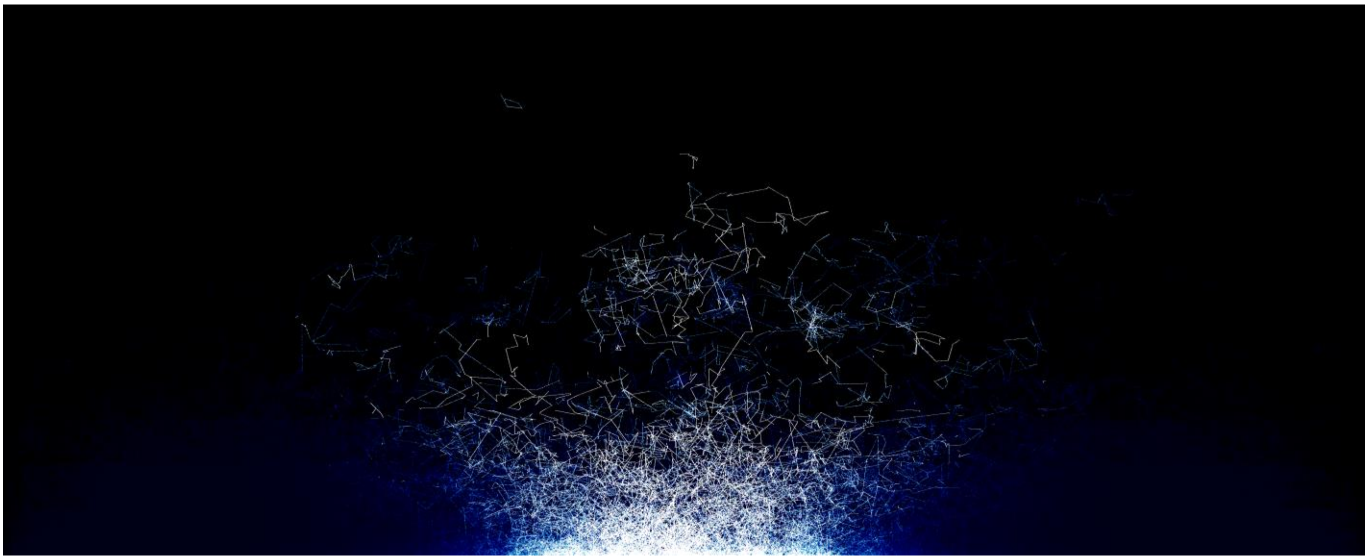
**RESEARCH REPORT** VTT-R-00050-25



# Validation of the coupled photon transport mode in Serpent 2.2 with the Baikal-1 skyshine benchmarks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**Summary**

This report summarizes validation of the coupled neutron-photon transport mode in the Serpent 2.2 Monte Carlo code using the Baikal-1 skyshine benchmarks distributed with the ICSBEP. In the Baikal-1 skyshine experiment the atmospheric scattering of neutrons and photons was studied. Dose rates and flux levels above the reactor and at ground level up to 1500 m from the reactor axis were measured. The goal of the experiment was to provide a detailed study of the spatial energy dependency of atmospherically scattered particles as basis for a radiation safety analysis validation database. In addition to reference measurements, MCNP5 results are provided as part of the benchmark description.

The benchmarks were calculated using a development version of Serpent 2.2.2. Excellent agreement is observed with the MCNP5 results in the above core neutron dose rates and reasonably agreement in the photon dose rates. However, neutron dose rates on the two upper measurements levels are in subpar agreement with the measurement results. Photon dose rates agree well at all the elevations. On-site detector results for fast neutron flux as well as neutron and photon dose rates are in good agreement with the measurement and MCNP5 result across the entire spatial range. However, on-site results for thermal neutron flux agree poorly with the reference measurements especially at increasing distance from the reactor axis. In all cases Serpent and MCNP are in good agreement.

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Contents

# 1. Introduction

Serpent 2 is multi-purpose continuous-energy Monte Carlo transport code developed at VTT [1]. Serpent was originally developed for reactor physics applications but has since been expanded with features in support of radiation shielding and safety use cases among others. The topics of this report are related to photon transport physics, CAD-based geometries, and Serpent's built in variance reduction methods.

