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Monte Carlo Simulation Study on the Optimal Neutron Energy and Boron Concentration for SARS-COV-2 Inactivation through BNCT

Eulogio S. Auxtero, Jr.[1*], Jessa Mae T. Lazarte[2], Orneth C. Payac[3]

[1,2,3]*Department of Physics, Caraga State University, Ampayon, Butuan City, Philippines.*
E-mail: esauxtero@carsu.edu.ph

Abstracts: Researchers have been exploring various radiation therapies to treat COVID-19 patients ranging from mild to severe. One technique that has shown promise is Boron Neutron Capture Therapy (BNCT). This therapy involves administering of 10B isotope to the targeted area, which is then exposed to chargeless neutrons. These neutrons can be absorbed by areas with high concentrations of 10B. When the neutrons react with the 10B (10B + n→7Li + 4He reaction), it results in the transfer of highly ionizing energy, causing confined lethality and destroying the targeted area. In this study, we used the Particle and Heavy Ion Transport Code System simulation to evaluate whether Boron Neutron Capture Therapy could be effective as an anti-viral therapy. The study involves creating a model of the SAR-COV-2 target phantom's geometry and defining its chemical composition to collect data. It was found out that when tested at different neutron energies and concentrations (30 ppm, 50 ppm, and 100 ppm), a sufficient amount of dose to cause biological damage to the Sars-CoV-2 enveloped protein could be achieved with 30 ppm boron concentration and a neutron energy of 1.0x10-10 MeV.

Keywords: BNCT, COVID-19, 10B + n→7Li + 4He reaction, Monte Carlo simulation, neutron energy, boron concentration, PHITS.

1. INTRODUCTION

The use of ionizing radiation is nothing new and has been studied for decades as a method to kill viruses. It has been used for many years to kill harmful microorganisms on medical equipment and food products [1]. In the light of COVID-19 outbreak, many researchers are exploring ways to optimize the use of radiation therapy, one example of this is Low Dose Radiation Therapy (LDRT). This radiation therapy shows promises on radiation regimen for treating pathological diseases like COVID-19 pneumonia by modulating the inflammatory response of cytokine, however, despite its effectiveness in clinical trials, the understanding of this process is still under investigation, there is not enough data that has been establish about the optimal dose fraction and the mechanism through which LDRT (which uses X-ray photons) modulates the various phases of the anti-inflammatory response [2], [3]. In this study, we are investigating the use of BNCT with the help of Particle and Heavy Ions Transport Code System (PHITS) Monte Carlo simulation to evaluate the inactivation of Sarscov-2 virus.

BNCT is a unique type of radiation therapy that differs from other in terms of its nature and deployment. To achieve the desired outcome of this complex therapy, it is critical to accurately localize the delivery of boron enriched agents and ensure their variable uptake in the target areas [4].

After the preferential uptake of the boron enriched agents in the target areas, the next stage of treatment involves providing an adequate flux of neutron energy. Chargeless neutrons having low atomic interactions also have lower chance to interact with the elements present in other phantom (e.g,. human tissue) thus, can easily penetrate and only react with high boron concentrated area. Boron has a higher neutron capture cross section than healthy cells, making BNCT an ideal radiotherapeutic approach as it restricts the lethality solely to the target cells, even if they are spread throughout the body [4].

2. METHODOLOGY

To prepare for BNCT simulation, an input file was developed through PHITS for modelling a space that fits the target phantom and neutron source, this will act like a treatment room. It incorporates data showing the geometry, the source definition, material's biochemical composition, and the tallies essential for each dose calculation. The model is consisting of mono-energetic axial source projecting incident neutrons that is placed centimeters away from the phantom.

Due to the intricate nature of the structure of SARS-CoV-2 and the variability of the surrounding functional proteins, this study opted for a simpler geometry since the main aim of this study was to only determine the level of radiation required to disrupt the E-protein's ability to protect the virus. A simplified molecular formula was used for this protein, obtained from the National Center for Biotechnology Information, in order to achieve this goal. The data regarding the chemical composition is given in Table 1.

Table 1. Chemical Composition of SARS-CoV-2 envelope protein.

E-Protein	C5.2297H10.203O1.2523N2.3514S0.0360		
	C	H	N
Atomic Weight	12.0107	1.0078	14.0067
Mass Fraction per Gram	0.494	0.081	0.157

3. RESULTS AND DISCUSSIONS

During the interaction of neutron with matter containing boron, part of neutrons may be slowed or absorbed resulting some nucleus to be left in an excited state (radioactive). The latter then deexcites with the emission of one or more particles (e.g alpha, proton, 7-Li, gamma) [5]. These reactions create a mixed radiation field causing an indirect ionization that have a higher chance to break the molecular chain on the envelope protein and will eventually inactivate SARS-CoV-2. Table 2 shows the cumulative dose deposited in the target phantom for at least four distinct neutron energies with varying boron concentration. In a related work, Guabao Feng et al., 2020 concluded that when irradiating, the envelope protein suffers the most biological damage which accumulates 2.8 x 106 eV [6]. Also, it is noteworthy to mention that their research involves direct electron irradiation, which runs counter to the desire of this study for selective treatment. In comparison with the corresponding data that they've obtained, it is evident that in Table 3.3 the closest value to achieve those results is when the neutron source is fixed at 1 MeV paired with 30 ppm boron concentration.

