Cement-polymer composites containing PANI/B_4C: Neutron shielding performance by Monte Carlo simulation

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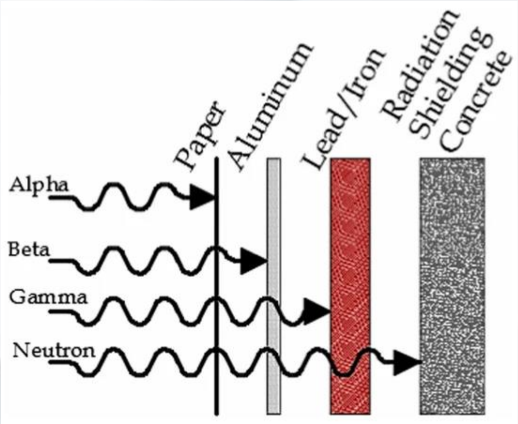
1. Purpose of the Study

- **Investigating the use of cement composites containing Polyaniline (PANI) and Boron carbide (B_4C) to develop a new material for neutron shielding:**

Neutron radiation requires special protection provided by shielding materials due to its high penetration ability.

Cementitious materials are common neutron shielding materials due to their cost-effective and reliable shielding performance.

Enhancing the radiation shielding capabilities of cementitious materials is essential for ensuring the safety of neutron radiation facilities.



Wang, K.; Ma, L.; Yang, C.; Bian, Z.; Zhang, D.; Cui, S.; Wang, M.; Chen, Z.; Li, X. Recent Progress in Gd-Containing Materials for Neutron Shielding Applications: A Review. Materials 2023, 16, 4305. https://doi.org/10.3390/ma16124305

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2. Earlier Work

Radiation Physics and Chemistry 219 (2024) 111675

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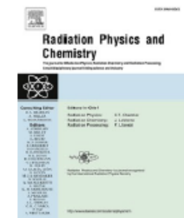
journal homepage: www.elsevier.com/locate/radphyschem



Neutron and gamma-ray shielding effectiveness of novel polyaniline composites

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- Novel thermal neutron shielding polyaniline composite was prepared by boric acid.
- Experiments, theoretical calculations, and Monte Carlo simulations were done.
- A detailed uncertainty evaluation of results was performed.

➢ **Boron carbide (B_4C):**

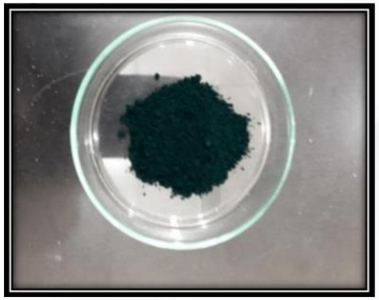
- Highly efficient neutron shielding material due to its high ^{10}B content.
- Its use is limited in cementitious materials because of the formation of boric acid, which reduces durability.

https://www.samaterials.com/spherical-boron-carbide-powder-b4c.html

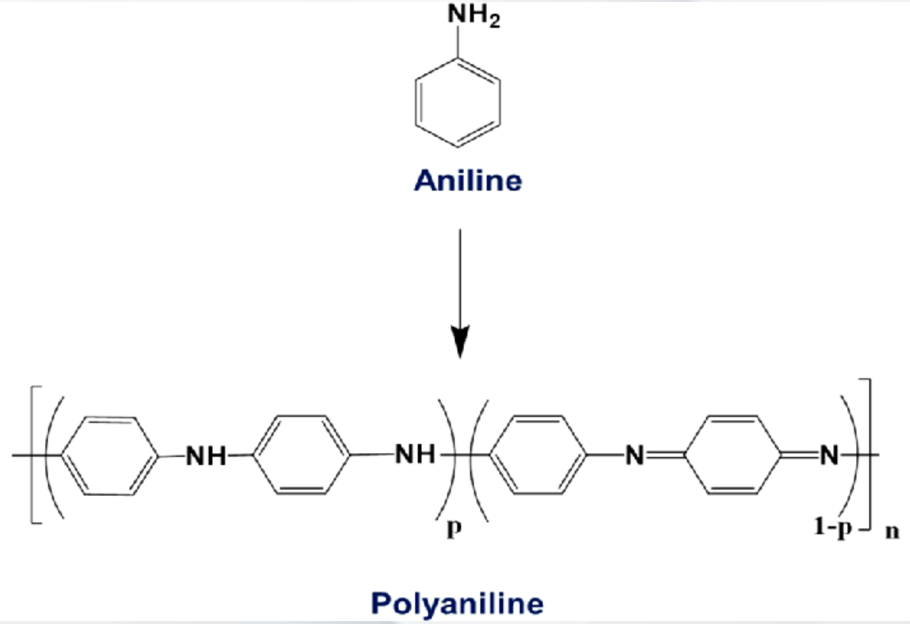
To offer an alternative solution to this problem, polymers are widely used because of their low cost, versatility, precise controllable synthesis, and availability, making them an excellent option for radiation shielding.

