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Monte Carlo Simulation of TLD Response Function: Scattered Radiation Application

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1. Introduction

Thermoluminescence dosimetry (TLDs) are routinely used for in-vivo dosimetry as well as other application in medicine and industry [1, 2]. The most commonly used TLD material is Lithium flouride based doped with small quantities of Mg and Ti that is denoted by LiF:Mg,Ti (TLD-100). This popularity is due, in part, to approximate tissue equivalence and low signal fading [3]. Knowledge of TL response, especially at commonly used photon energies, is useful to estimate the uncertainty of dosimetry system, and experimental methodology has elsewhere been regarded as the most reliable option [4]. TLDs are relative dosimeters and therefore have to be calibrated against absolute dosimetry systems such as a calibrated ion chamber. In radiotherapy application it is convenient to calibrate them in $^{60}$Co $\gamma$-ray beam or in a low-energy megavoltage x-ray beam of $^{137}$Cs $\gamma$-rays [4, 5]. It is therefore important to know quality dependence and energy correction factors that should be applied if the TLDs are used in photon beams other than calibration beam such as scattered beams [4].

In the present study, quality dependence of TLD-100 response was measured in different beam qualities followed by mcnp simulation. It was done to model the behaviour of dosimetry at low energy x-ray beams to improve the TLD usage in scattered radiation field.

2. Materials and methods

We used fourty cubic chips of lithium fluoride (LiF) crystals doped with Magnesium (Mg) and Titanium (Ti) presented at concentrations of 200 and 10 ppm by weight, respectively. Chips sizes were $3.1 \times 3.1 \times 1 \text{ mm}^3$ with density of $2.64 \text{ g cm}^{-3}$ and manufactured by Harshaw.
company. Our protocol for using TLD-100 was described in detail by Mckeever [2]. Briefly, the chips were first annealed at 400°C for 1h, followed by a second annealing at 100°C for 2h. After irradiation, and before reading, the TLDs were stored for 24h at room temperature (20°C) to clear the low energy traps. To produce radiation beams with different energies, Co-60 radiotherapy and orthovoltage x-ray therapy machines were used as specified in Table 1.

To determine the sensitivity of each individual TLD efficient correction coefficient (ECC) were obtained by the following equation after irradiation on a perspex holder.

$$Ecc_i = \frac{R_i}{R}$$  \hspace{1cm} (1)

where $Ecc_i$ is the ECC of each TLD, $R$ and $R_i$ are individual reading and average reading of the total TLDs, respectively.

The TLDs were calibrated against an ionization chamber at depth of 5 cm of water phantom at a distance of 50 cm from the radiation source. Water absorbed dose of 60Co $\gamma$-rays was measured by using IAEA protocol 277 [6]. To obtain absorbed dose calibration factors in cGy/Count, TLD chips in groups of three or four were irradiated with different beam qualities (120 kVp- 300 kVp). Then, the average counts (corrected for background counts) of the TLDs at each dose group were determined. Calibration factor at each energy quality was defined as the inverse of the tangent of TLD absorbed dose response curve. This factor allows to convert the TL signal to the received dose:

$$(CF)_q = \text{CalibrationDose} / \text{TL}$$ \hspace{1cm} (2)

Where “calibration dose” is the given dose for calibration of TLD and TL is the dosimeter response in cGy after irradiation with beam quality of “q” [7]. The quality dependence factor $(F_{\text{Co}}^X)$ is then defined as:

$$F_{\text{Co}}^X = \frac{TL(X) / D_{\text{med}}(X)}{TL(\text{Co}) / D_{\text{med}}(\text{Co})}$$ \hspace{1cm} (3)

