Designing a boron nitride polyethylene composite for lunar radiation shielding

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Recently, there has been an interest in integrating boron-based materials into critical radiation shielding and sensing components for space applications. The isotope $^{10}$B (19.9% of natural boron) has a large capture cross section for thermal neutrons, converting them into alpha particles and lithium ions, which are stopped within a few microns of material. With high density polyethylene (HDPE) as a thermalization medium and hexagonal boron nitride (hBN) as a capture medium, we model the maximum shielding effectiveness by optimizing the boron distribution within HDPE composites using the Geant4 Monte Carlo simulation toolkit. The shielding materials are optimized for the distribution of neutrons near the Moon’s surface, which are ubiquitous due to interactions of high-energy galactic cosmic radiation with the lunar regolith. From optimizing the $^{10}$B distribution within HDPE composites (through internal layering), we improve the shielding effectiveness by 4x to 30x over Al, the current space industry standard for radiation shielding, and 1.5x to 2x over HDPE. Interestingly, we find that the optimal solutions tend to be multilayered, with the HDPE layer thicknesses comparable to the neutron thermalization length.

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I. INTRODUCTION

Astronauts receive the most radiation exposure of any occupation, significantly more than air flight crew members. Radiation can result in changes to bone, muscle, and cartilage microstructures, increased risk of cancer,
cognitive decline, and degeneration of astronaut’s circulatory systems. From the guiding principle of radiation safety (ALARA, “as low as reasonably achievable”), there are three protective measures for limiting radiation exposure: minimizing time, maximizing distance, and shielding. Minimizing time and maximizing distance are often limited by mission constraints, while using shielding is limited by mass considerations due to the high cost of transporting materials and limitations of in-situ resource utilization. Therefore, the shielding afforded to astronauts by spacesuits and habitats is an impactful area for improvement. In this paper, we focus on optimizing the internal distributions of elements for shielding radiation on the surface of the Moon. We are specifically interested in materials that are effective against shielding neutrons and have a potential utility in additive manufacturing, a necessary tool for the creation of lunar habitats.

In the space environment, there are three sources of radiation: galactic cosmic radiation (GCR), solar energetic particles (SEPs), and trapped radiation belts. Each of these radiation sources presents its own health risks. GCR, produced during supernova explosions, consists of 83% protons, 13% alpha particles, 3% electrons, and 1% heavy nuclei. These particles have a wide range of energies, ranging from tens of MeV per nucleon (MeV/n) to hundreds of GeV/n, and thus pose a serious threat to astronauts. For GCR and other high-energy radiation, the threat is amplified by the extensive production of secondary radiation through interaction of the primary particles with matter.

Another source of dangerous radiation is SEPs, which are an enhancement of energetic particles above the thermal energy of solar wind particles. These enhancements arise from solar flares and coronal mass ejections. SEPs mostly consist of energetic protons and other heavy charged particles with energies ranging from tens of keV/n to several GeV/n. The relative abundances and fluxes of these particles vary with solar activity. During solar maximum, the interplanetary magnetic fields that carry the SEPs are heightened and make them the dominant radiation exposure risk for astronauts. But during solar minimum, the astronaut radiation exposure is dominated by GCR.

The last source of radiation relevant for earth-origin missions is the trapped radiation belts. There are two radiation belts spanning between ~1.5-3 and ~3-10 Earth radii, respectively. These consist of energetic electrons (from ~100 keV to >10 MeV), protons, and heavier charged particles (alpha particles, C/N/O ions, etc.). The protons and other charged particles range from a few eV/n to ~100 keV/n, with the relative abundances and fluxes of particles in the radiation belts dependent on geomagnetic disturbances. The trapped radiation belts only affect astronauts during mission transit, so their exposure to this intense radiation environment is limited.
Current and upcoming lunar missions include research tasks to improve the characterization of space radiation at
the lunar surface and enhance the understanding of potential human exposure \(^9\). Recently, the first measurements of
radiation dose on the lunar surface were made in the Lunar Lander Neutrons and Dosimetry experiment aboard China’s
Chang’E 4 lander \(^{10}\). From these measurements, the average absorbed dose rate in silicon is \(13.2 \pm 1 \mu\text{Gy/hour}\) \(^{10}\).
The CRaTER (Cosmic Ray Telescope for The Effects of Radiation) on board the Lunar Reconnaissance Orbiter is
also used to measure the lunar radiation and has determined the most conservative permissible mission duration of
\(~204 – 290\) days based on the measured radiation dose \(^{11}\).

From ALARA, the best way to limit the absorbed dose for astronauts is to develop improved shielding materials.
The mass attenuation coefficient generally increases as the atomic number of the shielding material increases. Thus,
lead and concrete are typically used as shielding materials for ground-based systems. However, due to the limited
flight mass of spacecraft, these materials are not suitable. Instead, spacecraft typically use aluminum to provide
shielding and structural support. Recently, high density polyethylene (HDPE) panels have been incorporated into the
ISS (International Space Station) to provide astronauts with additional protection \(^{12}\). Outside of the spacecraft,
astronauts receive limited shielding from the existing fabrics in the spacesuit, which consists of reinforced aluminized
mylar, nylon ripstop, and polyester \(^{13}\).

In this study, we optimize polymer composite shielding materials which could be incorporated into radiation
shielding for space applications (e.g., spacesuits and habitats) to provide additional shielding and further protect
astronauts from ionizing radiation. For a lunar mission, a significant component of the ambient radiation is originate
from GCR interacting with the lunar surface and the resulting cascade effects, such as spallation and inelastic
collisions, releasing leakage radiation \(^{14}\). The energy distribution of lunar neutrons rapidly decreases with increasing
energy, resulting in a distribution heavily weighted towards thermal and epithermal neutrons \(^{14-16}\). We are specifically
interested in optimizing shielding for albedo neutrons because of their high penetration depth and extreme health
effects, making shielding neutrons of central importance for human exploration beyond low Earth orbit. We focus on
shielding materials made from flexible, thermoplastic HDPE and hBN/HDPE composite materials which could be
additively manufactured (AM), expanding potential applications to include inflatable and AM habitats. Incorporation
of AM-compatible shielding materials provides the framework for expanding the materials palette and development
of designs strategies which could be used to effectively protect astronauts during long duration lunar missions \(^3\).
Layering different materials is not an uncommon approach for shielding materials; however, prior studies of layered shields typically focus on shielding for multicomponent radiation sources, with different layer materials devoted to attenuation of different particles \(^{17-19}\). In this study, we focus on a single radiation type—neutrons—and consider the effect of layering two components, high-density polyethylene (HDPE) and hexagonal boron nitride (hBN), to discover whether a “metamaterial” concept could affect the shielding property. Our modeling work focuses on optimizing the internal configuration of composites because of their shielding properties and prior experimental work suggests that the internal configuration of hBN in a polymer matrix can affect shielding effectiveness \(^{20-24}\).

