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Geant4 Simulation of Number of Event Effect on the TLD LiF: Mg, Cu, P Energy Response

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Abstract — The effect of different number of events on the energy response of a bare thermoluminescent dosimeter (TLD) LiF: Mg, Cu, P chip has been simulated using Geant4. This simulation aims to determine the optimum number of events with minimum computational time. Fourteen photon energies in a range of $16-1250 \text{ keV}$ with a range of $2\times10^7 - 2\times10^{12}$ events were applied. A LiF: Mg, Cu, P chip with 4.5 mm diameter and 0.9 mm thick on the surface of $30 \times 30 \text{ cm}^2$ water phantom and a thin 10 µm slice of water (at 10 mm deep in the phantom) were considered as the sensitive volumes to calculate the respective absorbed dose *DTLD* and *DW.* The relative energy response *R* was calculated from *DTLD* and *DW*'s ratio for each energy normalized to D_{TLD} and D_W ratio of energy 662 keV. 2×10^9 number of events were found to be the optimum number of events with minimum computational time. The simulation results were validated to the measurement results and the mean deviation of 0,59% was yielded. As the deviation is within the acceptable limit of $\pm 25\%$, it was concluded that the results were considered satisfactory and the materials and physics processes applied in the code were correct.

Keywords – TLD, LiF:Mg,Cu,P, Geant4, energy response

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I. INTRODUCTION

Thermoluminescent dosimeter (TLD) is a passive dosimeter used to measure a person's level of radiation exposure [1]. Radiation workers widely use it as a badge type personal dosimeter to monitor the cumulative radiation doses received over periods of weeks or months [2]. This dosimeter can measure the whole body dose $[H_p(10)]$ and skin dose $[H_p(0.07)]$ from X-ray and gamma radiation (energy range <12 keV - 3 MeV) [3]. Because of its broad energy coverage, TLDs are also widely used in environmental monitoring and diagnostic examinations [4].

The most common material used for TLD is lithium fluoride (LiF) in a chip form. Its atomic number $(Z =$ 8.2) is similar to that of tissue, so the sensitivity is not strongly dependent on the X-ray spectrum [5]. TLDs can be doped by a particular material to increase its responsiveness. The most commercially used TLD is doped by Mg, Ti (TLD-100) and Mg, Cu, P (TLD-100H) [6]. However, over the last decade, LiF: Mg, Cu, P (TLD-100H) seems to be gradually replacing LiF: Mg, Ti (TLD-100) due to its higher sensitivity, lower detection limit and almost negligible fading [7].

The working principle of TLD makes use of the luminescence phenomenon that occurs when the LiF chip receives heat stimulation. When subjected to radiation, free electrons in the LiF are trapped under unstable conditions. To get this radiation reading, the TLD chip goes through a reading process that is heating up in an oven inside a light-tight enclosure called the TLD reader. This heating causes the free electrons to return to their original position while emitting light. The quantity of light emitted is measured by a photomultiplier tube (PMT) on the TLD reader and the output is described in a temperature function called a radiating curve. The quantity of light emitted on this emission curve corresponds to the radiation dose received by TLD [8].

The ability of the TLD to interpret the amount of radiation energy absorbed to the measured radiation energy is called the energy response. The ideal TLD has a flat energy response where the energy measured is equal to the energy absorbed in the entire energy range [9]. However, based on previous studies, it was reported that a flat energy response, especially for TLD: LiF: Mg, Cu, P can only be achieved at high

energy ($> 500 \text{ keV}$). Whereas at low energy (< 500 keV), this has not been materialized [10][11][12].

Extensive simulation studies have been carried out by several researchers in search of this flat response for the lower energy region [13][14][15]. Several phases need to be conducted to achieve this goal. The initial step is to simulate the energy response of a single bare TLD chip (without any filter). The results need to be validated by comparing it to another simulated or measured results to ensure the simulation accuracy. A deviation of ±25% between the measured and simulated response is acceptable, as reported by Eakins et al. in 2008 [16].

The general-purpose radiation transport codes, such as GEANT4, can be utilized to perform this simulation. GEANT4 is an object-oriented toolkit written in C++ language. It can be used in different application domains such as high energy physics, radiation protection, and medical physics [17].

