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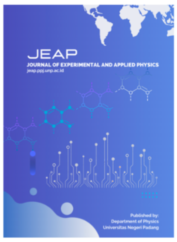

Modification of Thermal Column in Kartini Reactor Using Briquettes and Powder of Coconut Shell for BNCT: Monte Carlo Simulation

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Abstract: This study was analyzed the distribution of thermal neutron flux and gamma ray dose rate in the Kartini rector thermal column modified by replacing graphite material with briquettes and coconut shell powder as a moderator using Monte Carlo simulation, PHITS. The particle source uses neutrons with energies of 3 MeV, 4 MeV, and 5 MeV placed in front of the thermal column. The results showed that of the four modifications, only design 2 of the thermal column with briquettes at 3 MeV energy met the IAEA standard for Boron Neutron Capture Therapy (BNCT). The thermal column material with coconut shell powder does not meet the IAEA standard. This shows that coconut shell briquettes are more effective in moderating fast neutrons than coconut shell powder because the briquettes have the characteristic of greater density, which is almost the same value as the density of graphite.

Keywords: BNCT, briquette, Coconut shell, PHITS, thermal column.

1. Introduction

Cancer is known as the most recognized disease due to its expensive treatment and healing process. Medical treatments for cancer are usually chemotherapy, surgery and radiotherapy. In its development, some clinical treatments for brain tumors are considered not optimal. These treatment techniques have risky side effects [1]. Therefore, the need for new treatments that are more effective is needed, one of which is Boron Neutron Capture Therapy (BNCT) [2]. Radiation therapy using charged particles such as BNCT can improve the dose distribution to targets with higher relative biological effectiveness (RBE) than conventional photon therapy and minimize the dose to surrounding healthy tissues [3-5].

BNCT therapy is a type of radiotherapy that uses a nuclear reaction that occurs between thermal neutrons and ^{10}B atoms, which have a large thermal neutron absorption cross-section.

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BNCT can selectively kill tumor cells and ensure minimal damage to normal body tissues by accumulating ^{10}B atoms inside tumor cells prior to neutron radiation [6-7]. BNCT utilizes boron carrier compounds capable of being concentrated, namely Sodium Boronocaptate (BSH) or Boronophenylalanine (BPA), which are injected into tumor patients. Both compounds accumulate at different locations in the body. BSH tends to accumulate in the extracellular fluid, and BPA tends to accumulate in the cancer cells [8-9].

The Kartini reactor is a research reactor type TRIGA MARK II (Training, Research, and Isotope Production by General Atomic) which is used for neutron activation or irradiation services, education and training, and research in the field of nuclear technology. Kartini reactor is operated with a nominal power of 100 kW based on the license issued by BAPETEN (Badan Pengawas Tenaga Nuklir) in 2000 [10]. Supporting facilities at the Kartini reactor are thermal columns to produce neutron flux in accordance with IAEA (International Atomic Energy Agency) standards for BNCT, namely 1.0×10^9 n/cm^{2}s [11]. However, it is necessary to modify the thermal column to reduce the neutron flux because the neutron flux produced by the Kartini reactor terrace is high enough to exceed the IAEA standard.

BNCT research can be conducted using Monte Carlo simulation in recent years for brain cancer cases. Monte Carlo is a method used to simulate a stochastic process that can be used to duplicate statistical processes and various complex problems that cannot be done with deterministic methods [12-13]. PHITS (Particle and Heavy Ion Transport Code System) performs calculations with the Monte Carlo method. PHITS is a Monte Carlo-based code released by JAEA (Japan Atomic Energy Agency) that can simulate charged and neutral particles. This program is equipped with calculations that can visualize 2-dimensional particle trajectories and calculations of various other physical parameters [14]. BNCT study using Monte Carlo simulation has been conducted by several researchers [4, 15-16]. The NCTPLAN code, a Monte Carlo-based treatment planning code developed by Zamenhof et al. (1996) computationally produced dose distributions that matched the experimental results [15]. Another study used Monte Carlo simulations to assess the potential of the Tehran Research Reactor (TRR) thermal column as an epithermal neutron beam generator for BNCT. The best moderator to produce epithermal neutrons in this TRR is 20 cm aluminum [16].