Based on the energy distribution of lunar neutrons, it is advantageous to include boron-10 \(^{10}\)B as it has a large capture cross section for thermal neutrons (~3,800 barns) and produces the following capture reactions:

\[
\begin{align*}
\text{^{10}B} + \nu_{\text{th}} & \rightarrow \text{^\text{3}Li}^* (0.84 \text{ MeV}) + \text{^\text{4}He}^* (1.47 \text{ MeV}) \ [94\%], \\
\text{^{10}B} + \nu_{\text{th}} & \rightarrow \text{^\text{3}Li} (1.015 \text{ MeV}) + 4\text{He} (1.777 \text{ MeV}) \ [6\%].
\end{align*}
\]

Here, \(^{10}\)B captures the thermal neutrons \((\nu_{\text{th}})\), converting them into alpha particles and lithium ions, which have a relatively short stopping range of only a few microns at the relevant energies – much shorter than the neutron attenuation length. However, most of these alpha and lithium ions are created in an excited state that immediately decays, releasing additional gamma radiation, which carries its own health risks.

Experimental studies of boron-containing HDPE composites have been reported previously, where neutron transmission measurements reveal an improvement in the shielding effectiveness in hBN blended into HDPE, compared with composites made with B\(_4\)C, another boron-containing material \(^{20,21}\). Hexagonal boron nitride, a quasi-2D material with a large bandgap of ~5.9 eV, has naturally occurring boron (19.9\% of \(^{10}\)B and 80.1\% of \(^{11}\)B) and can undergo the capture event shown in Equations 1a-1b. However, hBN can be boron-10 enriched, further increasing the probability of undergoing the capture reaction \(^{25}\). Since there is a wide energy range of albedo lunar neutrons, HDPE is used to convert the high energy lunar neutrons to lower energy neutrons to increase the probability of undergoing a capture event with \(^{10}\)B.

This work builds upon previously published works that study the shielding effectiveness of layered hBN and HDPE \(^{20-23,26}\). However, in this study, we use Monte Carlo (MC) simulations to optimize the shielding composition and structures for hBN/HDPE composites. Sections II and III discuss hBN and HDPE interactions with neutrons and introduces the figure of merit that is used to evaluate the effectiveness of the simulated shielding composites. In
Section IV, we explore three different geometries for the hBN/HDPE composites: blended, ideal layered, and manufacturable. The blended composite is a homogenous mixture of HDPE and hBN, which has been previously experimentally studied by examining materials made by melt blending platelets of hBN into HDPE matrices. The ideal layered composite consists of pure hBN interlayered with layers of pure HDPE to understand the advantage of layering versus blending. The poor mechanical properties of pure hBN layers and the poor interfacial bonding between pure hBN and pure HDPE layers makes this ideal structure difficult to manufacture at the size scale needed for spacesuits and habitats. Therefore, in this study, we also consider a manufacturable composite, which consists of blended layers of hBN/HDPE interlayered with pure HDPE. Integration of blended hBN/HDPE layers in place of pure hBN layers improves both the manufacturability and the mechanical properties of the hBN-rich layers.

II. NEUTRONS INTERACTIONS WITH hBN AND HDPE

Design of effective shielding is driven by consideration of the basic neutron capture event, $^\text{10}\text{B}(n,\alpha)$. Figure 1a shows the capture cross-section $\sigma$ (right-axis, blue), from the ENDF/B-VIII.0 database, of this capture event for boron-10 enriched hBN (i.e. $^\text{10}\text{BN}$) and natural hBN (i.e. $^\text{Na}\text{BN}$). Correspondingly, the capture mean free path ($\lambda$ or mfp; $\lambda = 1/Na$ where $N$ the density of boron atoms) is orders of magnitude smaller for thermal neutrons than fast neutrons (Figure 1a: left-axis, $^\text{Na}\text{BN}$ – red and $^\text{10}\text{BN}$ – black). Figure 1b shows the elastic scattering cross section for $^\text{1}\text{H}$ and $^\text{12}\text{C}$ (right-axis, blue) and the mfp of lunar neutrons in HDPE (left-axis, black). The elastic mfp provides us with an estimate of the amount of HDPE required to moderate lunar neutrons, showing that the elastic mfp is ~0.5 cm of HDPE for thermal and epithermal neutrons and rapidly increases for fast neutrons.
FIG. 1. (a) Capture mean free path (mfp), obtained from ENDF/B-VIII.0 database, in $^{10}$BN (left axis, black line), $^{10}$BN (left axis, red line), and the scattering cross section for $^{10}$BN reaction with neutrons (right axis, blue line) as a function of energy. The dotted line marks the mfp of 10 μm. (b) Elastic mfp in HDPE (left axis, black line) and elastic scattering cross section for $^1$H and $^{12}$C with neutrons (right axis, blue lines) as a function of energy. The dotted lines mark the mfp of a 1 MeV neutron. For both subplots, the thermal, epithermal, and fast neutron regions are shown.

On the surface of the Moon, approximately ~70% of the neutrons lie within the thermal and epithermal region because the neutron flux decreases as the energy increases. Based on the capture mfp shown in Figure 1a, these neutrons are captured by a $^{10}$BN layer between 10 μm and ~10 cm for thermal and epithermal neutrons, respectively. To capture the full energy range of neutrons, we would need between ~10 μm and 2 m of $^{10}$BN (Figure 1a, black) and ~35 μm and 13 m of $^{10}$BN (Figure 1a, red). Production and incorporation of large area hBN layers with thickness approaching or exceeding 10 cm is extremely difficult due to poor mechanical stability of hBN layers and high rigidity. Therefore, to enhance neutron capture, it is reasonable to consider a second material component which is effective at thermalizing the neutron flux to increase the probability of undergoing a capture event in hBN layers of reasonable thickness.

Thermalization requires a high rate of momentum transfer to the material, which is best accomplished by compounds with high hydrogen content due to the near equality of neutron and proton masses. A good moderator is capable of slowing down fast neutrons without capturing the neutrons and undergoing radiation damage. For these reasons, water ($\rho \approx 1$ g/cm$^3$), graphite ($\rho \approx 2.26$ g/cm$^3$), and polyethylene ($\rho \approx 0.90 - 0.97$ g/cm$^3$) are commonly used as neutron moderators. HDPE, ($C_2H_4)_n$ for n between 3,500 and 9,000, is ideal for space applications due to its high hydrogen content, low density, and large elastic neutron scattering cross section. Additionally, unlike water and graphite, HDPE has suitable physical properties to be used as a stand-alone flexible radiation shielding material across the broad range of operating temperatures on the lunar surface.