The accuracy of the GEANT4 simulation result depends on many factors, one of them is the number of events given in the simulation. The maximum number of events that can be generated is not unlimited but restricted to the CPU capability. The higher number of events will produce a more precise calculation but requires a longer computing time [18]. Therefore, determining the number of events that can provide good results of energy response in the least amount of time is crucial. Hence, this study aims to present the effect of the different number of events on the simulation of TLD LiF: Mg, Cu, P energy response to achieve an adequate number of events.

II. RESEARCH METHOD

A. Simulation model

The Monte Carlo Geant4 Toolkit was used to simulate TLD LiF: Mg, Cu, P energy response. The toolkit uses C++ programming language to simulate particle movement through matters. The Geant4's toolkit was installed on a self-built High-Performance Computing (HPC) Grid consist of six 3.4 GHz i-7 Quad Core CPUs with 8 GB RAM each. These CPUs are capable of executing a maximum value of 2×10^{12} number of events.

Photons and electrons are chosen as the basic particles in this simulation because photon energy ranges from 16-1250 keV. The physical processes that govern the interaction of these particles are G4PhotoElectricEffect, G4Compton Scattering, and G4GammaConversion for photons and G4eIonisation, G4eMultipleScattering, G4eBremsstrahlung, and G4eplusAnnihilation for electrons. Threshold values for secondary particle production defined as range cut are set to 0.05 mm across all geometries.

In this simulation, only the whole body dose $[H_p(10)]$ energy response was simulated since it provides an effective dose value sufficiently precise for radiological protection purposes. In the real condition, a TLD is worn inside a badge that has a specific filter for $H_p(10)$ measurement. The complex geometry and material used for the filter could contribute to the complexity of the simulation. Hence for the initial phase of the energy response simulation, only a single bare TLD chip was simulated.

For verification purposes, this simulation was made based on the measured energy response of bare TLD LiF: Mg, Cu, P chip conducted by Obryk [19]. The dimension of the TLD chip used in Obryk's experiment was 4.5 mm diameter and 0.9 mm thick. This TLD chip was placed on the 30×30 cm² surface of the water phantom (water phantom dimension: $30 \times 30 \times 15$ cm3) and exposed to X-ray and gamma radiation. The energy of the X-ray were 16, 20, 24, 33, 48, 65, 83, 100, 118, 164, 208 and 250 keV) and gamma 662 keV (Cs-137 source) and 1250 keV (Co-60 source). The distance of the radiation source to the TLD was 2 m for X-rays and 2.5 m for gamma radionuclides (Cs-137 and Co-60).

Fig.1. The Simplified Geometry of The Simulation Model

The simulation model was made as closely as possible with the Obryk experimental settings, as shown in Fig. 1. Three types of materials, namely LiF, water, and air, were used. Two types of sensitive volumes were defined, namely (1) a chip of TLD LiF on the surface of a water phantom and (2) water with a thickness of 10 µm at a depth of 10 mm in the water phantom. These two volumes are indicated by numbers (1) and (2) in Fig. 1. Several events were tested in the range of $2\times10^{7} - 2\times10^{12}$ photons for each energy measured to determine the optimum number of events on the simulated energy response. The number of events represents the amount of the photon energy emitted by the radiation source. A large number of photons are used to reduce the possibility of systematic errors.

Simulation optimization was done by adding a build-up to the TLD radiation exposure model. Buildup is an additional structure placed in front of the radiation receiving object to facilitate the Charged Particle Equilibrium (CPE) balance. CPE can only occur if the number of charged particles leaving a volume equals to the number of particles entering that volume [20]. It is necessary for calculating the absorbed dose because, with the form of CPE, the amount of dose absorbed in size is the same as the absorbed dose in the air or air kerma. Air kerma can be defined as the amount of radiation energy (in Joule) deposited in a unit mass (kg) of air. Water was used as a build-up material in this simulation because water's density is considered the same as air.

The area of radiation exposure given to the TLD was equals to the surface area of the water phantom (30 \times 30 cm²). It was done to produce a broad spectrum of light and not just focus on the object receiving the light. The built-up area was 5×5 cm² with a thickness following the approximate range of continuous slowing down an approximation of electrons in the water.