➢ Polyaniline (PANI):

- PANI ($C_6H_5NH_2$) is made up of a chemically flexible amino group in the polymeric chain that is bonded to any side of the phenylene ring.
- Stable in the environment
- Easy to synthesize
- Stable electrical conductivity
- Low-cost
- High-temperature resistance



Essa, Abbas & Hasan, Salma & Jerjack, Najlaa & Hassan, Salma. (2021). Optical and Structural Properties of Prepared Polyaniline - Graphene (PANI/GN) Nanocomposite.



Ahmad, S., Hammad, R. & Rubab, S. Gamma Radiation-Induced Synthesis of Polyaniline-Based Nanoparticles/Nanocomposites. J. Electron. Mater. 51, 5550–5567 (2022). https://doi.org/10.1007/s11664-022-09823-0

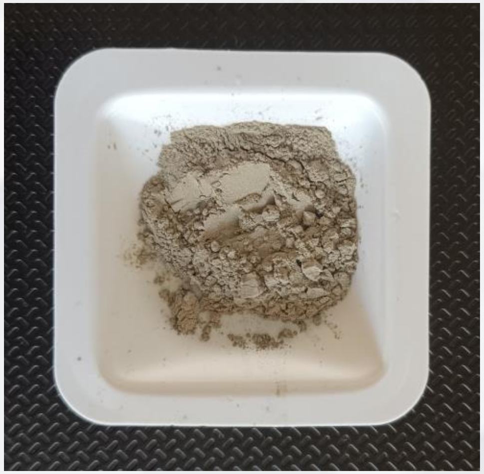
➢ Cement:

Type: CEM I 42,5 R Portland Cement

Usage areas:

- In the production of all kinds of reinforced concrete structures such as residential buildings, bridges, foundations, viaducts, concrete road pavements, precast structural elements where early strength is important

- Ideal for use in the production of shotcrete, dry mix mortars, construction chemicals.



➢ Chemical Composition of Cement:

Symbol	Concentration
CaO	70.14
Na_2O	10.47
Al_2O_3	6.16
Fe_2O_3	3.86
SiO^2	3.43
MgO	3.43
SO_3	1.38
K_2O	0.67

➢ Composition of cement composite materials

		wt.%/cement			
Sample code	Sample Content	Cement	DI water	PANI	B_4C
S1	OPC (ordinary portland cement)	100	30		
S2	OPC + 4 wt.% PANI	100	30	4	
S3	OPC + 4 wt.% B_4C	100	30		4
S4	OPC + 4 wt.% PANI/B_4C	100	30	2	2

➢ Neutron Shielding

The Beer-Lambert law was used to compute the macroscopic cross-section of the composites by Geant4 simulation.

$$I = I_0 \, e^{-(\Sigma . x)}$$

where I_0 and I are incident and transmitted neutron flux ($cm^{-2} \cdot s^{-1}$) respectively, Σ is macroscopic cross-section (cm^{-1}), and x is material thickness (cm).