III. FIGURE OF MERIT: EFFECTIVE DOSE

In radiation physics, there are three dose quantities that are used to assess the radiation exposure: absorbed dose, equivalent dose, and effective dose. The absorbed dose is defined as the mean energy imparted by ionizing radiation in matter per unit of mass (the SI unit of absorbed dose is the Gray, with 1 Gy = 1 J/kg). The equivalent dose ($H_T$) weights the absorbed dose by the radiation type to determine the effect of the ionizing radiation on a specific organ or tissue. Mathematically, the equivalent dose reads
\[ H_T = \sum_R w_R D_{T,R} \]  

where \( w_R \) is the radiation weighing factor, and \( D_{T,R} \) is the mean absorbed dose from a radiation type, \( R \), in specific organs or tissues, \( T \). The effective dose \( (E) \), provided in units of Sieverts (Sv), takes the equivalent dose and sums over the organ/tissue as

\[ E = \sum_T w_T H_T = \sum_{T,R} w_T w_R D_{T,R} \]  

where \( w_T \) is the tissue weighting factor. Although the weight factors are dimensionless, both \( H_T \) and \( E \) are assigned the SI unit Sievert, when \( D_{T,R} \) is in Gy units.

The International Commission on Radiological Protection (ICRP) provides a set of protection quantities based on radiation transport simulations for a monoenergetic particle emitted in various directions (rotational, left lateral, right lateral, isotropic, etc.) incident on a human phantom. ICRP provides the necessary coefficients to convert incident energy to effective dose for sex-averaged models of human phantoms. These coefficients are used to estimate the effective dose an average human receives for a given radiation type and energy. Here, we use the sex-averaged conversion coefficients for an isotropic input distribution as it more accurately represents the radiation in space. ICRP 103 provides the radiation weighting factors\( \text{ }^{29} \); ICRP 116 and 123 provide the conversion coefficients for a given fluence \( (\Phi) \)\( ^{30,31} \).

Figure 2 shows the effective dose per fluence \( (\Phi) \) as a function of the incident energy for different radiation types. The heavy ions have the largest effective dose and can, therefore, be the most damaging for humans in comparison to other ionizing particles. However, significant damage occurs for energetic heavy ions (greater than \( \sim 1 \text{ MeV} \)). In contrast, neutrons are quite damaging across all incident energies. For this reason, we integrate \( ^{10} \text{B} \) into the shielding components to capture high doses of hazardous thermal neutrons. Gammas, positrons, electrons, and protons have a similar effective dose and are also important to shield against.
FIG. 2. Effective dose per fluence (pSv cm\(^2\)) for a sex-averaged human as a function of the incident energy, calculated for various radiation types emitted isotropically. The effect of different radiation types is shown in color. ICRP 116 and 123 are used to obtain the conversion factors from energy to effective dose.

IV. RESULTS AND DISCUSSION: hBN/HDPE COMPOSITES

We use the MC simulation toolkit, GEometry ANd Tracking (Geant4, version 4.10.07-p02), to simulate the passage and interactions of particles through the shielding material\(^{32,33}\). Geant4 was selected as it can be used to model particle interactions in small-scale geometries on a single particle basis, while allowing the user to control all relevant parameters, including the geometry and materials composition, fundamental particles of interest, physics processes governing the interactions, tracking of particles, storage of events/tracks, etc\(^{32}\). We validate the physics models in Geant4 using Monte Carlo N-Particle code (MCNP), a well-established neutron transport code (see Appendix B for details of the validation with MCNP). These materials, HDPE and hBN, are specifically chosen to thermalize and capture the lunar neutrons, by the mechanisms discussed in Section II. The effective dose per fluence, described in Section III, is used as the figure of merit to evaluate the effectiveness of various composite configurations, and determine the optimal composition and structure. In this section, we present the shielding effectiveness of hBN/HDPE composite shielding materials, starting with a description of the simulations, and followed by the results for various hBN/HDPE configurations.

A. STRUCTURE OF THE SIMULATIONS

We restrict our design space to address a simple question related to the use of hBN and HDPE to perform the two-step shielding process, neutron thermalization and neutron capture. There are many possible configurations of the
hBN/HDPE composite structures, including blended and layered geometries with varying weight percentages of hBN. Within the layered geometry, the number and thickness of HDPE and hBN layers can also be varied. Our goal is to explore the design space of all possible configurations of hBN/HDPE composites using the effective dose as a figure of merit to obtain the optimal boron distribution in HDPE composites.

For the blended geometry, three free design parameters are considered: total composite thickness, global weight percentage of hBN, and material identity of hBN (either h^{10}BN or h^{11}BN). The thickness is varied between 1 mm and 150 mm to simulate a lunar shielding material for various applications, such as lining for space suits or habitat shielding. We note that one could run one simulation at the largest thickness, namely 150 mm, and extract the exiting distribution for smaller thicknesses (<150 mm). However, for simplicity, we run each thickness as a separate run to minimize the personnel time required for post-processing. The global weight percentage of hBN is varied between 0 and 100%, in increments of 10%. The range of weight percentage is simulated to cover the entire design space of all possible blended configurations even though blended composites with >30wt% of hBN are difficult to manufacture via traditional blending methods. Including higher weight fractions of hBN also allows this dataset to be used to evaluate the cost-benefit relationship for implementation of advanced manufacturing methods which could be used to produce composites with higher weight percentages of hBN.

For the ideal layered geometry, we consider four parameters: total composite thickness, number of HDPE and hBN layers within a composite thickness, global weight percentage of hBN, and hBN material (either h^{10}BN or h^{11}BN). This configuration consists of interlayering pure HDPE and pure hBN layers to explore how spatial distribution affects the effective dose compared to a blended structure. Based on the capture reaction (Equation 1), it is best to terminate the structure with an HDPE layer so that the heavy charged particles—which would significantly increase the effective dose (see Figure 2)—can be stopped before exiting the composite shielding. For this reason, there is always one less hBN layer than HDPE layers. Figure 3 shows an example of two layered structures with global hBN weight percentage of (a) 20% and (b) 80% for 5 layers of HDPE (4 layers of hBN) within a total thickness of 10 mm. Changing the global weight percentage of hBN changes the relative thicknesses of the hBN layers within the internal structure. This figure also shows that the ideal layered composites are modeled with step-function transitions between the HDPE and hBN layers. For this portion of the study, we vary the number of HDPE layers between 2 (1 layer of hBN) and 100 layers (99 layers of hBN) and the global hBN content between 0-100wt%. The number of layers can be alternatively characterized in terms of the period of the repeating hBN/HDPE unit.
FIG. 3. Cross-section view of two ideal layered composites with a global weight percentage of (a) 20% and (b) 80% of pure hBN for 5 layers of HDPE within a thickness of 10 mm. The relative thicknesses of the layers are determined by the global hBN weight percentage in the composite structure.