This study aims to analyze the epithermal neutron flux distribution and gamma-ray dose rate in accordance with the parameters recommended by the IAEA for BNCT carried out by modifying the thermal column by replacing graphite material with coconut shell briquettes and coconut shell powder using Monte Carlo simulation.

2. Method

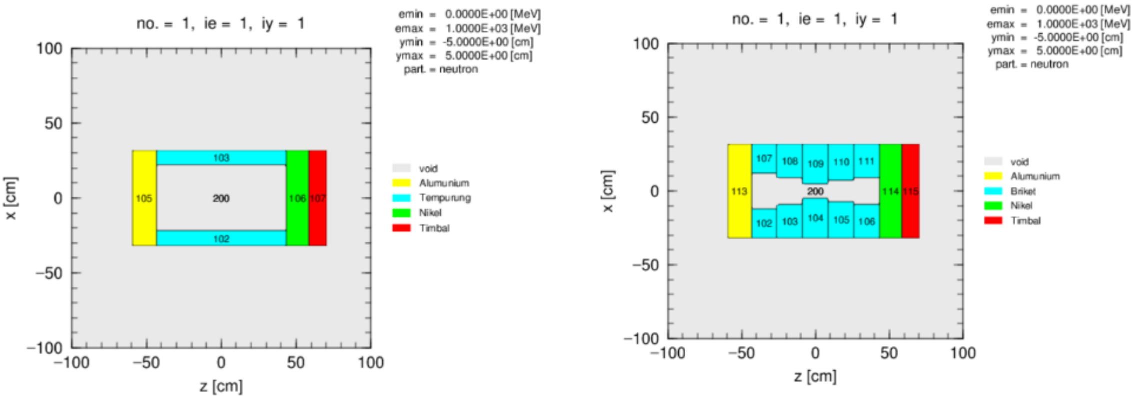
In this study, a thermal column was designed to produce epithermal neutron flux in accordance with IAEA standards to be applied for BNCT. Modifications were made to optimize the thermal column using PHITS 3.341 version. PHITS can simulate particle transport in complex media by utilizing random numbers [14]. The design of the thermal column modification involves adjusting the components of the neutron moderator, thermal neutron filter, gamma shield, and coconut shell powder or coconut shell briquette material block which is considered capable of producing the neutron flux dose recommended by the IAEA for BNCT applications. Table 1 shows the mass fraction of coconut shell briquettes and powder used in the simulation.

Source of PHITS is an input section that defines the energy source used. The energy source comes from neutron particles in the fast neutron range in the form of point and monoenergetic sources with energy variations of 3 MeV, 4 MeV, and 5 MeV. This source is placed 1 cm before the thermal column as shown in the Figure 1 (z=-65 cm).

Tabel 1. Mass fraction of briquettes and powder of coconut shell

Briquettes [17]		Powder [18]	
Composition	Mass fraction	Composition	Mass fraction
C	0,8567	C	0,5076
Si	0,0042	O	0,4511
O	0,0706	H	0,0071
Al	0,0056	Lu	0,0150
Fe	0,0079	Si	0,0004
Ca	0,0064		
Mg	0,0045		
K	0,0031		
H	0,0410		

Five materials were used to design thermal reactor, namely coconut shell briquettes, coconut shell powder, Al as moderator, Ni as neutron filter, and Pb as gamma filter. Aluminum was chosen as the moderator material because it is more effective in moderating fast neutrons, with minimal interaction with epithermal neutrons [16, 19-20]. Nickel was chosen as the material for the neutron filter because it has a high scattering cross section for epithermal neutrons, resulting in a higher epithermal neutron flux than the thermal neutron flux and fast neutron flux.