Coupled neutron-photon transport capabilities were introduced to Serpent 2 in 2017 [2]. The coupled and non-coupled photon transport physics have previously been validated for radiation shielding [3] [4] and reactor dosimetry applications [5] [6] with experimental data and code-to-code comparisons against MCNP. This report aims to continue the Serpent 2 validation efforts with the Baikal-1 Skyshine experiments [7] distributed in the ICSBEP [8].

In addition to being relevant for photon-neutron transport validation the Baikal-1 benchmark provides an apt opportunity to further verify the functionality of CAD-based geometries in Serpent 2. CAD support has been available in the Serpent code since 2014 [9], and a relevant publication on the methodology and applications was published later in 2022 [10]. CAD-based geometry models have previously been applied in radiation shielding calculations [11] and fusion neutronics [12] with good results. The methodology has been shown to have great potential for various radiation transport uses where typical geometry models are lacking due to the complex and irregular geometries present. This makes CAD-based models especially relevant for radiation safety and reactor dosimetry applications.

In this report the atmospheric scattering of neutrons and photons is simulated. Neutron and photon surface fluxes at near and remote on-site measurement locations are tallied for various particle energies. Particle energy driven conversion factors are used to estimate dose rates based on tallied flux levels. In addition, above core dose rate readings were used to confirm the correctness of the source.

# 2. Baikal-1 skyshine experiments

## 2.1 Experiment

The Baikal-1 skyshine experiment was carried out between the years 1996 – 1997 at the Kurchatov Institute of Atomic Energy in the Kazakhstan National Nuclear Centre. The goal of the experiment was to provide a detailed study of the spatial energy distribution of atmospherically scattered photons and neutrons. The radiation source used was the RA reactor built in 1987, originally a prototype nuclear rocket engine adapted to a research reactor. The reactor was cooled by forced atmospheric air and fuelled with highly enriched 90 % $^{235}$U rods. The approximate structure of the reactor and the surrounding structure can be seen in Figure 1.

The skyshine experiment entailed removing the upper biological shielding block of the containment structure, see Figure 1, exposing the reactor to the outside environment and releasing intense photon and neutron radiation to the atmosphere. On-site dosimetry measurements were taken on ground level, at distances between 50 m and 1500 m from the reactor axis. In addition, dose rate measurements immediately above the core were taken at three elevations and various radial positions.

A much more detailed description of the experiment is provided in the ICSBEP reference [7].

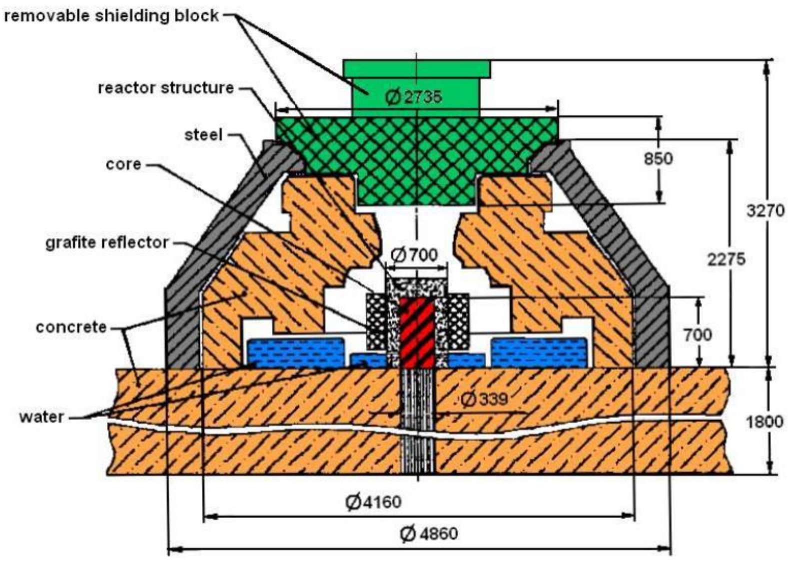


*Figure 1: Schematic of the RA research reactor, approximate dimension in cm. Adopted from [7]*

## 2.2 Benchmark description

The benchmark model in [7] has been defined realistically, with some key simplifications. These include the assumed radial symmetry of the surrounding facility, homogenization of the fuel composition, moderator element, lateral beryllium reflector assembly, and the various shielding zones above the core. Additionally, the effect of elevation on atmospheric conditions has been considered by defining altered material definitions for different elevations based on measurement taken at the site. Radial detectors are modelled as annular bands with radial width of 10 m, centred around the measurement location. To better visualize the scale of the geometry the detector positions are pictured in Figure 2. The benchmark defines another, more simplified point source model which was not reproduced here. Quality of the model approximations has been extensively assessed in the benchmark report [7].