Where $TL(X) / D_{\text{med}}(X)$ is the light output of material TL per unit dose for the x-ray beam quality or the inverse of calibration factor for the beam quality. $TL(\text{Co}) / D_{\text{med}}(\text{Co})$ is the light output per unit dose in the same medium for 60Co gamma-rays or inverse of calibration factor for the 60Co gamma-rays. Assuming the $D_{\text{LiF}}$ to be the dose of TLD material that is directly proportional to the output light of TL(X) at any x-ray beam quality, $F_{\text{Co}}^X$ can also be written as:

$$F_{\text{Co}}^X = \frac{(D_{\text{med}} / D_{\text{LiF}})_{\text{Co}}}{(D_{\text{med}} / D_{\text{LiF}})^X}$$ \hspace{1cm} (4)

To measure the absorbed dose cavity theory defines the relation between the dose absorbed in a medium $(D_{\text{med}})$ and the average absorbed dose in the detector or cavity $(D_{\text{cav}})$:

$$D_{\text{med}} = D_{\text{cav}} f_{\text{med,cav}}$$ \hspace{1cm} (5)
Where $f_{med,cav}$ is a factor that varies with energy, radiation type, medium, size and composition of the cavity. For a cavity that is large enough in comparison to the range of electrons, the dose in the medium can be obtained from the mass energy-absorption coefficient ratio of that medium to the cavity material:

$$f_{med,cav} = \frac{\mu_{en}}{\rho}_{med,cav}$$  \hspace{1cm} (6)

Where $\left( \frac{\mu_{en}}{\rho} \right)_{med,cav}$ is the ratio of the mass-energy absorption coefficient of medium to the cavity, averaged over the photon energy fluence spectrum present in the medium. This expression completely neglects any perturbation effects or interface effects that may occur by the introduction of the detector material into the uniform medium [8]. As a consequence, for kilovoltage x-rays the dose ratio of water to LiF is equal the mass energy-absorption coefficient of water to Lif. This is justified as the range of electrons generated by kilovoltage x-rays are very short compared to the smallest distance across the cavity in the beam direction. From equation 5 quality dependence was re-designed as:

$$\frac{\left( \frac{\mu_{en}}{\rho} \right)_{w}}{\left( \frac{\mu_{en}}{\rho} \right)_{LiF}} = \frac{\left( \frac{\mu_{en}}{\rho} \right)_{w}}{\left( \frac{\mu_{en}}{\rho} \right)_{LiF}}$$  \hspace{1cm} (7)

The mass energy absorption coefficients for water and LiF are taken from Hubble (1982) [9].

3. Monte Carlo simulation

MCNP-4C Monte Carlo system was used for all simulations reported in this study. Monte Carlo calculation did not show any difference in behaviour of pure LiF and TLD-100 in kilovoltage or megavoltage x-ray ranges. This is expected since the concentration of Ti and Mg by weight is negligible in TLD-100 [10]. The TLD chips were represented by 3.1 mm ×3.1 mm×1 mm. In all cases the phantom material was represented by a 20cm×20cm×12cm cube of water same as experimental method. The incident photons were transported in a water medium and the dose scored in a water cube of the same dimension as the TLD placed with its center at a particular depth. The depth of irradiation of the TLD in kV x-rays and $^{60}$Co gamma-rays was 5 cm. We used energy cut-off variance reduction technique in this simulation. Electron and photon transport were terminated at 10 keV and 1 keV, respectively. The photons were assumed to be perpendicularly incident on the flat surface of the chip. Non-divergent beam and field size of 6cm×8 cm were applied to simulate the experimental method. The recent publishing photon beam spectra for theratron 780 E cobalt machine was also used as input. Kilovoltage spectra was taken from results of our previous investigation.

The mean energies simulation shown in the table 1 were calculated from the expression:

$$E_{mean} = \left( \frac{1}{n} \sum_{i=1}^{n} \phi(E_i) E_i \Delta E_i \right) \left( \frac{1}{n} \sum_{i=1}^{n} \phi(E_i) \Delta E_i \right)^{-1}$$  \hspace{1cm} (8)
where $E_i$ is the phantom energy and $\phi(E_i)$ is the number of photons in the energy bin of width $\Delta E_i$ at phantom surface.