➢ Neutron Shielding

The theoretical macroscopic cross-section was calculated from microscopic cross-section (σ, cm^2) and the atomic number density (N, atoms·cm^{-3}) as follows:

$$\Sigma = \sigma N$$

If the material is a compound instead of a simple element, the total macroscopic cross-section is the sum of the macroscopic cross-sections of the individual elements

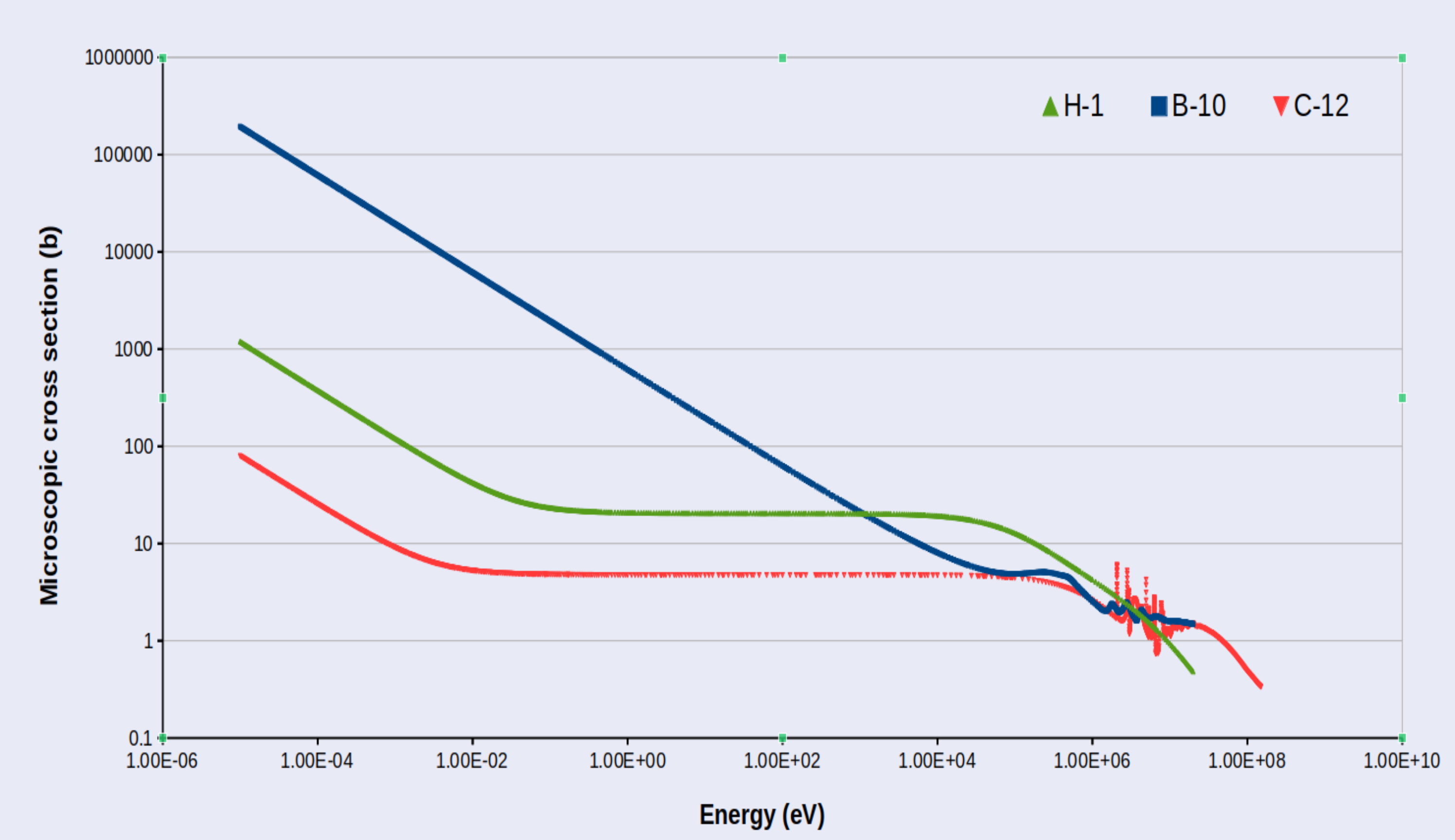
$$\Sigma = \sum_i w_i \frac{\rho}{A_i u} \sigma_i = w_i \Sigma_i$$

The material thicknesses required to reduce radiation intensity to 50% of their initial intensity is known as the half-value layer (HVL, cm). For neutrons, they were calculated by:

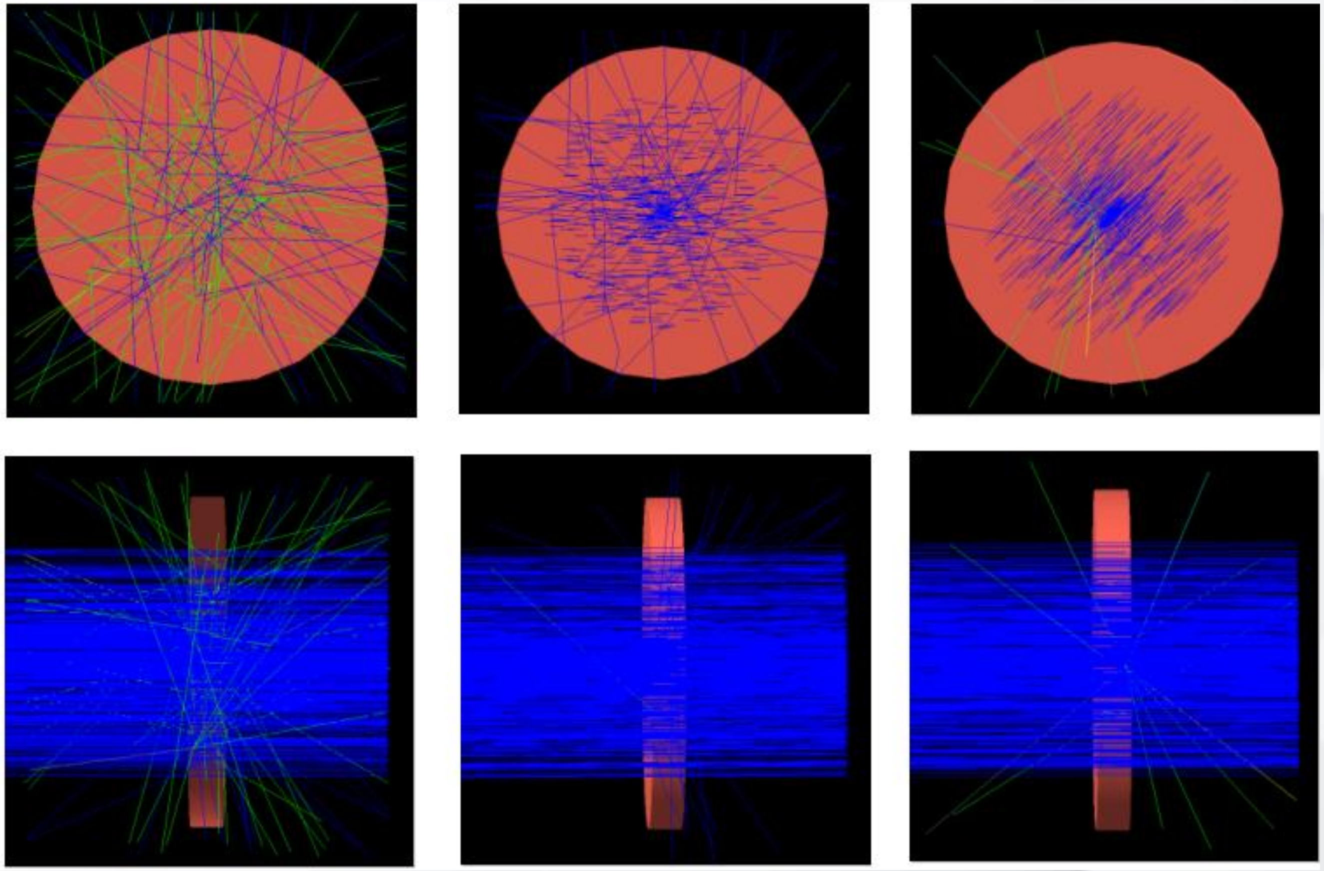
$$HVL = \ln(2)/\Sigma$$

3. Materials and methods

➢ Neutron Shielding



➢ Monte Carlo Simulations



a) **b)** **c)**

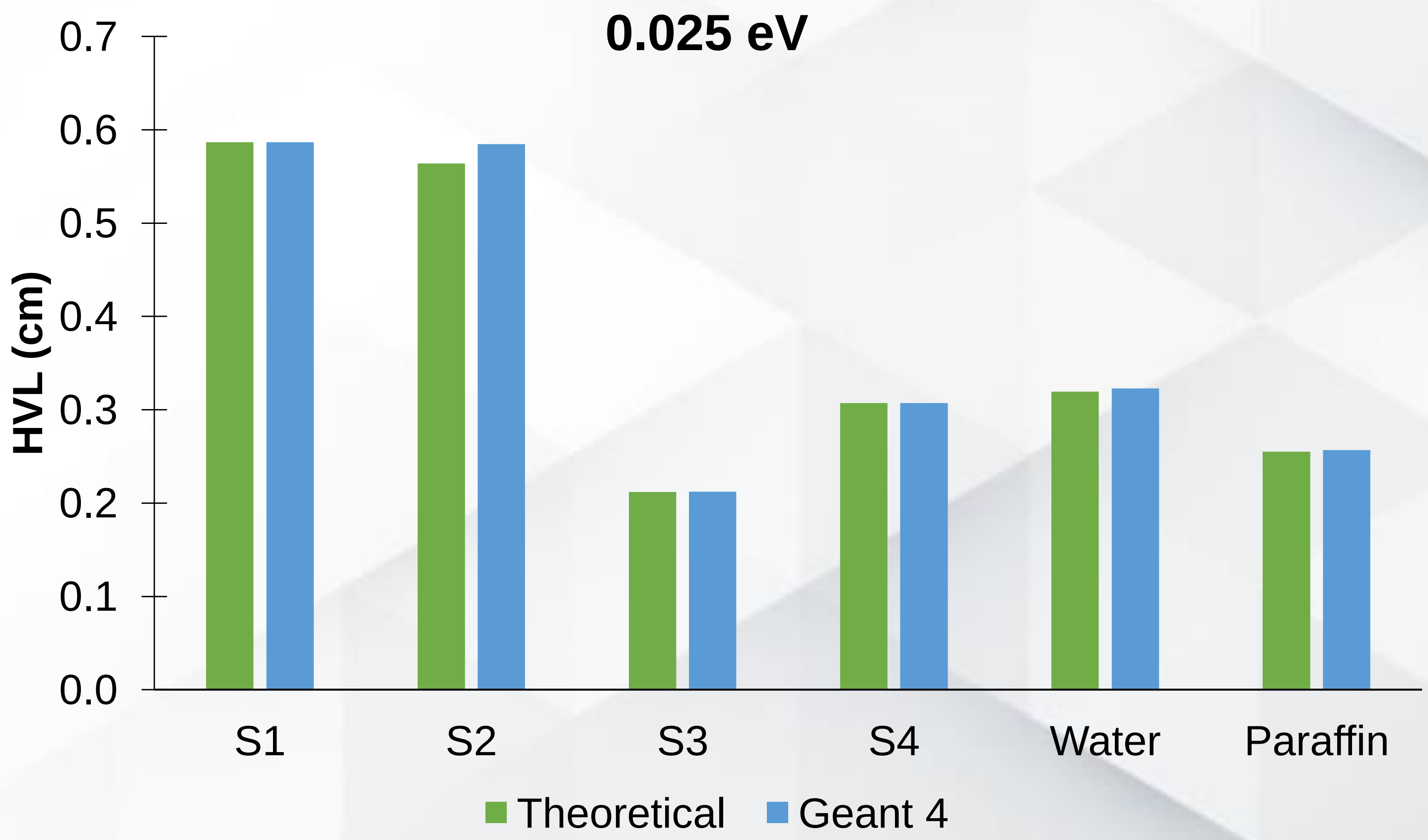
Interaction of neutrons with S4 in Geant4 **a)** 0.025 eV **b)** 1 keV **c)** 10 MeV

4. Results and discussion

➤ **Macroscopic cross-sections (cm^{-1}) for cement-polymer composites :**

	0.025 eV		1 keV		10 MeV	
	Σ_{theo}	Σ_{Geant4}	Σ_{theo}	Σ_{Geant4}	Σ_{theo}	Σ_{Geant4}
S1	**1.18**	**1.18**	0.84	0.83	0.12	0.12
S2	1.23	1.19	**0.87**	**0.86**	0.12	0.12
S3	**3.27**	**3.27**	0.84	0.83	0.12	0.12
S4	2.26	2.26	**0.85**	**0.86**	0.12	0.12
Water	2.17	2.15	1.49	1.49	0.11	0.11
Paraffin	2.72	2.70	1.87	1.88	0.12	0.13