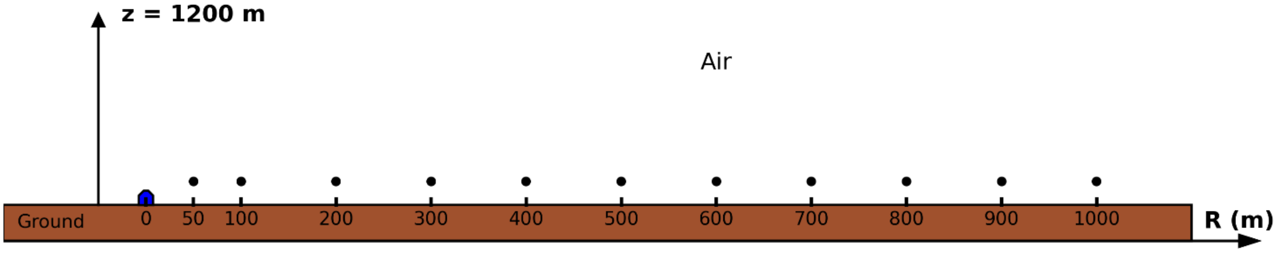


*Figure 2: Visualization of benchmark universe. Detector positions are marked with dots, reactor building is represented with a blue rectangle at R = 0m. Picture is not to scale.*

## 2.3 Serpent 2 model

The Serpent 2 model was built according to the benchmark definitions. Constructive Solid Geometry (CSG) was used for reactor internals and other simple geometries. CAD-based solids were utilized for the inner and outer shielding structures. The entire environment was defined as the background universe of the CAD-based geometries, further simplifying the universe definitions. The geometry was bound inside a cylinder of radius and height of 1200 m, ground level was defined at z = -8.8 cm. The core bottom was centred at ground level. The model geometry has been plotted in Figure 3.

Void boundary condition was used for all directions. All material definitions used were directly from the model definition. Radially binned surface flux detectors were used for both neutrons and photons at on-site and above core positions at the defined heights and energies. This differs from the annular bands used in the benchmark description. However, continuous radial binning allows for tallies across the entire range, rather than at distinct positions. On-site detector results are directly comparable as the radial bin width was set at 10 m, similarly to the band dimensions in the benchmark. The above core detectors were binned at 1 cm radial intervals, so that the desired tallies could be extracted easily.