Table 2. Measured Dose Irradiated at Varying Neutron Energy and Concentrations.

Incident Neutron Energy	Boron Concentration		
	30 ppm	50 ppm	100 ppm
	Total Absorbed Dose		
1x10-10 MeV	3.1369x10-12 MeV	3.7479x10-12 MeV	3.4674x10-12 MeV
1x10-8 MeV	3.6303x10-12 MeV	3.8019x10-12 MeV	3.9811x10-12 MeV
1x10-6 MeV	3.7928x10-12 MeV	4.0083x10-12 MeV	4.1218x10-12 MeV
1x10-4 MeV	3.8124x10-12 MeV	4.7468x10-12 MeV	5.2481x10-12 MeV
1x10-4 MeV	3.8124x10-12 MeV	4.7468x10-12 MeV	5.2481x10-12 MeV

The neutron flux and its spatial distribution were presented in Figure 1. It was calculated and graphed using coupled software (Angel code). In this study, there are 1000 particles tested and 50 batches were examined.

Assuming homogeneity of boron concentration in the target phantom, a gradual shift can be observed in Figure 1a which is probably due to energy attenuation when the neutrons bump into a number of nuclei present in the target phantom. Though the energy loss from the outgoing beam is not clearly visible in Figure 1b, the scattering of nearby particles serves as sufficient proof that 10B + n7Li + 4He occurs simultaneously. The presence of the scattered nearby particles can be attributed to the distance travelled from recoiled particles that are released from such reactions, increasing the possibility of escaping from the simulated geometry [7].

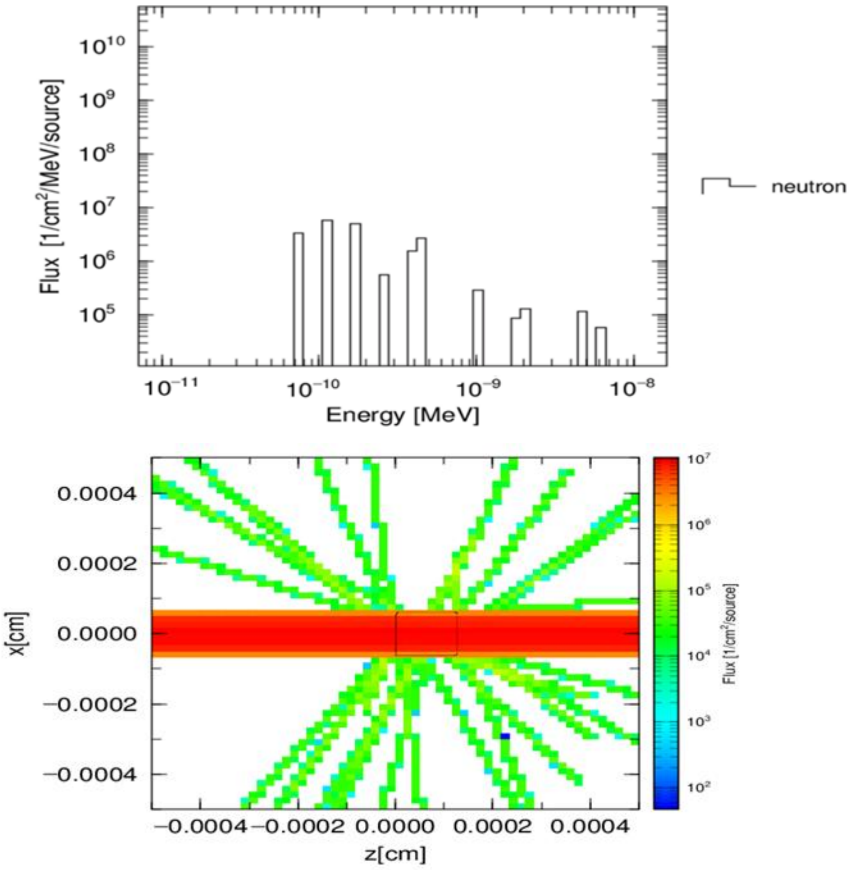

Figure 1. (a) Neutron Fluence track and (b) Spatial Distribution of Energies.

4. CONCLUSION

Radiation damage simulation in SARS-CoV-2 is quite fascinating for a variety of reasons. This study looks at how boron neutron capture therapy could be used to inactivate Sars-CoV-2 virus.

Using gamma rays or LDRT to inactivate a virus unavoidably destroys adjacent tissues or causes a cytokine storm, whereas an inactivated virus with restricted damage is deemed to be the most effective [8], [2]. This experimental data obtained in this study shows that when indirect ionizing radiation is applied particularly neutrons reacts with boron (10B + n→7Li + 4He), the overall deposited dose can be sufficient, ensuring virus inactivation. These are generally physical dose in the BNCT treatment planning, while it may not be an adequate index to justify its overall therapeutic effectiveness, the simulation study sure demonstrates that the energy needed to inactivate the SARS-COV-2 particle can indeed be attained.

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