➢ **Half Value Layers (cm) for cement-polymer composites:**



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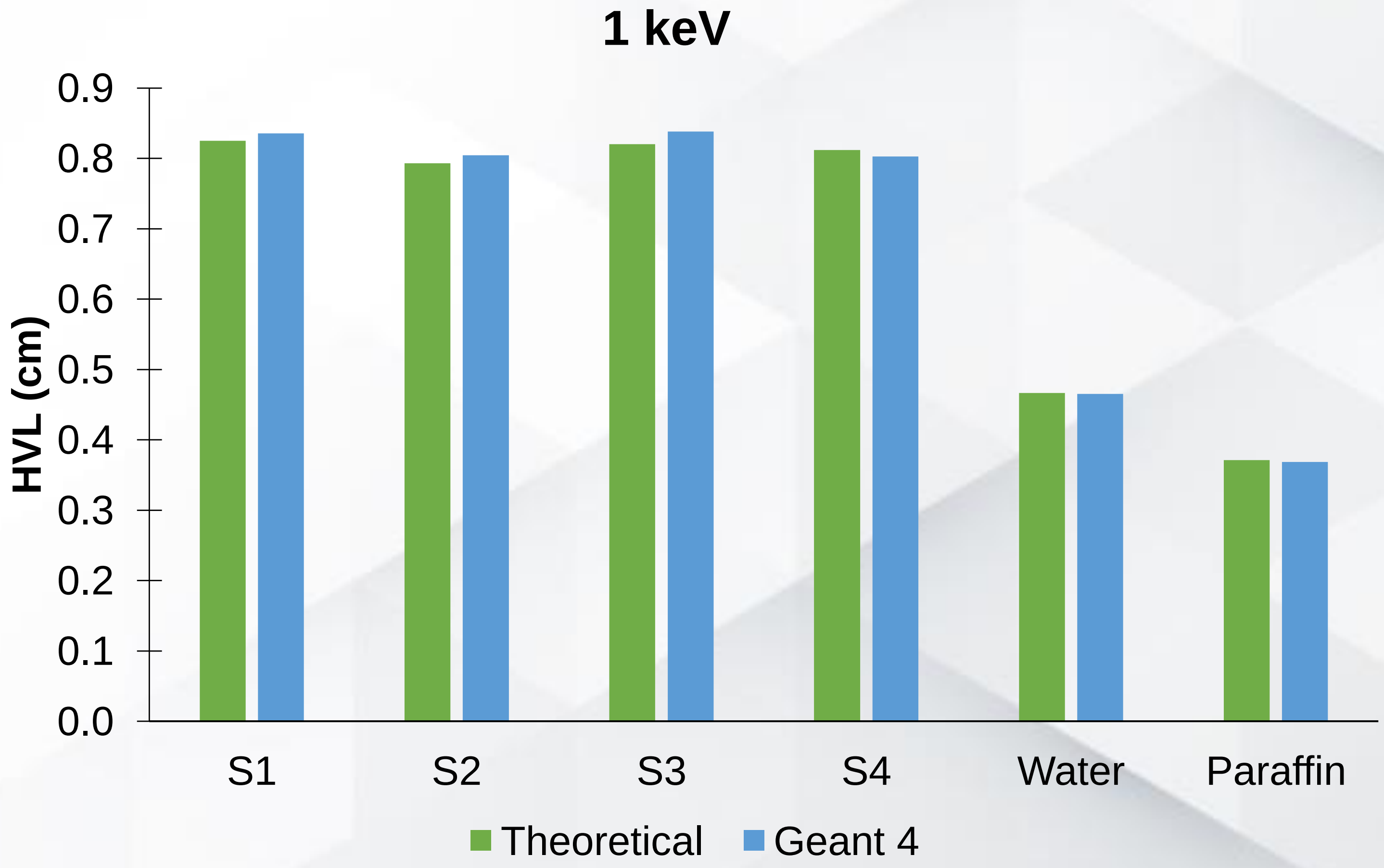