(a) (b)

Figure 1. Thermal column (a) Design 1 and (b) Design 2

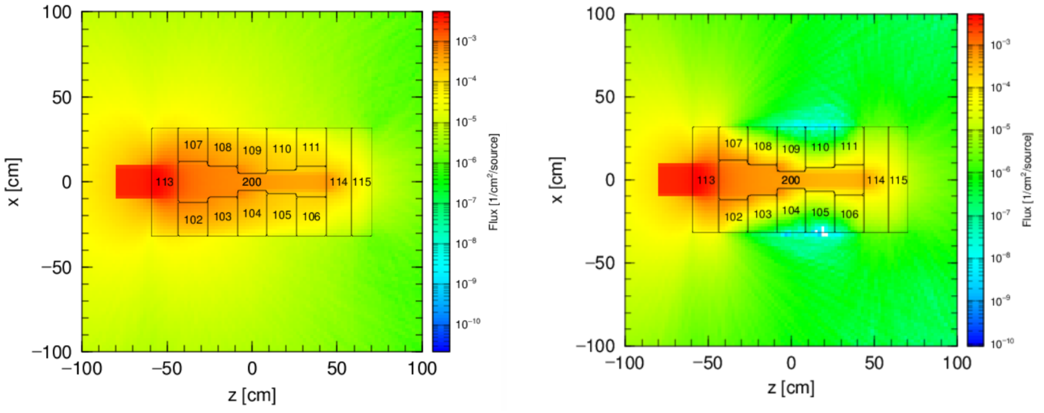
Thermal column design cannot be done directly through measurements but can be simulated first. This is aimed at cost efficiency and minimizing the risk of radiation accidents during direct measurements, so as to obtain a ready-made thermal column design. In general, there are several components of the collimator that can be optimized to obtain the appropriate neutron output, including moderators, filters, and gamma shields. The design 1 and 2 of thermal columns is depicted with beam visualization (rpp) with dimensions x_{min}, x_{max}, y_{min}, y_{max}, z_{min}, and z_{max} in the [surface] section in Figure 1. This thermal column design was modified from our previous study [21].

The output of this simulation was produced Track.out and Dose.out data. T-track is used to calculate the path length (cm) of particles by looking at the distribution of particles in a given region. The average fluence (/cm^2) in the region can also be deduced from this calculation by dividing the path length (cm) by the volume of the region (cm^3). T-track output in the form of track.out from PHITS simulation to determine the particle flux distribution in a particular region. Calculation [T-deposit] tally is to calculate the deposition energy (MeV) in a particular region. PHITS output is automatically saved in a file with extension.out. This file can be opened with Notepad++. The T-deposit output is dose.out which gives the particle dose in Gy/source.

3. Results and Discussion

3.1 *Total Neutron Flux*

Figure 2 show that aluminum shows a very effective moderation effect that can reduce the dose of fast neutrons. The main function of the filter is to attenuate fast neutrons and thermal neutrons and pass epithermal neutrons through and out of the reactor. Nickel material shows the best ability as a neutron filter to interact with fast neutrons to lower their energy. The highest flux value recorded in design 1 and design 2 of the briquette thermal column modification is 10^{-3} cm^2/source, which is marked in red in Figure 2(a) and 2(b), respectively. Meanwhile, the lowest flux value is located in the section marked in green, with a value of 10-6 cm^2/source.



(a) (b)

Figure 2. Total neutron flux at (a) Design 1 and (b) Design 2 in the briquette thermal column for 3 MeV neutron

The addition of coconut shell briquette blocks in design 2 shows better neutron moderation effectiveness, marked by a fainter red neutron beam when compared to the design 1. The thermal column design 1 and 2 that use coconut shell briquettes with coconut shell powder produce very different neutron fluxes. The highest flux value recorded in the thermal column modification of coconut shell powder is 10^{-3} cm^2/source, which is marked in red in the figure. The lowest flux value in design 1 using coconut shell powder is located in the section marked in green, with a value of 10^{-6} cm^2/source. Meanwhile, in design 2 using coconut shell powder, there are parts of the thermal column that are not passed by neutron particles at all, marked in white. In design 2 using coconut shell powder also shows better neutron moderation results compared to thermal column design 1.