Due to manufacturability constraints of creating thick continuous hBN layers bonded to HDPE layers in the ideal layered structure and high loadings in some blended structures, it is difficult, or impossible in some cases, to manufacture all the geometries that are explored in the blended and ideal layered geometries. For the blended geometries, only the configurations with <30 wt% of hBN can be manufactured by traditional melt blending processes due to poor particle dispersion and dramatically increased viscosity of the melt at higher loadings, particularly when hBN nanoparticles are used in the manufacture of blended composites 36. For the layered condition, it is also difficult to make a pure hBN layer of large size due to the restricted growth conditions required to obtain a pure hBN crystal 37. To address this issue, additional simulations were run in which pure HDPE was interlayered with hBN/HDPE blended composite layers with \( \leq 20 \) wt% of hBN. This configuration is explored as an easily manufactured configuration, via melt blending and hot compaction, and is compared with the blended and ideal layered simulation results. A weight percentage of \( \leq 20 \)% is chosen in hBN/HDPE composites as these loading levels show little degradation in mechanical or rheological properties increasing the ease of manufacturing. Additionally, due to the small impact of \( \leq 20 \) wt% on the rheological properties of the hBN/HDPE melt, it is reasonable to assume that these manufacturable geometries could be easily adapted to fused filament fabrication, a space proven additive manufacturing technology 3.

For the manufacturable geometry, there are five design parameters: total thickness of composite material (\( t \)), mixture weight percentage of the blended hBN/HDPE layer (\( \omega_{mix} \)), local weight percentage of hBN within the blended
layer ($\omega_{hBN}$), number of HDPE layers ($n$), and inclusion of either $h^{30}$BN or $h^{10}$BN. The thickness of each blended hBN/HDPE layer ($t_{\text{mix}}$) is:

$$t_{\text{mix}} = \frac{t}{n-1} \left[ \omega_{\text{mix}} \rho_{\text{total}} \right]$$

(4)

where $\rho_{\text{total}}$ is the total density of the composite material which includes both $t_{hBN}$ and $\omega_{\text{mix}}$, and $\rho_{\text{mix}}$ is the density of the blended hBN/HDPE layer. The thickness of each HDPE layer ($t_{\text{HDPE}}$) is:

$$t_{\text{HDPE}} = \frac{t}{n} - t_{\text{mix}}$$

(5)

The global weight percentage for the manufacturable configuration is calculated using both $\omega_{\text{mix}}$ and $\omega_{hBN}$. Equations 4 and 5 can be reduced to the thickness of each HDPE and hBN layer for the ideal layered geometry by making the following simplifications: $\omega_{\text{mix}} = \omega_{hBN}$ and $\rho_{\text{mix}} = \rho_{hBN}$. Because of the large number of design parameters for each configuration, we run 286 simulations for the blended structure, 2,420 for the ideal layered structure, and 11,340 for the manufacturable structure. The Geant4 output files produces a few terabytes of data that is parsed and presented in this study.

Additionally, simulations of a pure aluminum block are carried out to provide a direct comparison with the current radiation shielding used in spacecraft. These simulations are run for the same thicknesses as the blended, ideal layered, and manufacturable geometries to allow for a direct comparison. Comparisons with pure HDPE (0 wt% of hBN) and pure hBN (100 wt% of hBN) are also provided within the blended geometry.

For all simulations, neutrons, isotropic in angle, are uniformly incident on one side of the composite material with an energy uniformly varying from 1.5 meV to 17 MeV. During the post-processing, the incident neutrons are weighted according to the lunar energy distribution making these shielding results only applicable to lunar missions. The leakage flux is modeled using Geant4 for incident GCR particles, similar to the procedure presented in Mesick et al., 2018 28. Figure 4 shows the normalized flux that is applied during the post-processing to weight the exiting particle distribution from each incident neutron by the probability of incidence determined by the lunar energy distribution. This distribution is determined for the neutron leakage flux 10 cm away from the surface of the Moon for a solar modulation of $\phi = 530$ MV. The flux is normalized such that the area under the curve integrates to one.
FIG. 4. Neutron energy distribution simulated from 10 cm above the surface of the Moon. This distribution is calculated using the method provided in Mesick et al., 2018.

Within each Geant4 simulation, a “sensitive detector” is placed on the entry and exit surface of each composite structure to record the particles entering and exiting the material without saving all the interactions occurring within it (see Appendix A for details of Geant4). The composite material is set to have periodic boundary conditions (using the g4pbc module) in the lateral dimensions to simulate an infinite slab. The lateral dimension for all the simulations is 100 cm, which is ~10x larger than the thickest sample, namely 150 mm. We choose such a large lateral dimension to ensure that the periodic boundary conditions do not have a significant effect on the simulation results. Note that an equivalent method is the use of isotropically emitted neutrons from a point source and a large lateral dimension to ensure that the particles are not escaping through the lateral edges.

B. COMPOSITE SHIELDING RESULTS

1. Blended Geometry

We explore the shielding effectiveness of a homogenous distribution of boron in HDPE by varying the weight percentage of hBN in HDPE from 0% to 100%. As described in Section III, we use effective dose (per incident fluence) as the measure of shielding effectiveness because of its direct relation to health effects. However, before focusing on this single figure of merit, we describe in more detail how it is obtained from the raw MC results. Figure 5 shows the particles contributing to the effective dose per fluence (pSv cm²) in (a) and the energy distribution of the exiting particles in (b) and (c) for a 5-mm-thick composite shielding material with a blend of h⁰BN and HDPE. The contributions to the effective dose in Figure 5a are presented as a function of h⁰BN weight percent for neutrons in
blue and gammas in gray where each bar sums to 100%. There are other particles exiting the composite shielding material, like lithium and alpha particles; however, they do not contribute significantly to the effective dose (<0.1%). The number on each bar shows the effective dose per fluence for each weight percentage, in units of pSv cm². The histograms of the energy distributions for neutrons are shown in Figure 5b and gammas in Figure 5c. The only post-processing done here is the weighting of exit-particle distributions by the lunar distribution, shown in Figure 4. The histograms are normalized such that the area integrates to one and plotted on the same scale for each of the subplots. The absolute magnitude of the integrated number of particle counts is shown by the colorbar, which determines the color of the histogram.

