Monte Carlo Simulation of Neutrons Scattering in the Reactor

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ABSTRACT

The significance of Monte Carlo simulation to engineer and scientist is now broadly stated and maximum undergraduates have a few training within the use of computers and feature get right of entry to a laptop for the solution of their issues. Monte Carlo method became used to sample the probability laws that describe the behavior of the neutrons in the reactor Shielding. In this study the principles of Monte Carlo simulation were applied to describe the behavior of the high energy neutrons in two different shielding materials; lead and water, the method used is based on the postulate that the scattering is isotropic. Monte Carlo Simulation used to calculate neutron flux and neutron scattering in the reactor. This study had shown that the shield material of water is the one regarding that is best of energy and collision. The findings will be of interest to agree with theoretical results, showed that Monte Carlo method is a method that is efficient reasonable accuracy. Also, the neutron flux was calculated according to the mixture components, radial, energy spectrum in the reactor system for the selected fluids, library and structural material. Three-dimensional nucleonic calculations were performed using the Monte Carlo method. The analysis of Monte Carlo undertaken here, to the knowledge of the neutrons attenuation calculation, which is performed for two different materials in terms of their atomic mass numbers, show that the best diluted are those having an atomic mass comparable to the neutron's mass. Also, other average neutron flux distribution was investigated according to the neutron energy spectrum [0-20 MeV] in the system.

Key Words: Monte Carlo, Neutron Scattering, Neutron Flux, Energy Spectrum, Diluted, Shield Reactor.
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1. INTRODUCTION

Monte Carlo simulation uses random sampling and statistical modeling to assessment mathematical functions and imitative the process of complex systems [1]. This paper gives an overview of its principles and uses, followed by a general description of the Monte Carlo method, discussion the behavior of the neutrons in two different shielding materials; lead and water, and a brief survey of the methods used to sample from random distributions [2]. There is no single Monte Carlo method and any try to define one will inevitably leave out valid examples [3]. A Monte Carlo program may use a great many random numbers, and the path of the calculation through the program will depend on the numbers chosen in each run [4] with truly random numbers, every run of Mont Carlo calculation would follow a different path and produce a different result [5]. Such a program would be very difficult to debug [6]. A pseudo-random number generator usually called an RNG (with the pseudo-left out) [7], is a deterministic computer algorithm that produces a series of numbers that shares many of the characteristics of truly random samples [8]. numbers generator

can have written to be portable; that is, the sequence produced by the algorithm is independent of the computer hardware and language [9] so that a given program will produce the same result when running on different computers [10]. Most RNGs uniformly sample positive integer values between *0* and *N* [11]. To sample the uniform distribution on (0,1) [12], a sample, *u*, from the RNG is divided by *N*[13]. Most RNGs allow *N* to be large enough that the double precision numbers between 0 and 1 are quite uniformly sampled using this method [14]. A very common simple method for generating pseudo-random numbers to use a recurrence is the linear congruential generator (LCG). This recurrence has the form:

$$X_{n+1} = [aX_n + c] \mod m \dots\dots\dots\dots\dots\dots\dots\dots \text{(1)}$$

where *a*, *c*, and *m* must be carefully chosen for best performance, *a* and *c* are positive constant while m is usually chosen to be the size of the maximum positive integer that the machine can resent [15]. The applicability and utility of Monte Carlo methods to reactor problems rest in part upon both of random behavior and numerical solution of mathematical model descending the neutron in the reactor. First, the interaction of neutrons passing through matter is random [16]. A calculation may be often set up simply by simulating primary random variables and observing the behavior of imagined neutrons. Secondly, this process may be regarded as a numerical solution of the linear Boltzmann transport equation [17]. This consideration is helpful in removing irrelevant random process and essential establishing processes that are more efficient. Based on the above, it was noticed that Monte Carlo method is eligible for addressing these problems and provide suitable results for shield design data [18]. In Monte Carlo calculation it is possible to gain estimates of the error and set confidence limits for the result. One way to decrease uncertainty in the answer is to collect and base it upon more observations [19]. In other words, standard errors could be reduced by taking the average of *n* independent values of the quantity under the measurement, since the standard error is inversely proportional to the square root of the sample size *n*. This is, of course, in addition to the techniques that often used to improve the Monte Carlo procedure in terms of reduction of both the statistical errors and computation time [20]. Shielding against fast neutrons, as well as high energy γ rays, is an essential issue in the reactor shielding design. Really, it is found that among all kinds of radiation sources, the fast fission neutrons are the most difficult to shield against. Unfortunately, it is not possible to absorb fast neutrons, because absorption cross – sections are simply too small at high energies. Basically, attenuation of fast neutrons is accomplished by slowing down the neutrons through elastic and inelastic scattering in the shield of moderately heavy and heavy materials until the neutrons reach the thermal energies (1/40 eV), where they are readily absorbed in the material of the shield in the radioactive capture interaction [21]. The previous paper published was not discussing the flux distribution of the neutrons in a nuclear fission reactor, fusion reactor with the same simulation method. This paper will be provided all the empirical piece of evidences in the context of shielding; neutron flux and not just the correlation with the other variables. previous research also measuring and study the Shielding Reactors using Monte Carlo simulation method and this paper is relying on Monte Carlo with advanced computers. the previous study covered each topic on a case-by-case basis but this paper covered shielding reactors and neutron flux. The objective of research was to evaluate the Monte Carlo simulation method in study of shielding reactors and measuring the neutron flux.