3.2 *Epithermal Neutron Flux*

Modification of the thermal column by replacing graphite with coconut shell briquettes as moderator and reflector material provides good neutron moderation efficiency. The high density of coconut shell briquettes provides the ability to reduce the energy of fast neutrons to thermal or epithermal neutrons needed for BNCT. The porous structure of coconut shell briquettes also allows for effective neutron dispersion. Research conducted by Zhang (2014) and Kim (2018) showed that alternative materials with high density can increase the efficiency of epithermal neutron flux in BNCT [22-23].

Based on the simulation results of design 1 with coconut shell briquettes, the epithermal neutron flux at energy variations of 3 MeV, 4 MeV, and 5 MeV are 1.08×10^{9}, 1.03×10^{9}, and 9.53×10^{8} n/cm^{2}s, respectively. Meanwhile, in design 2, the output epithermal neutron fluxes resulting from energy variations of 3 MeV, 4 MeV, and 5 MeV were 1.35×10^{9}, 1.39×10^{9}, and 1.45×10^{9} n/cm^{2}s, respectively. The design of 1 thermal column using coconut shell briquettes with 5 MeV energy does not meet the IAEA criteria [11].

The results of research on design 1 with coconut shell briquettes get flux results that decrease as energy increases, while design 2 produces flux that increases with energy. The results of the research on the modification of the coconut shell powder thermal column did not meet the IAEA standard; this can be caused by the mismatch of the density of coconut shell powder, which is much smaller than graphite. Epithermal neutron flux is one of the important parameters in Boron Neutron Capture Therapy (BNCT) applications. According to IAEA standards, the epithermal neutron flux must fulfil certain criteria in order to produce a dose sufficient to kill cancer cells without damaging the surrounding healthy tissue. The appropriate epithermal flux standard is more than 10^{9} n/cm^{2}s.

3.3 *Fast Neutron Component*

Neutron moderators are materials used in nuclear reactors to reduce the energy of fast neutrons to epithermal neutrons. Fast neutrons produced by the reactor are neutrons produced from fission reactions with high energy. The fast neutron component $(\dot{D}_f/\Phi_{epi})$ is one of the parameters calculated and analyzed to select a value that is small enough.

Based on Figure 3 and 4, the design 1 coconut shell briquette with energy variations of 3 MeV, 4 MeV, and 5 MeV obtained a fast neutron component output of 3.73×10^{-13}, 4.30×10^{-13}, and 5.18×10^{-13} Gycm^2/n. The thermal column with coconut shell powder design 1 obtained the output of fast neutron components of 5.52×10^{-13}, 6.39×10^{-13}, and 7.21×10^{-13} Gycm^2/n, respectively. Design 2 coconut shell briquettes with the same energy variation obtained fast neutron component outputs of 1.55×10^{-13}, 1.74×10^{-13}, and 2.01×10^{-13} Gycm^2/n while in coconut shell powder obtained 9.41×10^{-13}, 1.04×10^{-12}, and 1.07×10^{-12} Gycm^2/n, respectively. The results of the four design there are only two thermal columns that meet the IAEA standard, which has a fast neutron component output less than 2.0×10^{-13} Gycm^2/n is a design of two thermal columns of coconut shell briquettes with energy variations of 3 MeV and 4 MeV.