In Figure 5, as the weight percentage increases from 0% (pure HDPE) to 10%, neutrons no longer dominate the effective dose. The number of gammas increases by an order of magnitude as the weight percentage increases to 10%, increasing the gamma contribution to the effective dose. The magnitude of the effective dose decreases as the gamma contribution increases as gammas have a lower effective dose than neutrons across all energies (see Figure 2). Upon
Further increasing h\textsuperscript{Na}BN from 10 wt% to 40 wt%, the effective dose stabilizes at 0.63 pSv cm\textsuperscript{2} and gammas contribute to >90% of the effective dose. From the histograms of the neutron energy distribution (Figure 5b), we observe that the low-energy neutrons are absorbed by the neutron capture event (shown in Equation 1), reducing the total number of neutrons and increasing the number of gammas. From the magnitude of the effective dose in Figure 5a, we find that it is more favorable to use a shielding material made from a composite blend of HDPE and h\textsuperscript{Na}BN with ≥30 wt% than to use pure HDPE. This indicates that incorporating a significant fraction h\textsuperscript{Na}BN into HDPE improves the shielding effectiveness for 5-mm-thick composites.

Figure 6 shows the results of the blended geometry for effective dose per fluence (pSv cm\textsuperscript{2}) versus the global weight percentage of h\textsuperscript{10}BN (Figure 6a) and h\textsuperscript{Na}BN (Figure 6b) for composites thickness ranging from 1 mm to 100 mm. The mass density of the composite structure for the corresponding weight percentage of hBN is shown on the top of each subplot. The effective dose is obtained from running five different random seeds of the blended geometry and computing the mean (dots) and 2\sigma uncertainty (error bars). As minimal checks, we note that the effective dose decreases with increasing thickness, as expected, and that the values at 0 wt% are the same in Figures 6a and 6b (pure HDPE). In Figure 6a, for small thicknesses, between 1 mm and 5 mm, there is a point of inflection which gradually shifts to lower weight percentage of h\textsuperscript{10}BN as thickness increases. At thicknesses beyond 5 mm, the point of inflection develops into a sharp local minimum at <2 wt%. A similar behavior observed in Figure 6b, though it occurs at a slightly larger loading of h\textsuperscript{Na}BN. These results show that, for even a simple homogenous blend of materials, the optimal configuration can be sensitive to the weight fraction of each component due to their varied influence on shielding capability.
FIG. 6. Effective dose per fluence (pSv cm$^2$) as a function of the global weight percentage of h$^{10}$BN in (a) and h$^{Na}$BN in (b). The equivalent density is shown at the top of each subplot. Different thicknesses simulated in this study are color-coded according to the legend. The error bars show 2$\sigma$ uncertainty among results obtained by varying the random-number seed for the MC calculations.

2. Ideal Layered Geometry

To further investigate the role of internal structure, we consider the next simplest modification, material layering, which effectively separates the two essential processes of neutron thermalization and neutron capture, into distinct repeating regions. We first consider a complete separation, where the layers are either HDPE or hBN—a situation we refer to as the ideal layering. Figure 7 shows the effective dose per fluence (in units of pSv cm$^2$) as a function of global weight percentage of h$^{10}$BN, in (a) and (b), and h$^{Na}$BN, in (c) and (d). The effective dose is shown for two example composite thicknesses: t = 5 mm in (a) and (c) and t = 60 mm in (b) and (d). The different colors correspond to a unique number of HDPE layers, changing the spatial period of the repeating structure. As a reference, the blended hBN/HDPE results are duplicated from Figure 6 for t = 5 mm and t = 60 mm at equivalent global weight percentages.

From Figure 7, we find the ideal layered geometry provides better shielding than a homogeneous blend across nearly all weight percentages and layer configurations. For t = 5 mm, two layers of HDPE and one layer of hBN (black data) minimizes the effective dose across all weight percentages of hBN and results reconverge to the blended...
configuration as the number of layers reaches 50+ layers. However, for \( t = 60 \) mm, greater than two layers HDPE minimizes the effective dose across most of the weight percentages with reconvergence to the blended conditions only beginning for 50+ layers. This is the first indication in our results that the spatial scale and organization of the internal material structure can significantly affect the macroscopic shielding properties. For example, at a global wt% of \(~20\%\) for a thickness of \( t = 60 \) mm, the optimal structure has seven layers of HDPE versus 2 layers for \( t = 5 \) mm, as shown in Figure 7b and 7d. This result also demonstrates that the optimal shielding configuration depends on the application requirements (e.g. spacesuits need a thinner material and habitats call for a thicker material).

Table I shows the optimal ideal layered structure of layering HDPE with pure \( h^{10}\text{BN} \) at 30 wt%, 60 wt%, and 90 wt% and for thicknesses of 10, 30, 60, and 100 mm. For each corresponding thickness and weight percentage, the areal density (mass/area), unit thickness of the HDPE \((t_{\text{HDPE}})\) and \( h^{10}\text{BN} \) \((t_{\text{hBN}})\) layers, and a diagram of the internal structure are also shown in Table I. The data reveals an interesting pattern: the optimal structure for composites with a total thickness \( t \leq 10 \) mm is trilayer, two layers of HDPE interlayered with one hBN layer. But, as the thickness increases, the number of layers in the optimal configuration increases, as shown in the last three rows of Table I.

| Total Thickness (\( t \)) [mm] | wt% | Mass/Area [g/cm²] | Unit Thickness of HDPE \((t_{\text{HDPE}})\) [mm] | Unit Thickness of hBN \((t_{\text{hBN}})\) [mm] | Optimal Structure |
|-------------------------------|-----|-----------------|---------------------------------|-----------------|------------------|
| 10 | 30% | 11.55           | 4.17                            | 1.65             | Gray             |
|    | 60% | 14.31           | 2.95                            | 4.08             | White            |
|    | 90% | 18.80           | 0.97                            | 8.05             | Gray             |
| 30 | 30% | 34.66           | 8.34                            | 2.47             | Gray             |
|    | 60% | 42.94           | 5.91                            | 6.13             | White            |
|    | 90% | 56.41           | 2.91                            | 24.17            | Gray             |
| 60 | 30% | 69.32           | 7.15                            | 1.65             | Gray             |
|    | 60% | 85.88           | 7.09                            | 6.13             | White            |
|    | 90% | 112.82          | 3.88                            | 24.17            | Gray             |
| 100| 30% | 115.55          | 9.27                            | 2.06             | Gray             |
|    | 60% | 143.14          | 5.91                            | 4.54             | White            |
|    | 90% | 188.04          | 4.85                            | 26.86            | Gray             |
The optimal configurations in Table I also change with weight percentage for $t > 10$ mm. For example, at $t = 60$ mm, the optimal configuration changes from seven HDPE layers to three as the global hBN weight percentage increases from 30% to 90%. A similar pattern is observed for $t > 10$ mm. While the correlations are not perfect, we note that $t_{HDPE}$ for all optimal structures is of the same order as the thermal and epithermal neutron elastic mfp (see Figure 1b). We anticipate that future work could focus on the development of an analytical model to better understand the physics underlying this observation.