2. MATERIALS AND METHODS

2.1 Model and sampling procedure: Criteria and Requirements

The model assumes that when the neutron scatters, it does so in a manner which can be regarded as isotropic in the center of mass of the coordinate system. The model targeted the nucleus is at rest in the laboratory system and the angular dependence of the scattering is isotropic in the center of the mass coordinate system. The neutron after a collision takes any direction in the space with equal probability. Founded on these assumptions the probability density function (PDFs), ρ [E], can be expressed as:

$$\rho[E] = \frac{1}{E_0(1-\kappa)} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \text{(2)}$$

Where E_0 is the initial energy of the neutron, *E* is energy of the neutron after scattering [22].

$$\kappa = [(A-1)/(A+1)]^2 \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \text{(3)}$$

Where *A* is the mass number of the target nucleus.

A suitable sampling scheme for ρ[E] for the canonical distribution can be expressed as:

$$E = E_0[a + (1 - \kappa)n] \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \text{(4)}$$

Where *n* is the random number in the range 0 -1. We use *n* from eq. (4) to find the energy of the neutron after an elastic scattering. To find the scattering angleθ, we use [23]:

$$\theta = \cos^{-1}\left[\left(\frac{A+1}{2}\right)\sqrt{\frac{E}{E_0}} - \left(\frac{A-1}{2}\right)\sqrt{\frac{E_0}{E}}\right] \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (5)$$

2.2 Mean Free Path [MFP]

To compute how long on average, a neutron will move before being involved in a collision, we use:

$$MFP = (n\sigma)^{-1} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (6)$$

Where *n* is the number of molecules per unit volume, σ is the effective cross – sectional area for collision and measured by m^2, which depend on the radii of the target and entering objects [24].

$$\sigma = \pi(r_i + r_n)^2 \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots.. (7)$$

Where r_i is the radius of the molecules of the target, and r_n is the radius of a neutron.

$$n_m = \frac{\rho}{Mt_{wt}} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots.. (8)$$

Where n_m is the number of mole per unit volume of the substance, ρ is the density(kg/m^3) of a substance and $Mt._{wt}$ (kg) molecular weight. This multiplied by the Avogadro number (6.022×10^{23}mol^{-1}) gives us the number of molecules per unit volume (N_m) [24].

2.2.1 Water

$n_m = \frac{1000}{0.018} = 55555.5 \approx 5.5 \times 10^4$ mol/m^3.

$N_m = 5.5 \times 10^4 \times 6.02 \times 10^{23} = 3.34 \times 10^{28}$ molecules/m^3.

To calculate σ, was using eq. (7).

Radius of neutron =10^{-14} m, Radius of water molecule = 10^{-10} m

$\sigma_{Water} = \pi(10^{-10} + 10^{-14})^2 = 3.14 \times 10^{-20}$m^2.

To calculate Mean Free Path, was using eq. (6).

$MFP_{Water} = (3.344 \times 10^{28} \times 3.14 \times 10^{-20})^{-1} = 9.5236 \times 10^{-10}$ m/molecules.

2.2.2 Lead

$n_m = \frac{11340}{0.2072} = 54729.7 \approx 5.47 \times 10^4$ mol/m^3.