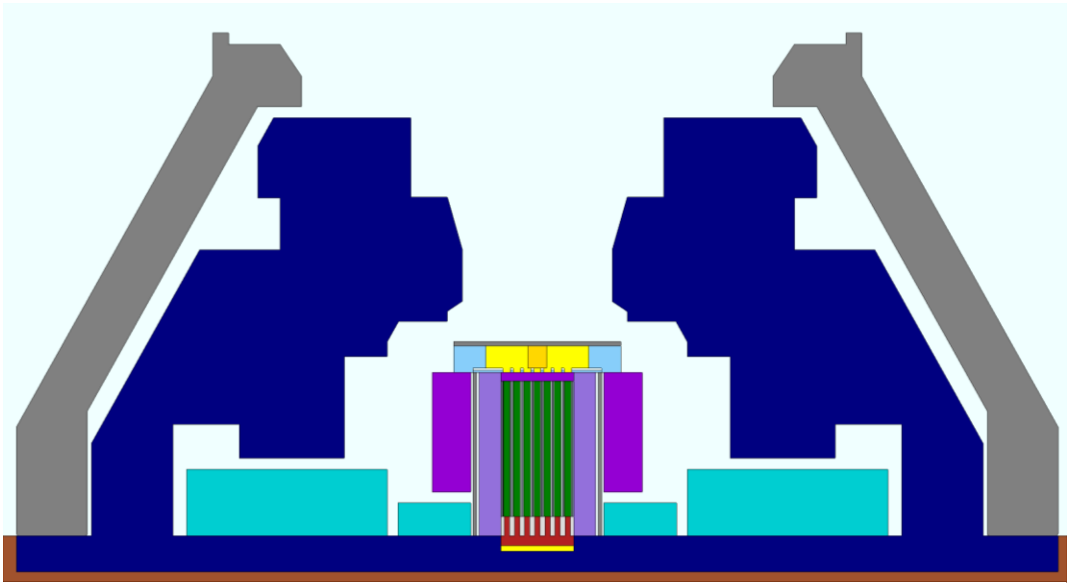

*Figure 3: Serpent 2 geometry of the RA reactor. Not to scale.*

Due to the considerable size of the geometry achieving acceptable statistics at the outer detector bins without variance reduction would have required an immense amount of particle histories. Serpent 2 has a built-in response matrix-based importance map solver [13] which was used to generate a weight-window mesh for the model. Best results were obtained with a coarse fixed cylindrical mesh using heavily increased splitting and roulette survival probability to promote better population across the entire geometry. This approach differs from a traditional shielding calculation using adaptive cell splitting, where the goal is to achieve statistics beyond a thick material boundary. In a skyshine benchmark a majority of the universe is thin air and especially density driven adaptive meshing has lacklustre results.

## 2.4 Results

The ICSBEP Baikal-1 skyshine benchmarks were calculated using a development version of Serpent 2.2.2. Neutron cross section data from ENDF/B-VIII library was used, with photo-atomic interaction data from the PAELib0.1/en71 library [14], which was purpose built for Serpent with data from ENDF/B-VII.1.

Calculation chain for the simulation begun with a criticality calculation to obtain the neutron source for the external source simulation. By using this neutron source in the coupled neutron-photon transport mode the actual calculation was run with the generated weight-window mesh. A photon source file was written during the coupled calculation, and with it a photon-only transport case was run to obtain better statistics specifically for the outermost photon detectors. Serpent does not support multi-particle weight-windows. Therefore, different weight-window meshes were used for the coupled and photon-only calculations created for neutrons and photons respectively.

The benchmark descriptions provides both reference measurements and MCNP5 results, against which the Serpent result are compared. All detectors used in the Serpent calculations were for tallying surface flux. Therefore, conversion factors for dose rate reported in the benchmark description were used, see Table 1. Further conversion was done from rem to sievert prior to visualizations. The spatial energy distribution of particles was not tallied from the Serpent input due to time constraints.

| Neutron Energy, Mev | NCRP-38, ANSI/ANS-6.1.1-1977 D(E), (rem/hr)/n/cm$^2$s) | Photon Energy, MeV | ICRP-21 D(E), (rem/hr)/photons/cm$^2$s) |
|---|---|---|---|
| **2.5E-08** | 3.67E-06 | **0.01** | 2.78E-06 |
| **1.0E-07** | 3.67E-06 | **0.015** | 1.11E-06 |
| **1.0E-06** | 4.46E-06 | **0.02** | 5.88E-07 |
| **1.0E-05** | 4.54E-06 | **0.03** | 2.56E-07 |
| **1.0E-04** | 4.18E-06 | **0.04** | 1.56E-07 |
| **1.0E-03** | 3.76E-06 | **0.05** | 1.20E-07 |
| **1.0E-02** | 3.56E-06 | **0.06** | 1.11E-07 |
| **1.0E-01** | 2.17E-05 | **0.08** | 1.20E-07 |
| **5.0E-01** | 9.26E-05 | **0.1** | 1.47E-07 |
| **1.0** | 1.32E-04 | **0.15** | 2.38E-07 |
| **2.5** | 1.25E-04 | **0.2** | 3.45E-07 |
| **5.0** | 1.56E-04 | **0.3** | 5.56E-07 |
| **7.0** | 1.47E-04 | **0.4** | 7.69E-07 |
| **10.0** | 1.47E-04 | **0.5** | 9.09E-07 |
| **14.0** | 2.08E-04 | **0.6** | 1.14E-06 |
| **20.0** | 2.27E-04 | **0.8** | 1.47E-06 |
| | | **1.0** | 1.79E-06 |
| | | **1.5** | 2.44E-06 |
| | | **2.0** | 3.03E-06 |
| | | **3.0** | 4.00E-06 |
| | | **4.0** | 4.76E-06 |
| | | **5.0** | 5.56E-06 |
| | | **6.0** | 6.25E-06 |
| | | **8.0** | 7.69E-06 |
| | | **10.0** | 9.09E-06 |