3. Manufacturable Geometry

As already mentioned, it is difficult to manufacture a pure layer of hBN with $t_{hBN} > 20$ mm, which is needed for the optimal configurations shown in Table 1. hBN is typically manufactured as a thin film as it requires high temperature and high pressure to obtain pure hBN single crystals. For this reason, the manufacturable geometry consists of layering pure HDPE with mixture of HDPE and hBN. By considering interlayers which are blended polymer-hBN, this geometry envisions constructions which use widely available feedstocks of hBN nanoplatelets blended or mixed into a variety of polymeric materials, including thermoplastics, such as HDPE. Additionally, by considering lower weight fractions ($\leq 20\%$) and interlayer thicknesses which are typically greater than 0.2-0.3 mm, these structures could be produced via multi-material fused filament fabrication, an additive manufacturing technique where thermoplastic filaments are successively deposited to build up 3D geometries. By using one blended feedstock and one pure HDPE feedstock interlayer composites of various geometries could easily be produced with layer thickness being controlled by simple programming. Alternatively, these materials could be manufactured into film materials which can be processed via melt compaction or roll-to-roll processes to create large surface area composite sheets suitable for habitat construction.

Figure 8 shows the effective dose per fluence as a function of global h$^{10}$BN weight percentage (bottom x-axis) and mass density (top x-axis) for homogenous blend of h$^{10}$BN in HDPE (black line with error bars) and the manufacturable geometries (colored lines). Figures 8 (a) and (b) show the results for $t = 5$ mm and $t = 60$ mm, respectively. The color bar in Figure 8 is split into three sections that show the local h$^{10}$BN weight percentage of 5% (shades of brown), 10% (shades of green), and 20% (shades of purple). The different shades of each color correspond to the number of pure HDPE layers interlayered with hBN/HDPE.
FIG. 8. Effective dose per fluence (pSv cm$^2$) as a function of global h$^{10}$BN weight percentage (corresponding density along the top-axis) for $t = 5$ mm in (a) and $t = 60$ mm in (b). The blended results are shown in black with error bars. The manufacturable results are split into three categories, which show the local weight percentage results for $\omega_{hBN} = 5\%$ (shades of brown), $\omega_{hBN} = 10\%$ (shades of green), and $\omega_{hBN} = 20\%$ (shades of purple). The different shades correspond to the different number of pure HDPE layers.

When comparing the manufacturable configurations to the blended geometry, we observe that the effective dose is further reduced by interlayering HDPE with h$^{10}$BN/HDPE blend at the same global weight fractions. However, the optimal number of pure HDPE layers is not the same across all composite thicknesses. For the manufacturable configuration with $t = 5$ mm, the optimal configuration is obtained with a global weight percentage of $\sim 12\%$ of h$^{10}$BN, two pure HDPE layers, and local weight fraction of 20%. However, for $t = 60$ mm, the effective dose is minimized when the internal configuration has the following parameters: global weight fraction of $\sim 10\%$ of h$^{10}$BN, five pure HDPE layers, and local weight fraction of 20% of h$^{10}$BN within the blended layer. These configurations shown in Figure 8 show that the optimal configuration occurs at $\omega_{hBN} = 20\%$ (shown in the shades of purple) for both thicknesses, which indicates that including as much h$^{10}$BN into the h$^{10}$BN/HDPE layer as possible reduces the effective dose the most. For all other thicknesses, we notice the same behavior: $\omega_{hBN} = 20\%$ is optimal within the hBN/HDPE layer. The optimal number of pure HDPE layers also changes in Figure 8b. The similar crossover in the number of layers as the thickness increases is also observed in the ideal layered configuration (Figure 7). This indicates that a similar process that occurs in both the ideal layered and manufacturable configuration.

In Figure 9, we compare the manufacturable configuration with the ideal layered to see the significance of layering pure hBN. Figure 9 is presented in a similar format to Figure 7 where the effective dose is for two thicknesses ($t = 5$
mm in (a) and (c) and \( t = 60 \) mm in (b) and (d)). The \( h^{10}\text{BN} \) results are shown in (a) and (b), and the \( h^{Na}\text{BN} \) results are shown in (c) and (d). The manufacturable results are shown in shades of purple to be consistent with Figure 8, where purple is for \( \omega_{h\text{BN}} = 20\% \) as this is the optimal local weight fraction across all thicknesses. The percent improvement is shown in each subplot to indicate the improvement from pure HDPE to the optimal manufacturable configuration and optimal ideal layered configuration.

![Figure 9](image)

**FIG. 9.** Effective dose per fluence (pSv cm\(^{-2}\)) as a function of global hBN weight fraction for \( t = 5 \) mm in (a) and (c) and \( t = 60 \) mm in (b) and (d). The top panel, (a) and (b), shows the results for \( h^{10}\text{BN} \) and the bottom panel, (c) and (d), shows the results for \( h^{Na}\text{BN} \). The blended results are shown in black. The ideal layered results are shown for varying numbers of HDPE layers, as described by the upper part of the color bar. The manufacturable configuration is shown for a local weight fraction of \( \omega_{h\text{BN}} = 20\% \) (shades of purple). The different shades of purple correspond to different numbers of pure HDPE layers.

For \( t = 5 \) mm (Figure 9a), the percent improvement from pure HDPE to the optimal manufacturable configuration and ideal layered configuration for \( h^{10}\text{BN}/\text{HDPE} \) is \( \sim 42\% \) and \( \sim 49\% \), respectively. When layering HDPE with \( h^{Na}\text{BN} \) (Figure 9c), the percent improvement from pure HDPE to the optimal manufacturable configuration and ideal layered configuration is \( \sim 29\% \) and \( \sim 46\% \), respectively. In Figure 9b and 9d, the percent improvement is approximately the same for both \( h^{10}\text{BN} \) and \( h^{Na}\text{BN} \); \( \sim 50\% \) for the optimal manufacturable configuration and \( \sim 60\% \) for the optimal ideal layered configuration, in comparison to pure HDPE. This indicates that shielding effectiveness is approximately the same between \( h^{10}\text{BN} \) and \( h^{Na}\text{BN} \) once \( t \) is large enough (\( \sim 60 \) mm). However, for thinner composites (\( \sim 5 \) mm), the choice of hBN material has a greater impact on the optimal design. Additionally, for the thinner composites, the manufacturable configuration could be improved at all global weight fractions by interlaying...
pure hBN rather than hBN/HDPE composite layers, while the blended interlayers outperform the ideal interlayers for a small range of global weight fractions in the thicker composite structures.