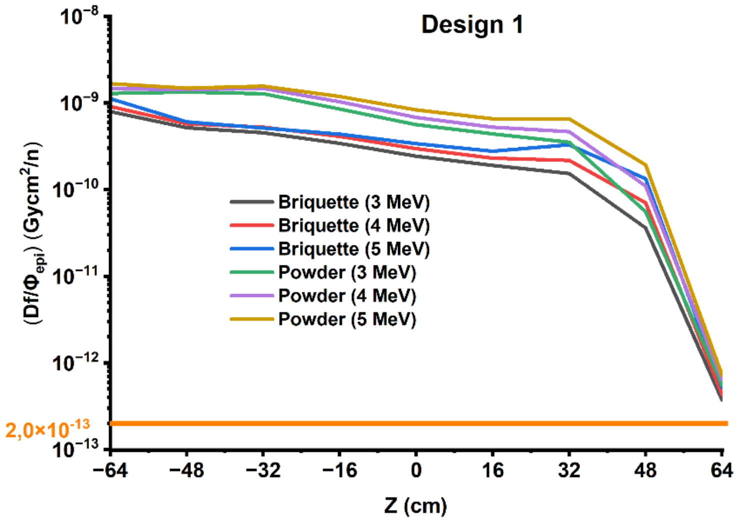


Figure 3. Fast neutron component in design 1 thermal column of briquettes and powder coconut shell

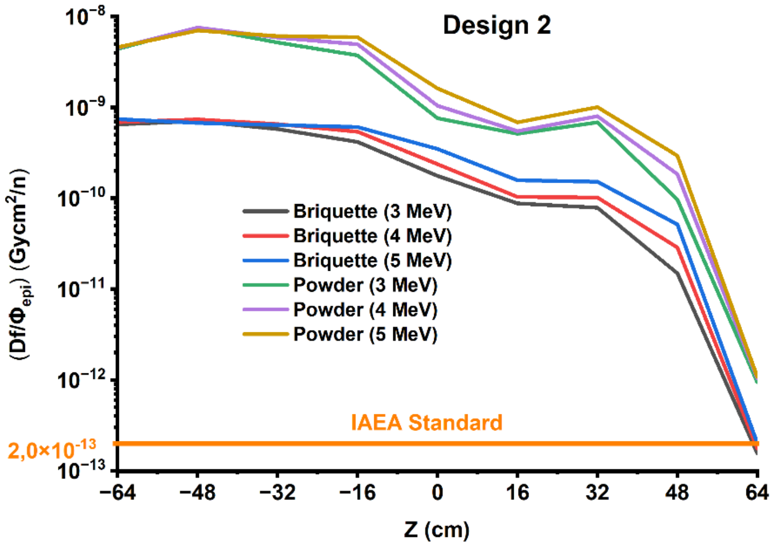


Figure 4. Fast neutron component in design 2 thermal column of briquettes and powder coconut shell

Coconut shell powder produces a larger fast neutron component than coconut shell briquettes. Coconut shell briquettes are made by compacting process, so they have higher density and lower porosity. The denser structure increases the chance of inelastic scattering that can slow down fast neutrons into epithermal neutrons.

3.4 Gamma Ray Dose Rate Component

One of the important parameters that must be considered in BNCT applications is the gamma-ray dose rate $(\dot{D}_{\gamma}/\Phi_{epi})$. The energy and intensity of the gamma rays generated by the neutron source must be evaluated because high-energy gamma rays can cause damage to healthy tissues around the tumour. At the end of the thermal column, a gamma shield is installed so that the gamma rays can meet the IAEA standard of $<2.0\times10^{-13}$ Gycm^2/n. The material that effectively absorbs gamma without reducing the epithermal neutron flux is lead (Pb). Therefore, a Pb gamma shield is installed at the end of the thermal column. The gamma-ray dose rate component is expected to be as small as possible.