The uncertainty was estimated by dividing the calculations into ten batches as well as calculating the variance on the mean. Each simulation was terminated when the uncertainty reached to lower than %1 and for this it needed between $3 \times 10^7$ to $2 \times 10^8$ x-ray photons.

| (Applied Kilovoltage) | (HVL) | Mean energy (MCNP) |
|-----------------------|-------|--------------------|
| 120 kVp               | 0.2 mm Cu | 58 keV            |
| 180 kVp               | 0.5 mm Cu | 74 keV            |
| 200 kVp               | 1.0 mm Cu | 88.6 keV          |
| 250 kVp               | 2.0 mm Cu | 114.5 keV         |
| 300 kVp               | 3.2 mm Cu | 140.2 keV         |
| 1.25MeV (average Co-60 energy) | 1.1 mm Pb | 1.08 MeV |

Table 1. Specifications of X or $\gamma$-ray beams that were used for measurements and calculations in this research

4. Results

The calibrated siemens stabilipan II superficial/orthovoltage therapy unit was used to irradiation TLDs with kilovoltage therapy beams as shown in Table 1. Table 2 shows the calibration factor values of the TLD’s which obtained as explained in method section.

| Photon specifications | Calibration factor (cGy/ Count) |
|-----------------------|--------------------------------|
| Qualities             | HVL                            |
| 120 kVp               | 0.2 mm Cu                      | 0.00718 |
| 180 kVp               | 0.5 mm Cu                      | 0.00740 |
| 200 kVp               | 1.0 mm Cu                      | 0.00795 |
| 250 kVp               | 2.0 mm Cu                      | 0.00862 |
| 300 kVp               | 3.2 mm Cu                      | 0.00894 |
| 1.25MV (Co-60)        | 1.1 mm Pb                      | 0.00923 |

Table 2. Calibration factors of different x-ray qualities were tabulated

Table 3 demonstrates the experimental quality dependence factor of different x-ray qualities and $^{60}$Co gamma rays. The data in Table 3 shows the experimental quality dependence factors of TLD at different beam qualities and $^{60}$Co gamma rays.

The data in Table 3 shows the experimental quality dependence factors of TLD at different beam qualities. Calculating the absorbed dose to water for different test beams based on the $^{60}$Co calibration factor shows some deviations in comparison to the related beam calibration factor. Table 4 shows the deviation between calculated absorbed dose to water based on $^{60}$Co calibration factor. Maximum deviation observed in the 120 kVp irradiation field.
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Table 3. Experimental quality dependence factors and their respective energy correction factors against Co-60 calibration factor were tabulated.

| Beam quality | HVL   | Quality dependence factor | Correction dependence factor |
|--------------|-------|---------------------------|----------------------------|
| 120 kVp      | 0.2 mm Cu | 1.28                      | 0.70                       |
| 180 kVp      | 0.5 mm Cu | 1.24                      | 0.80                       |
| 200 kVp      | 1.0 mm Cu | 1.16                      | 0.86                       |
| 250 kVp      | 2.0 mm Cu | 1.07                      | 0.93                       |
| 300 kVp      | 2.5 mm Cu | 1.03                      | 0.97                       |
| 1250keV      | 1.1mm Pb | 1                         | 1                          |

Table 4. The mean ± SD of error absorbed dose to water reading of TLDs at different beam qualities when they are calibrated with the energy of Co-60 (p<0.02).

| Qualities | HVL   | Mean diff.(%) | Standard deviation |
|-----------|-------|---------------|--------------------|
| 120 kVp   | 0.2 mm Cu | 19.9          | 2.1                |
| 180 kVp   | 0.5 mm Cu | 13.78         | 4                  |
| 200 kVp   | 1.0 mm Cu | 8.46          | 3.51               |
| 250 kVp   | 2.0 mm Cu | 3.60          | 2.64               |
| 300 kVp   | 2.5 mm Cu | 1.25          | 1.14               |
| 1250keV   | 1.1mm Pb | -             | -                  |

For calculation of Monte Carlo quality dependence factor, we obtained the ratio of absorbed dose in water and LiF (cavity) \( \left( \frac{D_W}{D_{LiF}} \right) \). Figure 1 shows the changes of the mass energy - absorption coefficient ratio and the Monte Carlo calculated dose ratio of water to LiF from 120 kVp to 1250 keV x-ray beams. It shows that experimental calibration factor varies as Monte Carlo calibration factor \( \left( \frac{D_W}{D_{LiF}} \right) \) changes.