C. OPTIMAL CONFIGURATIONS

The optimal boron distribution within the HDPE composites is determined by comparing the optimal configurations from each configuration: blended, ideal layered, and manufacturable. For space applications, it is critical that the shielding mass is minimized to reduce cost. From a simulation perspective, it is easier to sort runs by composite thickness; however, to assist design engineers for space structures, it is convenient to also consider the optimal configurations as a function of areal density, which combines the thickness and density of the shielding composite. For this reason, we sort by areal density to determine the optimal configurations so that the lowest areal density and effective dose can be used to design shielding composites.

Figure 10 shows the effective dose along the left axis and the effective dose ratio (output effective dose divided by the input dose) along the right axis versus areal density (mass/area, units of g/cm²) for the blended (yellow), ideal layered (green), and manufacturable (purple) configurations. All the data presented in Figure 10 are shown for the composites made with h₁₀BN and HDPE. The reference effective dose for Al, HDPE, and hBN are shown in dark gray, light gray, and light blue, respectively. The optimal h₁₀BN/HDPE configurations are determined for the lowest effective dose within a given range in mass/area. The ideal layered and manufacturable configurations are separated into two regions, trilayer and multilayer. The trilayer refers to the optimal configuration consisting of two layers of HDPE and one layer of hBN, as shown by the inset in Figure 10. Multilayer consists of configurations with greater than three layers of HDPE. For example, at ~1.0 g/cm², the optimal manufacturable configuration has two layers of pure HDPE within a composite thickness of \( t = 10 \) mm for local weight fraction \( \omega_{hBN} = 20\% \) and mixture weight fraction \( \omega_{mix} = 30\% \), corresponding to a global weight fraction of 6%, \( t_{HDPE} = 3.62 \) mm, and \( t_{mix} = 2.77 \) mm. At ~10 g/cm², the optimal manufacturable configuration has nine layers of pure HDPE within \( t = 150 \) mm for \( \omega_{hBN} = 20\% \) and \( \omega_{mix} = 60\% \), corresponding to a global weight fraction of 12%, \( t_{HDPE} = 7.13 \) mm, and \( t_{mix} = 10.73 \) mm.
FIG. 10. Effective dose per fluence (pSv cm\(^2\), left-axis) and effective dose ratio (output dose divided by input dose, right-axis) as a function of mass per area (g/cm\(^2\)) for the optimal h\(^{10}\)BN/HDPE configurations. The reference data for Al, HDPE, and h\(^{10}\)BN are provided in dark gray, light gray, and light blue, respectively. The optimal results for the blended (yellow), ideal layered (green), and manufacturable (purple) are shown. Multilayer consists of configurations with >3 layers of HDPE.

From the results in Figure 10, the blended geometry aligns with the effective dose of pure h\(^{10}\)BN for low areal density (i.e., small thicknesses), deviates from h\(^{10}\)BN in the middle region, and rejoins in the large areal density (i.e., large thicknesses). The ideal layered and manufacturable configurations are the most optimal configurations that were considered in this study for all areal densities. For configurations below \(~0.5\) g/cm\(^2\), the ideal layered is better than the manufacturable configuration. However, above \(~0.5\) g/cm\(^2\), the manufacturable configuration approaches ideal layered results. As the areal density increases (mass/area \(>3\) g/cm\(^2\)), the effective dose of the manufacturable configuration is lower than that of the ideal layered configuration, showing that the manufacturable configuration exceeds the performance of the ideal layered configuration for high areal densities. The internal structure of the ideal layered and manufacturable consistently changes from a trilayer to multilayer configuration around an areal density of \(~4.0\) g/cm\(^2\); however, further work is needed to better understand the physics driving this observation.

V. CONCLUSION

In this study, we optimize the boron distribution within HDPE composites using the lunar neutron distribution as the radiation source. Three different configurations are explored: blended, ideal layered, and manufacturable. The blended geometry consists of a homogenously blended hBN and HDPE. The ideal layered and manufacturable
configurations consist of layers of pure HDPE with interlayers of either pure hBN (ideal layered) or a composite blend of hBN/HDPE (manufacturable). The effective dose is employed as a figure of merit to evaluate the different shielding configurations. The ideal layered and manufacturable configurations reduce the effective dose by a factor of 4 – 30x in comparison to Al and by a factor of 1.5 – 2x in comparison to HDPE for similar areal density (Figure 10). This is a significant improvement in shielding effectiveness that could dramatically reduce the radiation exposure that astronauts receive for a long-duration mission to the Moon. In addition, the constraints placed on the manufacturable configuration ensure that the explored design space would be compatible with a multi-material additive manufacturing method via fused filament fabrication, a space proven additive manufacturing technology, as well as conventional large area methods such as roll-to-roll processing or melt laminated sheets for thermoplastic molding. Moreover, the HDPE and hBN/HDPE blends used in the manufacturing configuration are inherently flexible, allowing for easy incorporation into the linings of the spacesuits to reduce the astronaut exposure during extravehicular activities.

From the MC simulations, we discovered a dependence on internal structure when optimizing the distribution of the thermalization and capture processes. For the blended configurations with composite thickness above ~10 mm, the optimal configuration consists of incorporating a weight fraction of <2% into the hBN/HDPE composites. We observe that there are no incremental gains from increasing the weight fractions beyond 2%, which indicates that incorporating a small weight fraction of hBN can be highly beneficial to reducing the effective dose, informing the design for thick shields (>10 mm). From the optimal ideal layered and manufacturable configurations, we observe an interesting feature: the optimal configurations changes from a trilayer structure to a multilayer structure. This interesting result indicates that spatially separating the neutron thermalization and capture process reduces the effective dose. Future work involves: understanding the underlying physics driving this change in the internal structure, fabricating and irradiating the optimal manufacturable configurations to confirm shielding effectiveness in real-world composites.

We note that there are additional methods to improve the shielding effectiveness for the materials explored in this study. The particles that dominate the effective dose are mostly gammas for the blended configuration (Figure 5); the same behavior is also observed for the layered and manufacturable configuration. This indicates that the effective dose could be further reduced with the addition of a high-density material, such as bismuth or barium titanate, at the backend of the composite shielding materials to reduce the gammas that penetrate the shielding material and contribute to the effective dose. However, the addition of a high-Z material layer to attenuate the photons is outside the scope of this
work and will affect the inherent flexibility of the hBN/HDPE composites. We also note that our study targets lunar missions specifically and relies on the lunar neutron energy distribution. For other scenarios, such as a mission to Mars, another set of MC simulations could be undertaken, with GCR and SEP radiation interacting with a spacecraft or with the Martian surface. Such simulations would follow a path analogous to those described in this study but would require the appropriate incident radiation distributions.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

APPENDIX A: Details of Geant4

Geant4 (GEometry ANd Tracking) is used to model the hBN/HDPE shielding composites as Geant4 provides us with additional flexibility in the modeling software that is more difficult to achieve in other transport codes. There are several ways to record the relevant information in Geant4. The simulation toolkit allows the user to define a region as a “sensitive detector” (SD) and record information related to a “hit”. A hit is defined as a physical interaction on a single-particle basis, and SD is assigned to the logical volume that defines the geometry. For each hit, the kinetic energy, charge, and position vector can be recorded, providing the user with detailed information of the particle’s trajectory through a material. The sensitive detector method allows the user to record all the relevant information, then perform a post-processing on the simulation results. Alternatively, the user can define specific variables to tally within the code (e.g., deposited energy, surface flux, number of particles), which is useful when there is a specific variable of interest.