Table 2. $\dot{D}_\gamma/\Phi_{epi}$ in design 1 and 2 of coconut shell briquette with 3 energy variations

z (cm)	$\dot{D}_\gamma/\Phi_{epi}$ (Gycm^2/n)					
	Design 1			Design 2		
	3 MeV	4 MeV	5 MeV	3 MeV	4 MeV	5 MeV
-64	3.84×10^{-10}	6.41×10^{-10}	9.38×10^{-10}	3.27×10^{-10}	5.18×10^{-10}	6.35×10^{-10}
-48	1.32×10^{-10}	2.19×10^{-10}	3.21×10^{-10}	1.58×10^{-10}	2.34×10^{-10}	2.80×10^{-10}
-32	3.67×10^{-11}	5.87×10^{-10}	8.63×10^{-11}	8.17×10^{-11}	1.03×10^{-10}	1.18×10^{-10}
-16	2.79×10^{-11}	4.31×10^{-11}	6.37×10^{-11}	7.58×10^{-11}	8.74×10^{-11}	9.91×10^{-11}
0	2.19×10^{-11}	3.31×10^{-11}	4.90×10^{-11}	5.96×10^{-11}	6.54×10^{-11}	7.41×10^{-11}
16	2.07×10^{-11}	2.96×10^{-11}	4.36×10^{-11}	4.37×10^{-11}	4.88×10^{-11}	5.48×10^{-11}
32	5.34×10^{-11}	7.57×10^{-11}	1.11×10^{-11}	5.90×10^{-11}	6.97×10^{-11}	8.28×10^{-11}
48	3.30×10^{-11}	5.32×10^{-11}	8.48×10^{-11}	1.67×10^{-11}	2.58×10^{-11}	3.61×10^{-11}
64	2.80×10^{-11}	1.19×10^{-11}	2.57×10^{-12}	1.32×10^{-13}	5.37×10^{-13}	1.03×10^{-12}

Table 3. $\dot{D}_\gamma/\Phi_{epi}$ in design 1 and 2 of coconut shell powder with 3 energy variations

z (cm)	$\dot{D}_\gamma/\Phi_{epi}$ (Gycm^2/n)					
	Design 1			Design 2		
	3 MeV	4 MeV	5 MeV	3 MeV	4 MeV	5 MeV
-64	7.28×10^{-10}	1.19×10^{-9}	1.50×10^{-9}	2.66×10^{-9}	3.84×10^{-9}	4.28×10^{-9}
-48	4.39×10^{-10}	5.89×10^{-10}	6.82×10^{-10}	2.31×10^{-9}	2.66×10^{-9}	2.65×10^{-9}
-32	2.85×10^{-10}	3.21×10^{-10}	3.34×10^{-10}	1.57×10^{-9}	1.62×10^{-9}	1.53×10^{-9}
-16	2.27×10^{-10}	2.53×10^{-10}	2.65×10^{-10}	1.14×10^{-9}	1.19×10^{-9}	1.16×10^{-9}
0	1.84×10^{-10}	2.05×10^{-10}	2.15×10^{-10}	6.09×10^{-10}	6.48×10^{-10}	6.71×10^{-10}
16	1.68×10^{-10}	1.87×10^{-10}	1.99×10^{-10}	3.90×10^{-10}	4.10×10^{-10}	4.25×10^{-10}
32	2.42×10^{-10}	2.87×10^{-10}	3.19×10^{-10}	4.66×10^{-10}	5.32×10^{-10}	5.63×10^{-10}
48	5.76×10^{-11}	9.34×10^{-11}	1.30×10^{-10}	9.39×10^{-11}	1.50×10^{-10}	1.93×10^{-10}
64	4.57×10^{-13}	2.04×10^{-12}	3.84×10^{-12}	8.72×10^{-13}	3.49×10^{-12}	6.08×10^{-12}

In general, the results show a decrease in the gamma ray component for the design variation and the neutron energy used (Table 2 and 3). The gamma dose rate component in coconut shell briquettes is smaller than that in coconut shell powder. The gamma dose rate component increased with the addition of neutron energy at a thickness of -64 cm. In addition, an increase in the gamma dose rate component also occurs at a thickness of 32 cm to 48 cm because at that time thermal or epithermal neutrons interacting with nickel are able to radiate gamma rays with greater energy. However, the gamma dose rate decreases again at a thickness of 48–64 cm because the particles interact with the lead material, which functions as a gamma shielding.