*Table 1: Neutron and photon flux to dose rate conversion factors. Adapted from [7].*

Above core thermal neutron fluxes are presented in Figures 4 – 6 and converted photon dose rates in Figures 7 – 9. Serpent produces acceptable agreement with MCNP5 across all three elevations for both particles. Although, the simulated thermal neutron flux differs considerably from the measurements on the two higher elevations and near the centreline, it should be noted that the above core reference measurements have significant uncertainties reported in the benchmark descriptions. The above core detector tallies were mainly used for source confirmation before proceeding to the on-site transport problem.

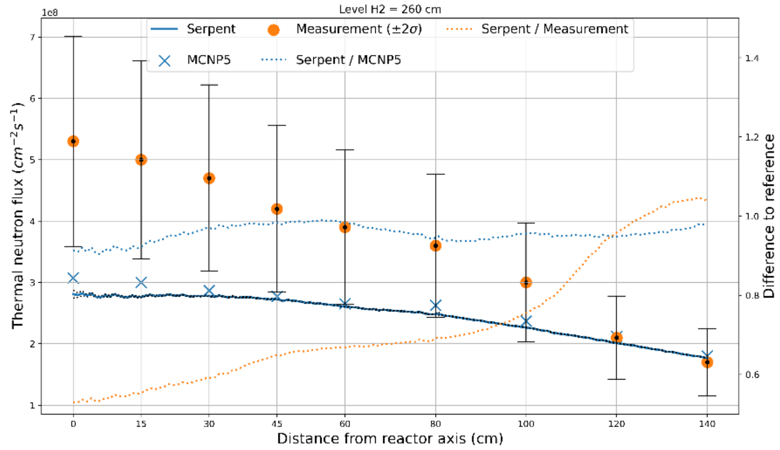


*Figure 4: Above core thermal neutron flux at H0 = 0 cm above the reactor*

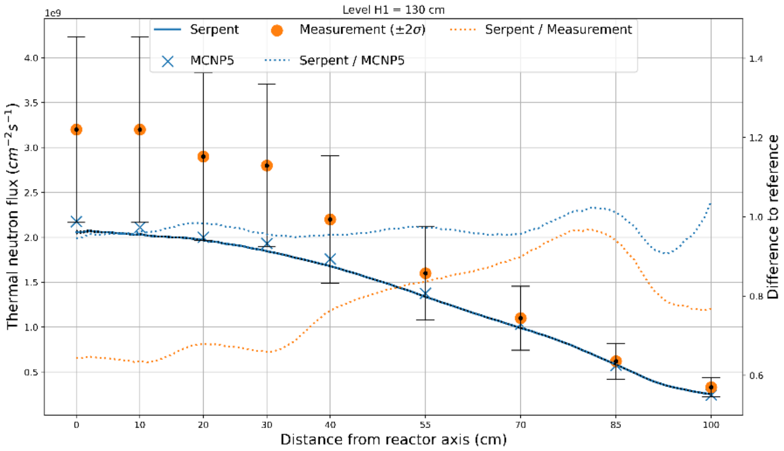


*Figure 5: Above core thermal neutron flux at H1 = 130 cm above the reactor*

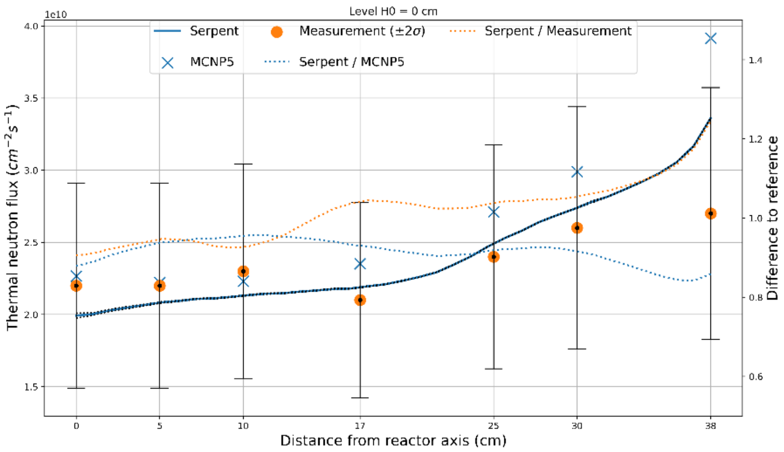


*Figure 6: Above core thermal neutron flux at H2 = 260 cm above the reactor*

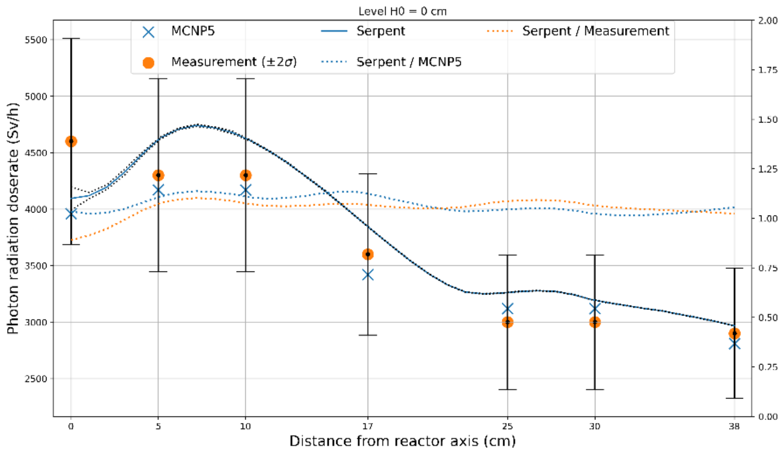


*Figure 7: Above core converted photon dose rate at H0 = 0 cm above the reactor*

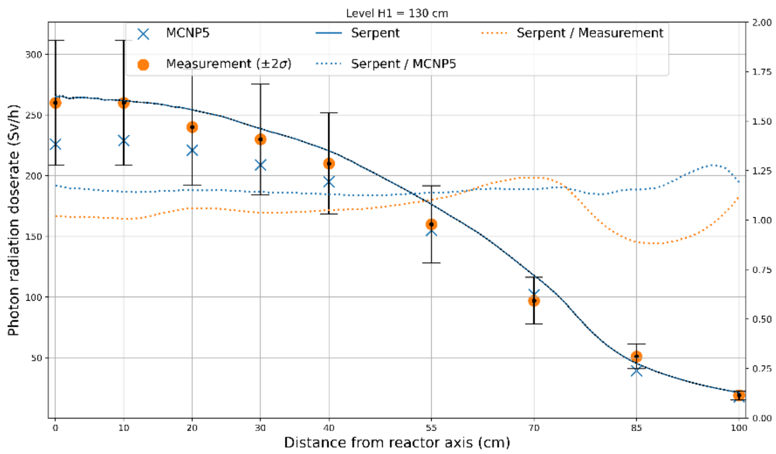


*Figure 8: Above core converted photon dose rate at H1 = 130 cm above the reactor*

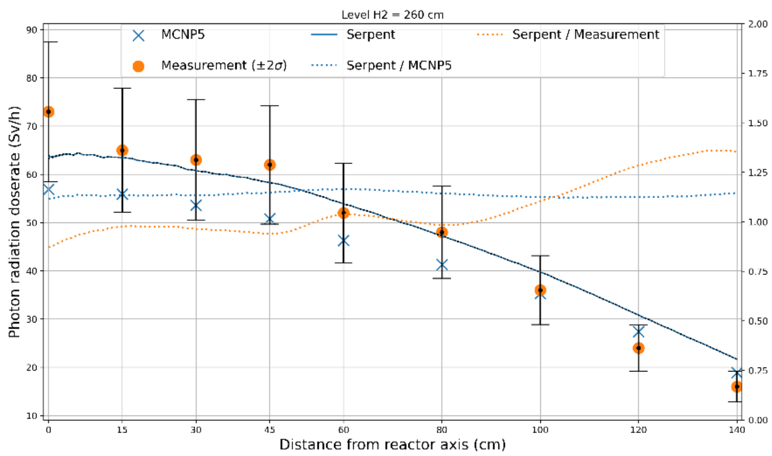


*Figure 9: Above core converted photon dose rate at H2 = 260 cm above the reactor*