$N_m = 5.47297 \times 10^4 \times 6.02 \times 10^{23} \approx 3.295 \times 10^{28}$ molecules/m^3

To calculate σ, was using eq. (7).

Radius of neutron =10^{-14} m, Radius of a lead atom = 5×10^{-14} m.

$\sigma_{Lead} = \pi(5 \times 10^{-14} + 10^{-14})^2 = 1.1304 \times 10^{-26}$m^2 .

To calculate Mean Free Path, was using eq. (6).

$\text{MFP}_{\text{Lead}} = (3.295 \times 10^{28} \times 1.1304 \times 10^{-26})^{-1} = 2.684 \times 10^{-3}$ m/molecule.

2.3 Neutron flux

It is important for neutronic calculations to know the flux distribution of the neutrons in a nuclear fission reactor, fusion reactor, and reactor that is hybrid. The neutron flux is defined as the path that is total of thermal neutrons in a unit volume around point *r* in a second. The neutron flux expresses a scalar value of dimensionsm^{-2} s^{-1}. In the nuclear reactors, fast neutrons are nearly exclusively produced in the fission reactions. The fast neutrons gradually slow due to collisions with the atoms of the moderator and the various nuclear processes taking place in the nuclear reactors [25]. The neutron flux distribution should also be expressed as a function of neutron energy as these formations are the functions of neutron energy. The flux of a neutron beam defined as [26]:

$$\Psi = \frac{\text{number of neutrons impinging on a surface per second}}{\text{surface area perpendicular to the neutron beam direction}} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \quad (9)$$

having the unit $n/(cm^2 \, s)$.

2.3.1 The differential scattering cross section

The angular dependence of the scattered neutrons is a most important aspect of all neutron scattering. To describe this, define the differential scattering cross section:

$$\frac{d\sigma}{d\Omega} = \frac{1}{\Psi} \frac{\text{number of neutrons scattered per second into solid angle } d\Omega}{d\Omega} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots.. \quad (10)$$

The total number of scattered neutrons is of course the sum of neutrons in all of the *4π* solid angle, whence:

$$\sigma = \int \frac{d\sigma}{d\Omega} \, d\Omega \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots...... \quad (11)$$

If one defines the following quantities a correlation to a general formulation of the reactor equations can be developed. Exact definitions of the various coupling parameters mentioned earlier can be obtained and these can then be explicitly evaluated. The parameters defined will be the steady state value [26].

Ψ (r, v)   The neutron flux as a function of position and velocity.

Ψ^* (r, v)   The adjoint flux as a function of position and velocity.

$v \sum_f(r, v)$ The product of the average number of neutrons emitted per fission and the macroscopic fission cross section (the product may be a function of position and of incoming neutron velocity).

x(v)   The normalized fission spectrum where $\int x(v)dv = 1$.

The data of the libraries that are ENDF/B-VII imperative for theoretical calculations. This study was performed with neutron wall loadings of 10 MW/m^2 and fusion power of 4000 MW. The transport equation is currently handled by the Monte Carlo method. An instrument is provided by the Monte Carlo method to solve the equations by simulating the neutron activities. In this study, neutron transport calculations of the neutron flux distributions were investigated equation that is using (10), (11) with Monte Carlo.

3. RESULTS AND DISCUSSION

Table 1 showed the Lead (pb) and water (H_2O) were considered here and subjected to neutrons" threshold energies as a lower limit for the model and is equal to 1.0 eV, also includes the average number of elastic scattering that brings the neutrons to energy that is minimum by the program and the corresponding average angle of scattering. Only 18 collisions are required for water shield to slow down a neutron of 13.99 MeV to 1eV whereas 1398 collisions are needed in the case of Lead to slow down a neutron of 0.57 MeV to1 eV. This is referring to the fact that the neutron in its elastic scattering collision forfeit energy that is most when the mass of the target nucleus is comparable to that of the neutron. Hydrogen as a mediator of little atomic mass, is then the best diluted for neutron between the two studied materials.

Table 1: Information regarding of different materials.

Materials	Alpha {α}	θ[Degree]	E_0 Mev	E Mev	Collision
Water	0.000	44.83	13.99	0.2×10^{-5}	18.009
Lead	0.977	89.73	0.57	0.001×10^{-5}	1398.2

Where θ is scattering angle, E_0 is the initial energy of the neutron, E is energy of the neutron after scattering.