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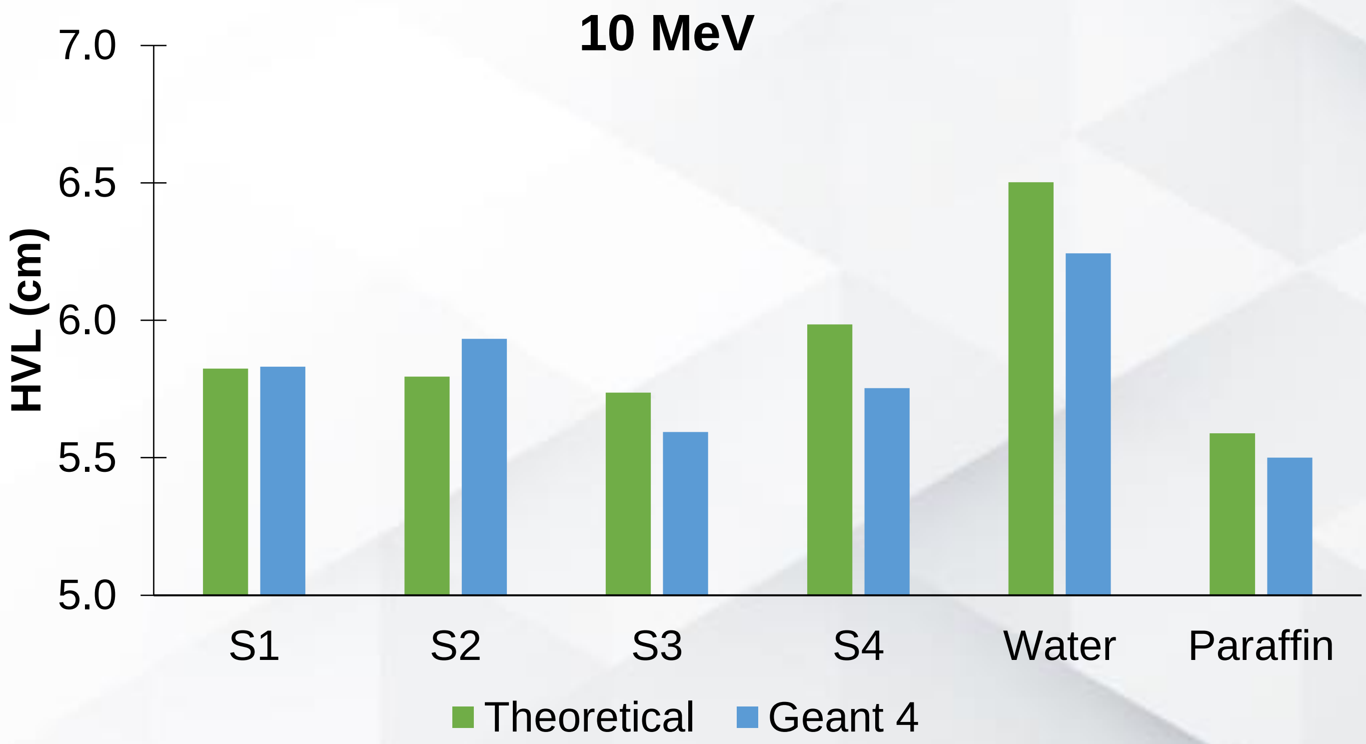

5. Conclusion

- This study investigated the shielding properties of cement-based composite materials for thermal, epithermal, and fast neutrons.
- The theoretical calculations and Monte Carlo simulations were conducted.
- The thermal neutron shielding performance of the composite containing 4 wt.% cement B4C was better than that of all composites, water, and paraffin.
- The thermal neutron shielding of the composite containing 2 wt.%/cement B4C and 2 wt.%/cement PANI was better than that of water.
- Due to PANI's hydrogen content, samples containing PANI had slightly better neutron shielding performance than other samples at 1 keV.
- The samples' shielding performance against fast neutrons is superior to that of water. Paraffin has a slightly better shielding performance than the samples.
- Experimental studies are ongoing.

THANK YOU!

Acknowledgments

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