On-site results were collected for thermal (E < 0.414eV), intermediate and fast neutrons as well as photons across various energies. Thermal neutron flux, in Figure 10, is significantly over reported by Serpent compared to the reference measurements and MCNP5 results. Combined fast and intermediate neutron flux, in Figure 11, is in good agreement with both MCNP5 and reference measurements throughout the entire detector range. The converted neutron dose rate based on the Serpent results is in very good agreement with the reference measurements, as seen in Figure 12. Additionally, Serpent does not reproduce the MCNP5's seemingly erroneous behaviour at the 800 m position. The converted photon dose rates by Serpent, in Figure 13, agree with the reference measurements more consistently than MCNP5. However, some noise can be observed at the outer detector positions, which can be explained by subprime detector statistics.

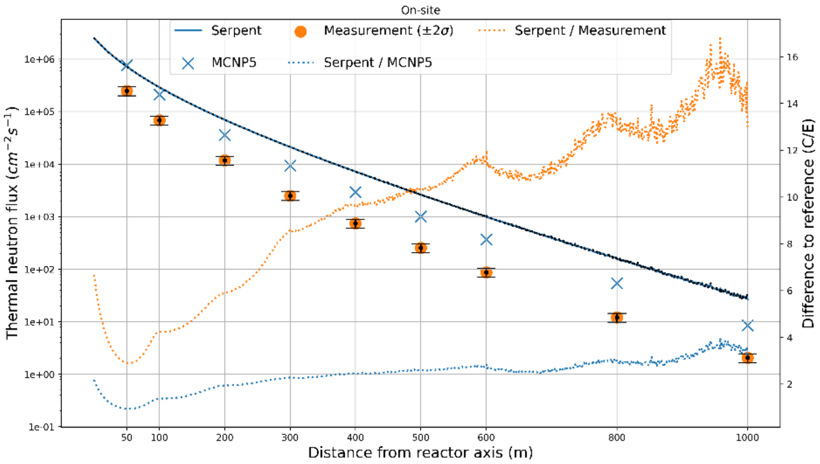


*Figure 10: On-site thermal neutron flux at ground level*

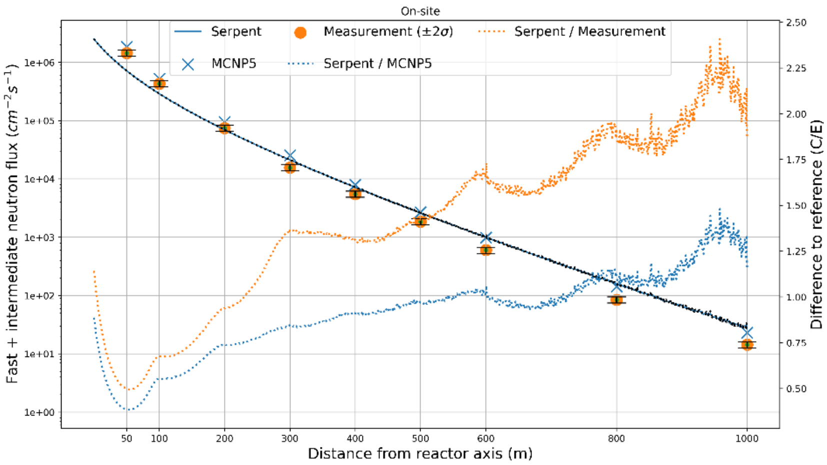


*Figure 11: On-site fast and intermediate neutron flux at ground level*

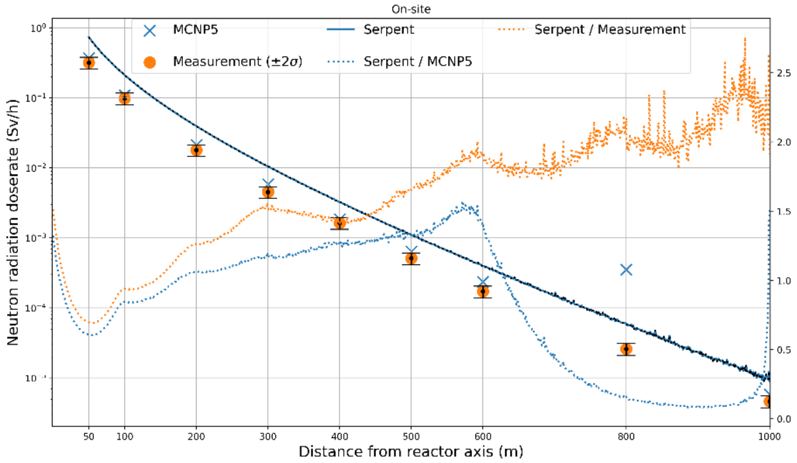


*Figure 12: On-site converted neutron dose rate at ground level*

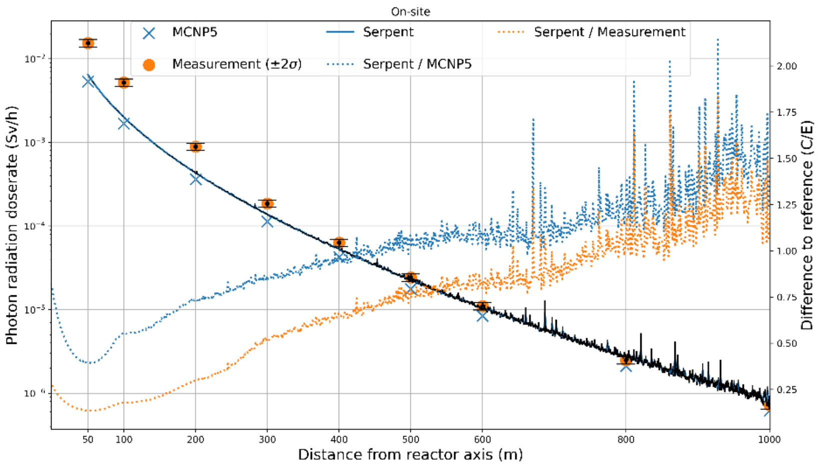


*Figure 13: On-site converted photon dose rate at ground level*

Generally good agreement between Serpent and MCNP5 is observed. However, at some cases larger than expected differences exist. For example, results of the on-site neutron flux rate are consistently overestimated by Serpent, compared to MCNP5. Across all cases, it can be noted that photon results agree better with the MCNP5 correspondents, as compared to neutron detector tallies. This can, at least partly, be explained by the different neutron cross-section libraries used. The MCNP5 results from over a decade ago were calculated using the ENDF/B-VI continuous-energy cross section library [7], whereas with Serpent the newer ENDF/B-VIII library was used.