Fig.1 showed the calculated number of collisions is directly proportional to the atomic mass of moderator's material.
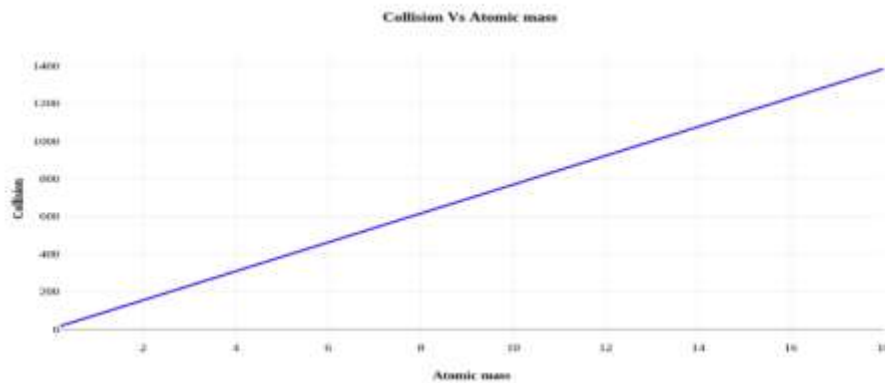

Figure.1: Collision Vs Atomic Mass

Fig. 2 showed the values of θ was found to be increasing with A values . This behavior was expected since the scattering was an elastic , and the higher values of θ reflect the scattering from heavy atoms.
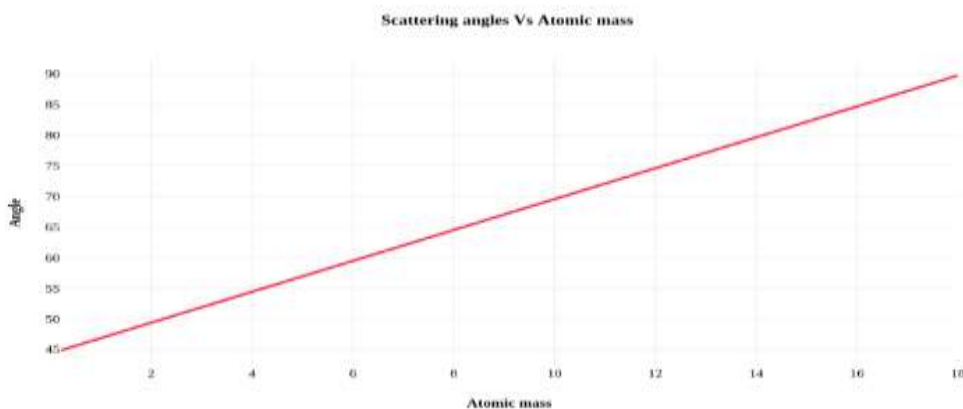

Figure.2: Scattering angle Vs Atomic

The values obtained are in good agreement with the average values reported by (A.S. Ham med et al [27], Dai Kunlun [28], S. Anim-Sampong et al [29].

For the average neutron flux distribution according to neutron energy spectrum (0-20 MeV) in the reactor system, it was seen that the average neutron flux distribution decreases between 0-14 MeV, a peak around 15 MeV and decrease, was shown in Fig. 3.
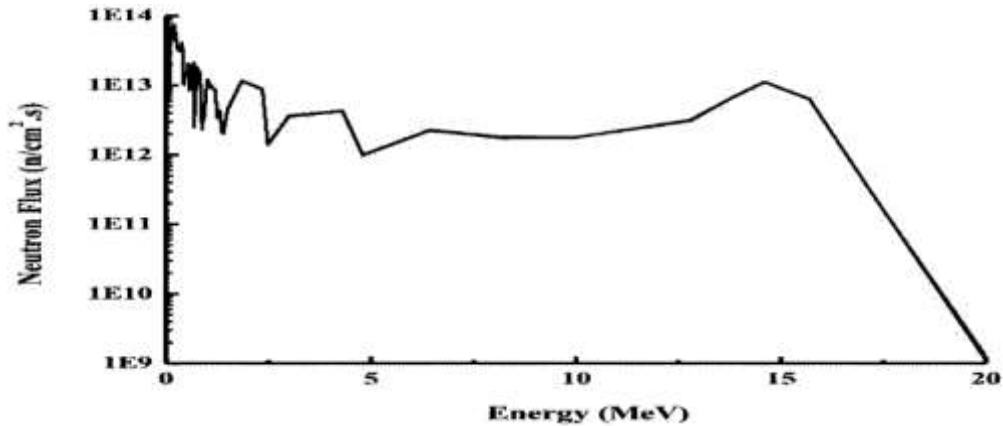

Figure. 3: Neutron flux Vs Energy

The values obtained are in good agreement with the average values reported by [Mehtap Günay et al [30], Boehmer, B. et al [31].