B. Energy Response Calculation

Energy response is a parameter calculated from the value of an absorbed dose of a certain material. The absorbed dose of a material *D* can be calculated using (1),

$$
D = \Psi\left(\frac{\mu_{en}}{\rho}\right) \tag{1}
$$

where Ψ is the energy flux (keV/cm²) and μ_{en} / ρ is the mass attenuation coefficient of a material $\rm (cm^2/g)$. The energy flux *Ψ* can be calculated from photon flux ∅ multiplied by energy *E*.

In the simulation, the *Ψ* value was determined by the user. At the same time, Geant4 calculated the amount of μ_{en}/ρ from the total number of cross-sections of the particle interactions defined in this simulation. If this equation is applied to Fig. 1, for specific photon energy, the absorbed dose in TLD (shown by number (1) in the figure) is now $D_{\text{TLD}} = \Psi \left(\frac{\mu_{en}}{a} \right)$ $\frac{\pi}{\rho}$ **TLD** , and the absorbed dose in water (indicated by number (2) in the figure) becomes $D_w = \Psi \left(\frac{\mu_{en}}{m}\right)$ $\frac{en}{\rho}$ w . For each energy, the D_{TLD} and D_w ratio will produce a standard energy response *Rstd*:

$$
R_{std} = \left(\frac{D_{TLD}}{D_W}\right)_E\tag{2}
$$

The relative energy response *Rrel* can be obtained by using the standard energy response for each measured energy was normalized to the standard energy response at 662 keV (Cs-137 calibration energy), as defined in (3),

$$
R_{rel} = \frac{\left(\frac{D_{TLD}}{D_W}\right)_E}{\left(\frac{D_{TLD}}{D_W}\right)_{662keV}}\tag{3}
$$

III. RESULT

Dose measurements on a bare TLD LiF: Mg, Cu, P chip located on in front of a water phantom was simulated using Geant4. Several events in the range of 2×10^{7} – 2×10^{12} were tested to simulate the emitted photon energy and determine the effect on the energy response. Fig. 2 shows the geometric simulation of the TLD with and without photon energy emission.

Fig. 2. Geometric Simulation of The TLD on a Water Phantom

The simulation results of absorbed dose values for each TLD and water, *DTLD* and *Dwater* were calculated using equation (1) – (3) for each of the energy measured. Each dose was normalized to Cs-137 (662 keV), resulting in a curve of relative energy response for each energy. Six numbers of events were tested in the simulation yielding six sets of energy response curves, which are presented in Fig. 3. In this figure, the simulated result was represented by curve A–F, which are A: 2×10^7 events, B: 2×10^8 events, C: 2×10^9 events, D: 2×10^{10} events, E: 2×10^{11} events, F: 2×10^{12} events; whereas curve G is representing the Obryk's result.

Fig. 3. Relative Energy Response of Bare TLD Lif: Mg, Cu, P Chip with a Different Emitted Number of Events

The computational time consume for each number of events in the simulation are given in Table 1. Along with that, the deviation value of each number of events energy response compared with Obryk's energy response were calculated and displayed in Table 1.

Table 1. The Computational Time and Deviation Value in Comparison with Obryks for Each Number of Events Used in This Study

Symbol in Fig.3	Number of Events	Computational Time (hours)	Deviation with Obryk [19] (%)
A	2×10^7	24	-7.73
B	2×10^8	48	10.59
C	2×10^9	72	0.59
D	2×10^{10}	96	3.43
E	2×10^{11}	120	3.87
F	2×10^{12}	144	4.02

The information given in Table 1, shows that the 2×10^9 number of events gave the smallest deviation value when compared to Obryk's results. We can assume that the value of energy response simulated using this number of events was more accurate than the other. A better comparison on each energy can be gain by using the detailed comparison of each energy response for 2×10^9 number of events in contrast with Obryk are given in Table 2.