3.5 IAEA Standard Parameter

The output results of designs 1 and 2 using coconut shell briquettes and coconut shell powder with energy variations of 3 MeV, 4 MeV, and 5 MeV that have been carried out using PHITS are shown in Table 4 and Table 5. Calculations based on simulation output results in PHITS software and multiplied by a multiplication factor, namely normalization. The normalization factor is 5.43×10^{11} n/cm^{2}s. Normalization is used to determine the PHITS output which is equivalent to the real Kartini reactor.

Table 4. IAEA parameters for coconut shell briquettes

Parameters	IAEA Recommendations [11]	IAEA Parameters					
		Design 1			Design 2		
		3 MeV	4 MeV	5 MeV	3 MeV	4 MeV	5 MeV
Φ_{epi}	$>1.0 \times 10^9$	1.08×10^9	1.03×10^9	9.53×10^8	1.35×10^9	1.39×10^9	1.45×10^9
$\dot{D}_f/\Phi_{epi}$	$< 2.0 \times 10^{-13}$	3.73×10^{-13}	4.30×10^{-13}	5.18×10^{-13}	1.55×10^{-13}	1.74×10^{-13}	2.01×10^{-13}
$\dot{D}_\gamma/\Phi_{epi}$	$< 2.0 \times 10^{-13}$	2.80×10^{-13}	1.19×10^{-12}	2.57×10^{-12}	1.32×10^{-13}	5.37×10^{-13}	1.03×10^{-12}
Φ_{th}/Φ_{epi}	< 0.05	0.006	0.008	0.008	0.021	0.021	0.020
I/Φ_{epi}	< 0.7	1.48	1.41	1.38	2.17	1.98	1.75

Table 5. IAEA parameters for coconut shell powder

Parameters	IAEA Recommendations [11]	IAEA Parameters					
		Design 1			Design 2		
		3 MeV	4 MeV	5 MeV	3 MeV	4 MeV	5 MeV
Φ_{epi}	$>1.0 \times 10^9$	6.50×10^8	6.28×10^8	6.28×10^8	1.91×10^8	2.03×10^8	2.28×10^8
$\dot{D}_f/\Phi_{epi}$	$< 2.0 \times 10^{-13}$	5.52×10^{-13}	6.39×10^{-13}	7.21×10^{-13}	9.41×10^{-13}	1.04×10^{-12}	1.07×10^{-12}
$\dot{D}_\gamma/\Phi_{epi}$	$< 2.0 \times 10^{-13}$	4.57×10^{-13}	2.04×10^{-12}	3.84×10^{-12}	8.72×10^{-13}	3.49×10^{-12}	6.08×10^{-12}
Φ_{th}/Φ_{epi}	< 0.05	0.069	0.071	0.065	0.092	0.091	0.091
I/Φ_{epi}	< 0.7	1.96	1.84	1.76	5.16	4.52	3.93

Tables show that only one thermal column meets the IAEA standards. namely the design of the thermal column of coconut shell briquettes with 3 MeV energy variation. However. overall design 2 with coconut shell briquettes does not meet the criteria set by the IAEA. Design 1 and 2 of the thermal columns using coconut shell powder did not meet the standard.

4. Conclusion

Modification of the thermal column design on the Kartini reactor for BNCT applications using PHITS software was carried out by replacing graphite moderator materials with coconut shell briquettes and coconut shell powder. Simulations were carried out with energy variations. namely 3 MeV. 4 MeV. and 5 MeV in each design modification. The moderator with coconut shell briquette material is able to moderate fast neutrons better than the moderator with coconut shell powder material and produces fewer gamma-ray components. The resulting output shows there is only one thermal column that meets the IAEA criteria to be applied to BNCT. namely design 1 and 2 thermal columns using coconut shell briquettes with 3 MeV neutron energy. In the modification of thermal columns using coconut shell powder. none of them meet the IAEA standards for BNCT.

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