4. CONCLUSION

These studies set out with the aim of assessing the importance of Monte Carlo in generate random numbers related to the process that is scattering. To show how this method that is numerical efficient and capable of addressing complicated problems of random processes, two different materials are used to slow down neutrons to thermal energies. The analysis of Monte Carlo undertaken here, to the knowledge of the neutrons attenuation calculation, which is performed for two different materials in terms of their atomic masses number, show that the best diluted are those having an atomic mass comparable to the mass that is neutron's. Also the neutron that is normal transition dissemination was explored by the neutron vitality range [0-20 MeV] in the framework. In the figuring was seen that the normal motion that is neutron a pinnacle roughly [14-16 MeV], diminishing from that point. The qualities between the [0-20 MeV] vitality hole were roughly similar estimations of the motion that is neutron indicated by the vitality in the framework.

SIGNIFICANCE STATEMENT
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DATA AVAILABILITY
The data required to reproduce these findings can be shared.

REFERENCES

[1] Press W.H. Teukolsky S.A Vetterling W.T., Flannery B.P. (2007), Numerical Recipes (Cambridge Uni. Press). books.google.com.sa/books?hl=en&lr=&id=1aAOdzK3FegC&oi=fnd&pg=PA1&dq=Press+W.H.+Teukolsky+S.A+Vetterling+W .T.,+Flannery+B.P.+(2007),+Numerical+Recipes+(Cambridge+Uni.+Press).&ots=3kOoHgDmpj&sig=XtKSgN53t2qB_f1nyCVT bm6W0Fg&redir_esc=y#v=onepage&q&f=false.

[2] Monte Carlo method. Wikipedia. en.wikipedia.org/wiki/Monte_Carlo_method.

[3] Robert L. Harrison, Introduction to Monte Carlo Simulation. AIP Conf Proc. 2010 Jan 5, 1204: 1721. https://doi.org/10.1063/1.3295638.

[4] Kroese, D. P., Brereton, T., Taimre, T., Botev, Z. I. (2014)." Why the Monte Carlo method is so important today". WIREs Comput Stat. 10.1002/wics.1314.

[5] P. Del Moral, G. Rigal, and G. Salut. Optimal nonlinear filtering in GPS/INS integration,(1997), IEEE Transactions on Aerospace and Electronic Systems, 10.1109/7.599254.

[6] Hubbard, Douglas (2007). How to Measure Anything Finding the Value of Intangibles in Business. John Wiley

[7] Kahneman, D., Tversky, A. (1982). Judgement under Uncertainty, Heuristics and Biases. Cambridge Univ. Press. people.hss.caltech.edu/~camerer/Ec101/JudgementUncertainty.pdf.

[8] Press, William H., Teukolsky, Saul A., Vetterling, William T., Flannery, Brian P. (1996) [1986]. Numerical Recipes in Fortran 77: The Art of Scientific Computing. Fortran Numerical Recipes. 1 (Seconded.). Cambridge University Press. websites.pmc.ucsc.edu/~fnimmo/eart290c_17/NumericalRecipesinF77.pdf.

[9] Ripley, B. D. (1987). Stochastic Simulation. Wiley Sons. 10.1002/9780470316726.

[10] Robert, C. P., Casella, G. (2004). Monte Carlo Statistical Methods (2nd ed.). New York: Springer. ISBN 0-387-21239-6.

[11] László Szirmay-Kalos, Monte Carlo Methods in Global Illumination (2000), citeseerx, citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.36.361.

[12] Vose, David (2008). Risk Analysis, A Quantitative Guide (Third ed.). John Wiley Sons.

[13] B. Meng and W. H. Weinberg, Monte Carlo simulations of temperature programmed desorption spectra, The Journal of Chemical Physics **100**, 5280 (1994); https://doi.org/10.1063/1.467192.