![Fig. 1. TLD-100 in kV x-ray beams and \(^{60}\text{Co} \) gamma rays: comparison of the Monte Carlo derived dose ratio, water to LiF, with the mass energy - absorption coefficient ratios, as a function of the maximum tube voltage in kV beams and \(^{60}\text{Co} \) gamma rays.](image)

The low and medium energy radiation of orthovoltage and superficial Siemens stabilipan were simulated by Monte Carlo calculation. The ratio of absorbed dose scored in water and LiF TLD \( \left( \frac{D_W}{D_{LiF}} \right) \) was calculated by Monte Carlo method. We also obtained the
theoretical prediction of the \( \frac{D_{WW}}{D_{LiF}} \) by the definition of cavity theory for LiF TLDs. Table 5 shows the different values of \( \frac{D_{WW}}{D_{LiF}} \) obtained from Monte Carlo calculation and theoretical prediction by means of cavity theory for different beam qualities.

| Qualities | HVL        | \( \frac{D_{WW}}{D_{LiF}} \) (Monte Carlo) | \( \frac{D_{WW}}{D_{LiF}} \) (Cavity theory) |
|-----------|------------|-------------------------------------------|-------------------------------------------|
| 120 kVp   | 0.2 mm Cu  | 0.91                                      | 0.97                                      |
| 180 kVp   | 0.5 mm Cu  | 1.00                                      | 1.05                                      |
| 200 kVp   | 1.0 mm Cu  | 1.05                                      | 1.09                                      |
| 250 kVp   | 2.0 mm Cu  | 1.13                                      | 1.15                                      |
| 300 kVp   | 2.5 mm Cu  | 1.16                                      | 1.17                                      |
| 1250keV   | 1.1mm Pb   | 1.196                                     | 1.20                                      |

Table 5. The ratio of absorbed dose in water and LiF TLDs by monte carlo calculation and prediction of cavity theory were shown.

In Table 6 the results of quality dependence factor obtained from Monte Carlo calculation, experimental study and cavity theory method were shown. The differences between experimental and mcnp values were also obtained. It was illustrated that calculated values of quality dependence factor by Monte Carlo and cavity theory predictions are more comparable at higher mean energies.

| Qualities | Quality dependence factor | Quality dependence factor (Monte Carlo) | Diff.(%) | Quality dependence factor (Cavity theory) |
|-----------|----------------------------|----------------------------------------|----------|----------------------------------------|
| 120 kVp   | 1.28                       | 1.134                                  | -11.41   | 1.237                                  |
| 180 kVp   | 1.24                       | 1.196                                  | +58.06   | 1.142                                  |
| 200 kVp   | 1.16                       | 1.139                                  | -1.81    | 1.100                                  |
| 250 kVp   | 1.07                       | 1.052                                  | -1.68    | 1.043                                  |
| 300 kVp   | 1.03                       | 1.034                                  | +0.04    | 1.018                                  |
| 1250keV   | 1                          | 1                                      | 0.00     | 1                                      |

Table 6. Value of quality dependence factors obtained by measurement, Monte Carlo calculation and cavity theory were shown. Percent of differences between measured values of quality factors and mcnp calculated factors were also tabulated.

