Validation of MCS Coupled Neutron-Photon Calculations with SINBAD Benchmark Experiments

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1. Introduction

This paper presents a validation study of the coupled neutron-photon transport calculation capability of the MCS Monte Carlo code developed at Ulsan National Institute of Science and Technology (UNIST). The validation is conducted against two shielding benchmark experiments from SINBAD (Shielding Integral Benchmark Archive and Database): the Fusion Neutronics Source (FNS) benchmark and the OKTAVIAN benchmark. SINBAD is a compilation of over 100 shielding benchmarks widely used for code [1] and nuclear data validation [2]. MCS has been developed since 2013 for the primary purpose of high-fidelity and high-performance criticality analysis of large-scale nuclear reactor with fuel depletion and thermalhydraulics feedback [3], [4]. Recently, to extend the range of MCS applications to reactor shielding studies and complex deep-penetration shielding problems, photon-transport and coupled neutron-photon capabilities have been implemented.

2. Description of Benchmark and MCS Models

2.1. FNS Benchmark

A 14-MeV neutron-transmission benchmark experiment on vanadium, one of the promising materials for fusion reactors, was conducted at the Fusion Neutronics Source (FNS) facility of Japan Atomic Energy Research Institute (JAERI) [5]. Neutron and photon leakage spectra were measured inside a vanadium experimental assembly composed of cubic vanadium blocks of side 5.08 cm piled up as a cubic experimental assembly of side 25.4 cm. Five of the six surfaces of the cubic vanadium assembly were covered with 5.08-cm-thick graphite to reduce the neutron leakage out of the assembly and the incoming background from the surroundings. A 14-MeV neutron source generated by deuterium-tritium (D-T) fusion reactions was located 20 cm away from the front surface of the assembly (the front surface is the only surface of the assembly not covered by graphite). Neutron and photon leakage spectra were measured in two experimental channels placed inside the assembly 7.6 and 17.8 cm away from the front surface. Four techniques were employed to measure neutron and photon spectra: (i) liquid organic scintillator for neutron spectra measurements above 2 MeV with uncertainties of about 3.5% for 2 < E < 6 MeV, about 11-20% for 6 < E< 8.3 MeV, and about 4% for E > 10 MeV; (ii) a pair of proton-recoil counters for neutron spectra measurements in the energy range 20 keV to 1 MeV with uncertainties of about 30% for 20 keV < E < 80 keV and below 10% for 0.1 MeV < E < 1 MeV; (iii) slowing down time (SDT) method for neutron spectra measurements in the range 1-300 eV with uncertainties of 11–40%; and (iv) BC537 scintillator for photon measurements with total uncertainty of about 15–20%. All the measurement uncertainties are assumed to be at 3 standard deviations (3 σ) since it is not clearly stated in the benchmark documentation.

The vanadium assembly is fully modelled with piled-up vanadium blocks and graphite blocks on five surfaces. The neutron source is modelled as a point isotropic source with energy and angular distribution as specified in the benchmark documentation. The experimental channels and detectors are not modelled and so the neutron and photon leakage spectra are directly calculated in the vanadium assembly, in vanadium cells located at the real position of the detectors in the experiment. The tallied multigroup flux in unit 1/cm² is converted into 1/(cm².MeV) by dividing by the width of the energy bin $(\Delta E_{\text{bins}} = E_{\text{up}} - E_{\text{low}})$. MATLAB subroutines provided by the benchmark documentation are used to post-process tallied flux and simulate the energy resolution of the liquid organic scintillator for neutron measurements above 2 MeV and the energy resolution of the BC537 scintillator for photon measurements.

2.2. OKTAVIAN Benchmark

Measurements of neutron and photon leakage spectra out of four spherical samples (Al, Si, W, and Mn) with a central 14 MeV neutron source were performed in the OKTAVIAN facility of Osaka University, Japan. The neutron source is produced by accelerating deuterons on a solid titanium-tritium target (D-T fusion reaction) placed at the centre of the spherical samples. Neutron and photon leakage spectra from the outer surface of the spherical sample were measured at 11 m and 5.8 m away respectively from the center of the sphere at 55° angle with respect to the deuteron beam axis. Two sizes of spheres were used in the measurements: 40-cm diameter spherical sample for Al and W and 60-cm diameter spherical sample for Si and Mn. For each spherical sample, 2-mm-thick stainless steel is placed on the inner and outer surfaces. Experimental uncertainties for neutron leakage spectra are about 60% for E < 0.2 MeVand around 6% for E > 0.2 MeV. For photon leakage,

experimental uncertainties are below 1.8% for energy range of 0.4 < E < 2 MeV, are about 11% for energy range of 2 < E < 3 MeV and range from 39 - 72% for E >3.5 MeV. All these uncertainties are assumed to be at 3σ .