## 3. Conclusions

In this report the Baikal-1 skyshine benchmarks [7] were calculated in Serpent 2.2 and used for further validation of the coupled neutron-photon transport mode. Neutron and photon surface flux was calculated at on-site ground level between 50 m and 1000 m away from the reactor axis. In addition, flux levels directly above the core were tallied at three different heights. Agreement between the calculated values and reference measurements was good. Excellent agreement between Serpent and MCNP was observed at the above core results neutron doses with good agreement in photon dose result. On-site result for neutron flux and neutron-photon dose rates are in good agreement with the measurements and MCNP5. However, on-site thermal neutron flux has poor agreement with the measurements at increasing distances. Agreement between the two transport codes was good across all calculated results. Differences were mainly observed with neutron result, which can partly be explained by the differing neutron cross-section libraries used in the calculations (ENDF/B-VI and ENDF/B-VIII). The coupled neutron-photon transport mode in Serpent produced generally very good results, especially for photons. Additional work to obtain the spatial energy distribution of neutrons and photons in the benchmark case could provide valuable information for further validation of the Serpent code.

Serpent's built-in importance map solver-based variance reduction scheme struggled with the almost entirely homogenous universe of the skyshine benchmark. Best results were achieved with a coarse cylindrical mesh and heavily increased splitting of particle histories. Nevertheless, statistics at the further detectors were suboptimal at some energies for both neutrons and photons. Further work could be related to refining the variance reduction methodology for sparse geometries like the one represented in this benchmark. CAD-based geometries were successfully used to model the reactor shielding structures and the background environment. This geometry type in Serpent has definite potential in applications requiring complex or irregular geometries, like fusion and realistic radiation safety analysis.

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