5. Discussion

The precision in TL dosimetry is very critical when the quality of radiations are to be considered. It is generally accepted that ±5% uncertainty in dose delivery to the target volume can be considered as a safe limit causing no severe radiotherapy treatment consequences [11]. The quality dependence factor is necessary if LiF TLDs are calibrated using a \( ^{60}Co \) photon beam but are used in lower or higher energy photon beams. In dosimetry it is frequently assumed that the quality dependence of thermonuminescence LiF:Mg,Ti detectors such as TLD-100, follows the ratio of the energy absorption coefficient.
for the LiF and water. It has been shown by Mobit et al (1998), that the quality dependence factor for LiF-TLD in kilovoltage x-rays relative to $^{60}$Co gamma-rays ranges from 1.36 for 50 kV x-rays to 1.03 for 300 kV which are comparable with our results [10]. Kearfott et al (1990) observed an quality dependence factor of LiF TL ribbon from 1.045 (50 keV) to 1.353 (100 keV) [12]. Study of Kron et al (1998) has also shown the quality dependence factor of 1.47 at 27 keV from synchrotron radiation [4]. Esteban et al (2003) reported results from experimental and cavity theory studies of LiF TLD in 20-29 photon beams, where the measured value of correction factor (approximately 0.78) are more comparable to the value determined from cavity theory for the effective energies of 25 keV and 29 keV [13].

We experimentally obtained the absorbed dose calibration factor (CF) for x-ray range of 120 to 1250 keV. The calibration factor varies from 0.00718 to 0.00923 cGy/Count for 120 kVp-1250 keV and quality dependence factor were in the range of 1.00 to 1.28 for Co-60 to 120 kVp x-rays respectively (Table 3). It shows that quality dependence factor decreases with increasing the beam energy and it reaches to the normalized one (in this case to the CF of Co-60). This is an important points for dosimetry out of primary radiation field. TLDs are used for dosimetry of scattered radiations and in such cases the calibration factor quality dependency may be a major consideration.

Finding dose ratio of water to LiF ($D_{W}/D_{LiF}$) and the mass energy absorption coefficient ratio, more comparable with increasing mean energy. This is reasonable because with increasing energy added filtration also increased and low energy portion of the spectrum is filtered out so that values of ($D_{W}/D_{LiF}$) obtained by two methods are more comparable. Same phenomenon was experienced by Esteban et al for LiF-TLD [13]. Quality dependence factors obtained from Monte Carlo method are in good agreement with experimental method except for 180 kVp and to a lesser degree for 120 kVp. The difference between quality factors at 180 kVp is about 3.5% which may be due to more exposure rate beam quality so that made its control more difficult. There is a significant difference of quality dependence factors between cavity theory and Monte Carlo quality dependence factors. As shown this difference decrease with increasing beam filtration. The same effect was also reported by Esteban et al (2003) that may be explained by attenuation of low energy photons [13].

Modelling the calibration factor of detectors can be used to predict the quality dependence factor. This model is to provide a tool for evaluation and not a physical explanation for the calibration factor. The energy model decrease with decreasing energy. The change of calibration factor with energy followed the equation:

$$\text{CF} = B_0 + B_1 E + B_2 E^2 + B_3 E^3$$  \hspace{1cm} (9)

Where CF and E are calibration factor and energy (in keV), respectively. $B_0$, $B_1$, $B_2$ and $B_3$ are 0.0058, 1.8E-5, 1.3E-8 and 1.2E-1. Equation 9 was fitted to the changes of calibration factors for different beam qualities.

Low energy x-rays are the major part of the scattered radiations which may arise partly from the primary irradiation field and partly from the any scatterer medium in the path of the primary beam. Using the data of the curve over the low energy range based on the equation 9 can lead to the more precise results in TL dosimetry. Our finding also showed significant difference between dose values when TLDs are calibrated at Co-60 beam. The greatest difference was equal to $19.9 \pm 2.1\%$ for beam quality of 120 kVp.
6. Conclusions

In conclusion, our study showed that the quality dependence of TLDs should be considered if LiF is calibrated in different beam quality than really wanted to be used. Dosimetry of non-primary radiation fields need more attention because of wide range of low energy photons contribution to dose formation. Obtaining a dose response curve may be helpful to calculate the calibration factor with more precision. The simplest way is to calibrate the chips against an ionization chamber using the beam quality that is to be used for the measurement.

7. References

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