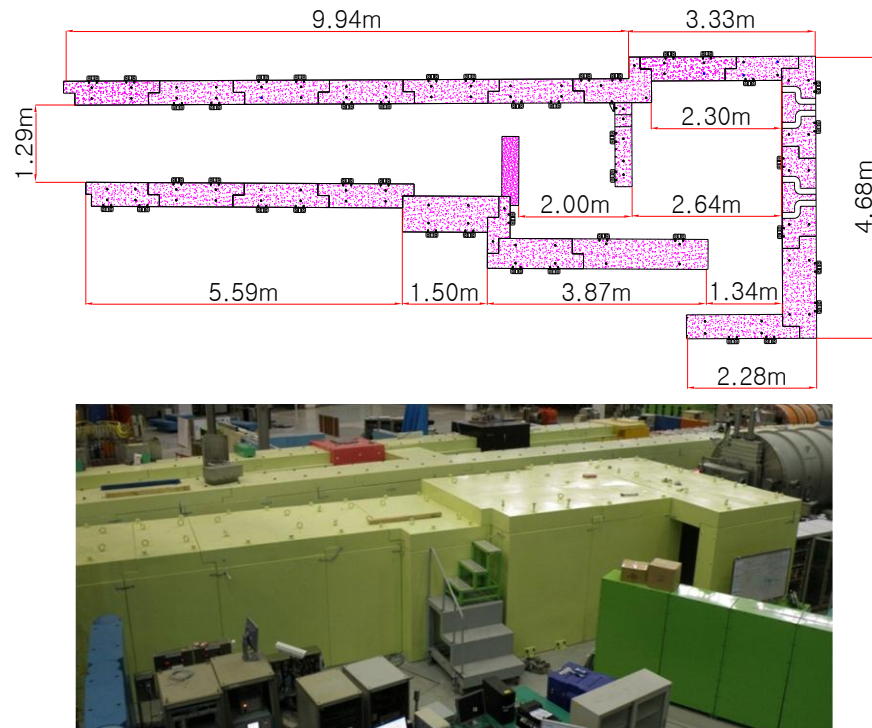


Fig. 2 (top) Top-view of the CONAS bunker, with the dimensions of the concrete shielding and wall thickness. (bottom) The real picture of CONAS bunker.

Table 1 The components of high-density concrete for casting in the CONAS bunker walls.

Component	Weight (kg)	Volume fraction (m ³)	Density (g.cc ⁻¹)
Cement	0.2	0.1	2.20
Water	0.1	0.1	1.00
B ₄ C	0.0	0.0	2.52
Steel ball	1.0	0.1	7.20
Iron ore	2.5	0.7	3.50
Total	3.7	1.0	3.70

By combining the application of AutoCAD and SuperMC tools, the CONAS bunker, as well as all components of the CN-NDP and CN-PGAA, were modeled in the MCNPX input text. Based on the dimensions of each compartment and CONAS bunker, the final MCNPX model of CONAS combines the four primary buildings and contains 127 MCNPX cells and roughly 900 surfaces. This model also integrated the material and air filling inside the blank of the model (Fig. 3).

A cluster of computers has utilized these simulations. The precompiled MPI of MCNPX 2.7.0 was installed on these computers with an MPICH 3.3.1 client based on CentOS 7. Using this setup, simulations can be executed in parallel to speed up the simulation by 32 processor cores with 2×10^9 histories.

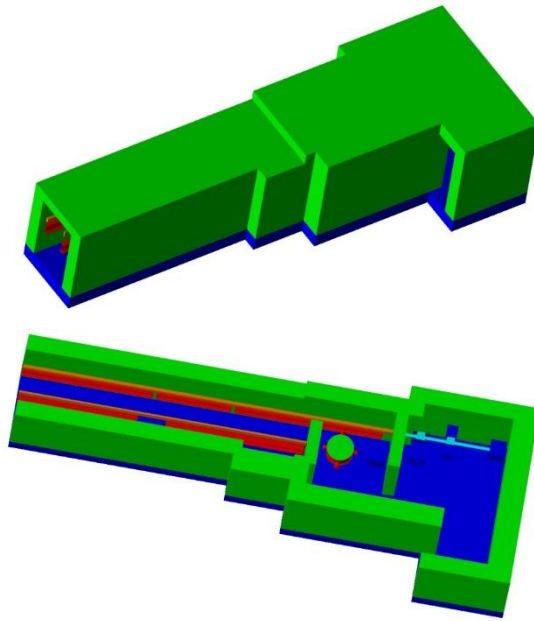
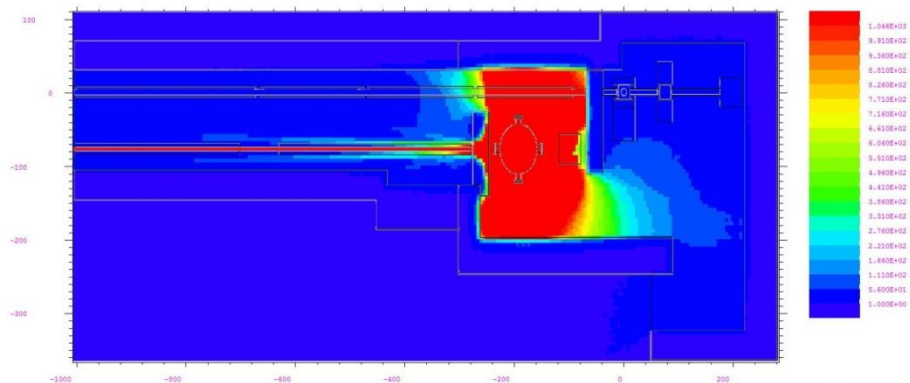


Fig. 3 The CONAS model by using MCNPX code. (top) The entire of CONAS bunker. (bottom) Cutaway view of internal walls and all components inside CONAS bunker.