For the simulations presented in this study, we record the following information associated with each hit: (1) particle type (e.g. neutron, gamma, alpha, etc.), (2) process type (e.g. inelastic collision, elastic collision, ionization,
transport, etc.), (3) particle kinetic energy, and (4) particle position in Cartesian coordinates. From this information, the exact interaction and energy deposited into the material can be determined and tracked through the particle cascade. However, to get valid results, it is critical to use the appropriate physics models. For these simulations, we use the following physics constructors: G4HadronPhysicsQGSP_BIC_HP, NeutronHPPhysics, G4EmStandardPhysics_option4, G4EmExtraPhysics, G4IonPhysics, G4DecayPhysics, G4RadioactiveDecayPhysics, and G4StoppingPhysics.

G4HadronPhysicsQGSP_BIC_HP is a physics reference list that uses binary cascade (BIC) to model inelastic collisions. The “QGSP” stands for Quark-Gluon String Precompound model, and “HP” stands for high-precision. NeutronHPPhysics constructor which computes the phonon density of states for both the coherent and incoherent part; this physics constructor has been verified and found to have reasonable agreement with other MC simulations codes along with experimental data. G4HadronPhysicsQGSP_BIC_HP and NeutronHPPhysics are both needed to accurately simulate thermal neutrons. The other physics constructors are used to account for the following physics: electromagnetic effects (G4EmStandardPhysics_option4, G4EmExtraPhysics), ion interactions (G4IonPhysics), decay channels according to the branching ratios (G4DecayPhysics), radioactive decay of isotopes (G4RadioactiveDecayPhysics), and nuclear capture at rest for negatively charged particles (G4StoppingPhysics). To ensure that we loaded the appropriate physics constructors, we compare the Geant4 results to another MC simulation code, Monte Carlo N-Particle code (MCNP), a well-established neutron transport code.

APPENDIX B: Validation of Geant4 using MCNP

MCNP is a general-purpose radiation tracking code developed by Los Alamos National Laboratory (LANL) for simulating neutrons, photons, electrons, and coupled particle transport. It has a wide range of applications, including nuclear reactors, radiation protection, medical physics, etc. In the past 40 years, it has been extensively evaluated and benchmarked, providing the standard simulation tool for nuclear engineers. This makes MCNP, specifically MCNP6, an ideal software to validate our Geant4 simulation results.

To compare the two MC codes, a simulation is run for a simple spherical geometry to remove any ambiguity due to boundary conditions. A solid sphere, placed in a vacuum environment, with a radius of 100 mm is filled with either HDPE or h^14BN. A monoenergetic neutron source is placed at the center of the sphere and emits neutrons
isotropically. For HDPE, we used a density of 0.96876 g/cm$^3$ and an energy of 2.5 MeV so that the neutron thermalization process is observed within the sphere. For h$^{11}$BN, a density of 2.1 g/cm$^3$ and an energy of 100 keV is used so that the neutron capture events are observed. For the MCNP simulation, the ENDF/B-VIII.0 cross section database and thermal scattering card are used. The surface current is tallied at each spherical shell, which are placed at 5 mm increments starting from the center of the sphere and propagating to the surface.

1. Calculation of Surface Current Tally

We use the surface current tally, denoted as F1 in MCNP, to compare the Geant4 and MCNP simulation results. This tally counts each neutron that crosses a specified surface and weights that neutron by the angle at which it exits the surface. The surface current tally is mathematically represented as

$$F1 = \int_A dA \int_E dE \int_\Omega d\Omega |n \cdot J(r_s, E, \Omega)|.$$  \hspace{1cm} (A1)

where $A$ is the specific surface area, $E$ is the neutron energy, and $J$ is the current vector. By computing the absolute value of $n \cdot J$, MCNP does not distinguish between forward and backward scattering. The same calculation is performed in Geant4 during the post-processing of the simulation results. The entire sphere is set as the SD and the direction is weighted by $|n \cdot J|$, replicating the process shown in Equation A1. For simplicity, the F1 tally is calculated for neutrons only in both Geant4 and MCNP.

2. Comparison Results

Figure A1a (top panel) shows the calculated neutron surface current, F1, at a shell radius of 30 mm, from MCNP6 (red) and Geant4 (black) for an isotropic source at 2.5 MeV located at the center of a HDPE sphere with a radius of 100 mm. Here, MCNP is run for $10^8$ neutrons, and Geant4 is run for 250,000 neutrons. We use a smaller number of neutrons for Geant4 as the computational time is higher when recording each individual interaction within the sphere. For direction comparison, the surface current is normalized by the number of incident neutrons, $n_{\text{incident}}^0$.

The difference between MCNP and Geant4 surface currents, at a shell radius of 30 mm, is shown in Figure A1a (bottom panel), where we observe a small discrepancy between the two MC simulation codes. In Figure A1b, the difference between MCNP and Geant4 is shown for each radial shell taken at 5 mm radius increments. The data are plotted with a diverging color bar, where white indicates that the two MC codes give the same results, red indicates
that MCNP has a larger surface current than Geant4, and blue indicates that Geant4 has a larger surface current than MCNP. From the stacked plot, we observe that MCNP and Geant4 results are in reasonable agreement for the neutron surface current results for all radial depths within the sphere (within 1% error between the two codes). After performing the same calculation for a BN sphere and 100 keV isotropic source, we also find that the MCNP and Geant4 results are in reasonable agreement (within 1% error). In the following section, we present the interactions of lunar neutrons with BN.

FIG. A1. (a) Top panel: MCNP (red) and Geant4 (black) neutron surface current comparison at a shell radius of 30 mm from an isotropic source at 2.5 MeV located at the center of a HDPE sphere of radius 100 mm. Bottom panel: The difference between MCNP and Geant4 in the top panel. (b) Stacked plot of the difference between MCNP and Geant4 as a function of energy. The difference is plotted on a diverging color bar, where white indicates that the MCNP and Geant4 surface current values are equal. The surface current is normalized to the total number of incident neutrons.
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