As for calculations, detailed geometry of the spherical sample (stainless-steel thickness, beam duct and beam tube) is included in the modelling but the tritium target, detector, collimator and walls are not modelled. Two isotropic sources (neutron and photon source) with energy distribution as specified in the benchmark documentation are calculated separately (one fixedsource neutron-photon run and one fixed-source photon run). The resolution function of the neutron detector is implicitly contained in the neutron source specification and therefore the tallied neutron results do not need postprocessing. The photon source corresponds to gamma photons produced by neutron interactions with the structural materials of the tritium target, with an intensity of 0.0862 gamma photon emitted per neutron source. Therefore, the calculated photon spectrum is the summation from the neutron and photon source calculations. Neutron and photon leakage spectra are tallied in the cell between the surfaces of radius 579 cm and 581 cm. The tallied flux unit in 1/cm² is converted into 1/MeV by multiplying by the surface area of the sphere of radius 580 cm and by dividing by the width of the energy bin. The energy resolution of the gamma detector is simulated with Gaussian energy broadening (GEB) of the tallies. The full width at half maximum is modelled as in Equation (1) with A = 0.04 MeV, B =0.0025 MeV^{1/2} and C = 100 MeV⁻¹. This modelling choice results in a relative energy resolution of about 3% for photon energies above 4 MeV. The 3% value is a rough approximation, but no information is provided in the OKTAVIAN benchmark documentation.

$$FWHM = A + B\sqrt{E + CE^2}$$
(1)

3. MCS Calculation Results

3.1. FNS Benchmark

Preliminary verification of MCS with ENDF/B-VII.I nuclear data library is conducted against MCNP 6.1 and good agreement is observed between the two codes (result figures are not included in this 4-page paper). Validation of MCS against experiment is shown in Figure 1 and Figure 2 for neutron and photon spectra respectively. Calculated neutron spectra match well with experiment except at low energy (SDT method), where MCS calculation is not well converged (3 standard deviations > 20%, variance reduction would be required for convergence). The shape of the calculated neutron peak at high energy after energy broadening matches well with experiment as shown in Figure 3. The error bars are plotted at 3σ . The statistical errors from calculations are represented with the thickness of the red

line. Overall, MCS results are in good agreement with experiments.

3.2. OKTAVIAN Benchmark

Excellent agreement is observed on neutron and photon leakage spectra for preliminary verification between MCS and MCNP6 at identical ENDF/B-VII.I nuclear data library (result figures are not included in this 4-page paper). Comparison of MCS calculation results against OKTAVIAN experimental data are shown in Figure 4 and Figure 5 for neutron and photon leakage spectra respectively. GEB is applied for the tallied photon leakage spectra. For the silicon sphere case, the experimental data for measured photon spectrum is shifted by 200 keV in the positive direction. This 200keV correction is applied because of inconsistencies spotted in the experimental information provided by the benchmark documentation [6]. The error bars correspond to the experimental uncertainties at 3σ . The statistical uncertainties of the calculated flux are very small and are represented with the thickness of the red line. Reasonable agreement is observed between calculation and experiment for both neutron and photon leakage spectra.



Figure 1. FNS benchmark: comparison of MCS neutron spectra without broadening against experiment



Figure 2. FNS benchmark: comparison of MCS photon spectra with & without broadening against experiment



Figure 3. FNS benchmark: effect of broadening the calculated neutron spectra above 2 MeV

4. Conclusion

Two benchmark experiments from the SINBAD shielding database have been interpreted to validate the coupled neutron-photon transport capability of MCS code. Calculation results on the vanadium cube of FNS benchmark and four spherical samples (Al, Si, W, and Mn) of OKTAVIAN benchmark show good agreement against experimental value for neutron and photon leakage spectra. Further investigations will concern the verification and validation of the variance reduction schemes currently developed in MCS. It is envisioned to simulate the OKTAVIAN benchmarks for this purpose with more details, including neutron source anisotropy, detector arrangement, collimator, and structural materials (walls) to model the effect of neutron scattering on those components. The variance reduction features would also allow to achieve great efficiency on calculation and to interpreted more complex experiments such as the tungsten (W) case of FNS benchmark.

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Figure 4. OKTAVIAN benchmark: comparison of MCS neutron leakage spectra against experimental data



Figure 5. OKTAVIAN benchmark: comparison of MCS photon leakage spectra with GEB against experimental data