2. 2. Results

The dose rate distributions ($\mu\text{Sv/hr}$) in CONAS bunker were simulated by using the MCNPX code by applying for the TMESH tally card. These values were carefully compared with the measured dose rate. The dose rate at the user position is less than about $0.1 \mu\text{Sv/hr}$.

The NCRP-38 Flux-to-Dose Equivalent Rate Conversion Factors using in these simulations and the unit of dose rate distribution is the micro Sievert per hour ($\mu\text{Sv/hr}$). The simulations of dose rate distributions have been carried out with CG1 or CG2B in operating status. The neutron and photon dose rate distributions for the horizontal planar views are presented in Fig. 4 and 5.



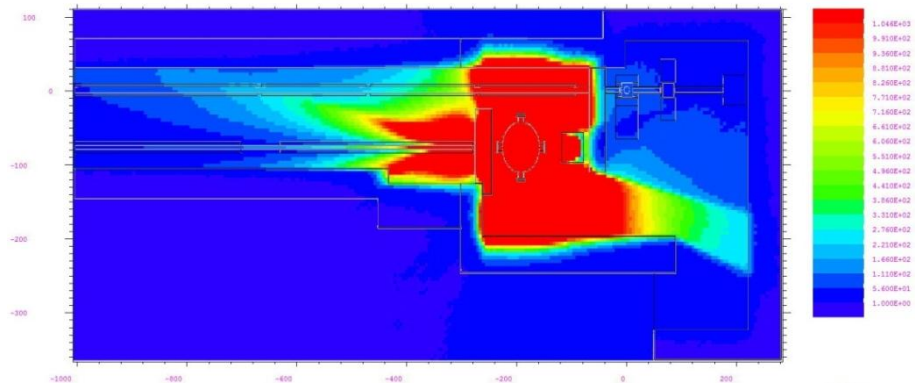


Fig. 4 Horizontal plane (plan view) of mesh tally neutron (top) and photon (bottom) dose rates ($\mu\text{Sv/hr}$) for the source from CG1. The plane is at elevation 176.5 cm from the floor.

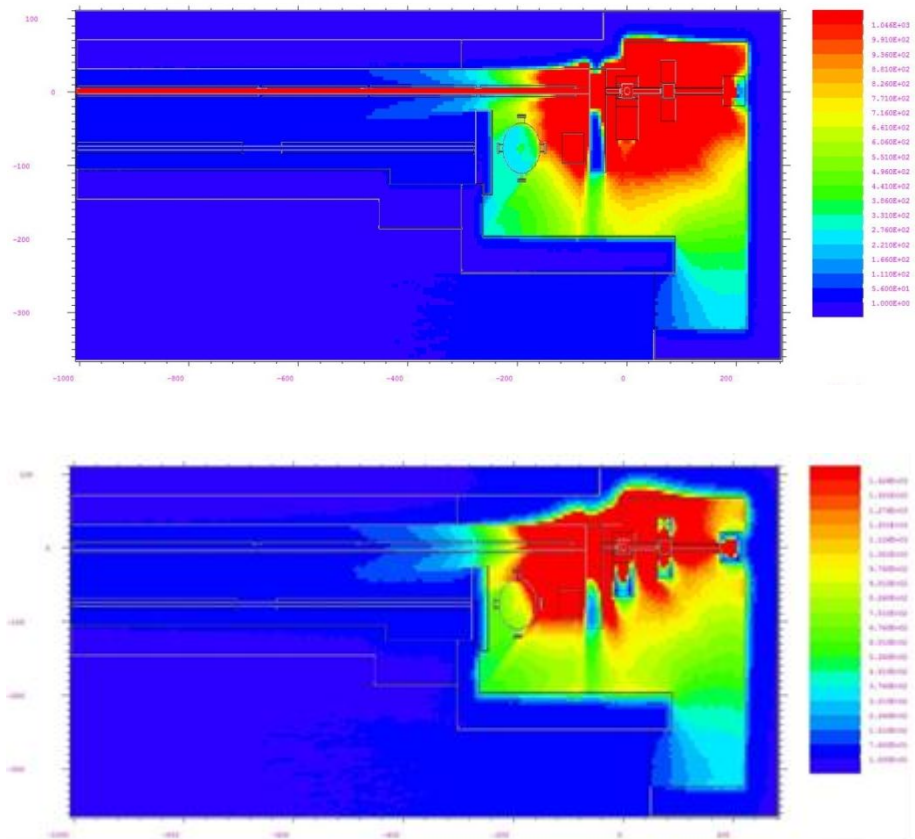


Fig. 5 Horizontal plane (plan view) of mesh tally neutron (top) and photon (bottom) dose rates ($\mu\text{Sv/hr}$) for source from CG2B. The plane is at elevation 154.5 from the floor.

3. CONCLUSION

We have applied the McStas-MCNPX interface in order to investigate the neutron and gamma background arising from the imperfect reflectivity of the guide, and the gamma background created by the activation of the supermirror multilayer and other components of the system. The method is capable of simulating the effect of changing the guide parameters and changing the shielding also. In this paper, the calculated dose rate at the user position is less than about $0.1 \mu\text{Sv/hr}$.

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