Table 2. The Energy Response Results from The Simulation with 2×10^9 Number of Events in Comparison with Obryk

Energy	Energy response			
(keV)	Simulation	Obryk [19]	Deviation $(\%)$	
16	3.68	3.50	5.13	
20	2.20	2.26	-2.79	
24	1.76	1.74	0.89	
33	1.40	1.50	-6.84	
48	1.17	1.24	-5.25	
65	1.09	1.05	3.56	
83	1.00	0.95	5.60	
100	0.96	0.90	6.82	
118	0.97	0.87	11.40	
164	0.91	0.87	5.15	
208	0.95	0.93	2.26	
250	0.99	0.99	0.42	
662	1.00	1.00	0.00	
1250	0.93	1.14	-18.12	
		Mean, μ	0.59	
		Standard deviation, σ	7.26	

IV. DISCUSSION

The simulation results of energy responses for each tested number of events were given in Fig. 3. As can be seen from this figure, the energy response curve for the TLD chip tends to be ideal (average) except the over-response that occurs at 16, 20, and 24 keV energy. Natural over-response occurs due to the photoelectric effect that contributes significantly to particle interactions in the low energy range (20–50 keV). In this range, almost all photons turn into photoelectron. Hence, when the primary photon energy increases, the energy of the secondary photon also increases, causing more responses in this energy range. Furthermore, the energy response curve of $H_p(10)$ chip of TLD without filter resembles the $H_p(0.07)$ energy response curve, which has a very thin filter (representing human skin).

The energy response for each number of events was then analyzed, and the deviation value in compared with Obryk's results was calculated. The results are shown in Table 1, along with the computational time consumed during simulation of each energy response. From these results, it can be seen that the results became more accurate when the number of events increased (only up until 2×10^9 number of events). However, the more number of events used requires a longer computational time.

The lowest deviation value with a minimum computational time was yielded when 2×10^9 number of events were selected. From this number upwards, both the deviation value and the computational time keep increasing until the maximum number of events that can be handled by the CPU (2×10^{12}) .

Since 2×10^9 number of events gave the lowest deviation value, a detailed comparison with Obryk for each energy measured is needed to ensure the accuracy of the simulation, as given in Table 2. The minimum and maximum deviation values obtained in the energy are 250 keV (deviation=0.42%) and 1250 keV (deviation= 18.12%), respectively. The mean deviation for 14 photon energies is 0.59%. All these values are within the criteria of an acceptable simulation result, which is less than $\pm 25\%$. It means that the results of the energy response simulation using Geant4 are in accordance with the results of the energy response measurements conducted experimentally by Obryk. Therefore, it can be concluded that the results of this simulation are accurate, and the selection of materials and physical processes used are correct.

Of all 14 deviation values (for 14 photon energies), ten energies give a positive deviation value. It means the simulation value is greater than the experimental value, and only four energies give a negative deviation value. It is quite interesting to note since it seems as if a systematic error has occurred in the simulation results. A one-sample t-test (student's t-test) was carried out to ascertain whether there was evidence that the simulation results were systematically higher than the experimental results. Based on the total value of $n = 14$, the average $(μ)$ and standard deviation $(σ)$ of all these deviations are: $\mu = 0.59$, $\sigma = 7.26$ (all in percent). One sample t test score for 13 degrees of freedom and 5% confidence level is 1.77. Since 1.77×1.94 is greater than 0.59, it can be concluded at a 5% confidence level. There is no evidence that the simulation results are systematically higher than the experimental results.

V. CONCLUSSION

Simulation of single bare TLD LiF : Mg, Cu, P chip energy response (without filter) for 14 energies in the range of 16-1250 keV has been carried out. This simulation is the initial phase of the TLD simulation in search of the flat response for the lower energy region. For this initial phase, the effect of a different number of events on TLD LiF: Mg, Cu, P energy response is analyzed. The simulation results showed that 2×10^9 events is the optimum number of events with the minimum computational time.

Accuracy of the simulation can be ensure from the results validation with the measured value and the mean deviation value of 0.59% was yielded. Since this value is much lower than the criteria of an acceptable simulation result $(\langle 25\% \rangle)$, it is indicated that the materials and physical processes used are correct.

Based on the one-sample t-test (student's t-test) at a 5% confidence level, there is no evidence that there is a systematic error in the simulation results. Therefore, it is concluded that these simulation results are accurate and the optimum number of events determined in this study can be utilized in the next TLD simulation phase.

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