[14] Random.org. random.org.

[15] Luby M., Pseudorandomness and Cryptographic Applications, Princeton Univ Press, 1996. ISBN 9780691025469.

[16] J.E. Hurtado, A.H. Barb, Monte Carlo Techniques in Computational Stochastic Mechanicsat, Archives of Computational Methods in Engineering, Vol. 5, 1, 330 (1998). doi.org/10.1007/BF02736747.

[17] Tenekedjiev KI, Nikolova ND, Kolev K. Applications of Monte Carlo Simulation in Modelling of Biochemical Processes,2011. ncbi.nlm.nih.gov/pubmed/28045483.

[18] Julius Goodman, ACCURACY AND EFFICIENCY OF MONTE CARLO METHOD, Bechtel Power Corporation 12400 E. Imperial Hwy. Norwalk, CA 90650, U.S.A. iaea.org/inis/collection/NCLCollectionStore/_Public/19/047/19047359.pdf.

[19] M. Piera, et al., Hybrid reactors: Nuclear breeding or energy production? , Energy Convers. Manage., 51, 1758, (2010). doi.org/10.1016/j.enconman.2010.01.025.

[20] B. Şarer, et al., Calculations of neutron-induced production cross-sections of ^{180,182,183,184,186}W up to 20 MeV, Ann. of Nucl. Energy, 36, 417 (2009). doi.org/10.1016/j.anucene.2008.11.025 .

[21] M.B. Chadwick, et al., ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology, Nucl. Data Sheets, 107, 2931, (2006). doi.org/10.1016/j.nds.2006.11.001.

[22] D.B. Pelowitz (Ed.), MCNPX User's Manual Version 2.7.0, LA-CP-11-00438, LANL, 2011.

[23] M. Günay, Investigation of radiation damage in structural material of APEX reactor by using Monte Carlo method, (2013).doi.org/10.1016/j.anucene.2012.06.038.

[24] Brünglinghaus, Marion." Mean free path". European Nuclear Society. Retrieved 2011-11-08. euronuclear.org/info/encyclopedia/m/mean-fee-path.htm.

[25] J.J. Duderstadt, G.A. Moses, New York: John Wiley & Sons, (1982). milproj.dc.umich.edu/pdfs/books/1982%20Inertial%20Confinement%20Fusion.pdf.

[26] Avery, R. Theory of coupled reactors. In U.N. (2nd Geneva) Conference on Peaceful Uses of Atomic Energy. Vol. 12, Pp. 182-191. New York, New York, United Nations. 1958. naweb.iaea.org/napc/physics/2ndgenconf/data/Proceedings%201958/NG900090.pdf.

[27] A. S. Hammed toda, A. M. Ali. "Monte Carlo Simulation of Neutrons Scattering in the Reactor Shielding for Lead and Water". University of Dongola Journal for Scientific Research, 9th edition June 2015. repository.uofd.edu.sd/handle/123456789/271.

[28] Dai Kunlun. "A Monte-Carlo Simulation for Neutron Transport in Spherical Reactor". National University of Singapore. April 4, 2016. physics.nus.edu.sg/student/Honours%20Projects%20Repository%202015-16/DaiKunLun.pdf.

[29] S. Anim-Sampong*, B.T. Maakuu, E.H.K. Akaho. "MONTE CARLO NEUTRON TRANSPORT SIMULATION OFTHE GHANA RESEARCH REACTOR-1" iaea.org 2005. inis.iaea.org/search/search.aspx?orig_q=RN:36069568.

[30] Mehtap Günay*, Hilal Bardakçõ. "The calculation of neutron flux using Monte Carlo method". EPJ Web of Conferences 154, 01025 (2017) 10.1051/epjconf/201715401025 TESNAT 2017.

[31] Boehmer, B., Konheiser, J., Noack, K., Rogov, A., Stephan, I., Hansen, W., Hinke, D., Unholzer, S., Grantz, M., and Mehner, H., "Measurements and Monte Carlo Calculations of Gamma and Neutron Flux Spectra Inside and Behind Iron/Steel/Water Configurations," Journal of ASTM International, Vol. 3, No. 8, 2006, pp. 1-8, doi.org/10.1520/JAI13457.ISSN 1546-962X.