Monte Carlo simulation studies on scintillation detectors and image reconstruction of brain-phantom tumors in TOFPET

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ABSTRACT

This study presents Monte Carlo Simulation (MCS) results of detection efficiencies, spatial resolutions and resolving powers of a time-of-flight (TOF) PET detector systems. Cerium activated Lutetium Oxyorthosilicate (Lu2SiO5: Ce in short LSO), Barium Fluoride (BaF2) and BriLanCe 380 (Cerium doped Lanthanum tri-Bromide, in short LaBr3) scintillation crystals are studied in view of their good time and energy resolutions and shorter decay times. The results of MCS based on GEANT show that spatial resolution, detection efficiency and resolving power of LSO are better than those of BaF2 and LaBr3, although it possesses inferior time and energy resolutions. Instead of the conventional position reconstruction method, newly established image reconstruction (talked about in the previous work) method is applied to produce high-tech images. Validation is a momentous step to ensure that this imaging method fulfills all purposes of motivation discussed by reconstructing images of two tumors in a brain phantom.

Key words: GEANT, Monte Carlo, phantom, PV method, scintillators, TOFPET

Introduction

The Department of Atomic Energy (DAE) of India is going to establish its first Medical Cyclotron Facility (MCF) in Kolkata with other existing facilities. It was scheduled to be commissioned by the end of 2008. MCF will primarily be used for the production of radioisotopes for symptom imaging in Single Photon Emission Tomography (SPECT) and in Positron Emission Tomography (PET), besides applications in other front line research. PET is a powerful metabolic imaging technique potentially used in small size brain tumor identification. The best radiopharmaceutical [18F]-fluorodeoxyglucose (FDG) is widely used in clinical oncology as a positron (e+, an antiparticle of e-) emitter which concedes of high quality images. Our objective is to design a sophisticated time-of-flight positron emission tomography (TOFPET) gamma camera to utilize one of the on-time shared beam lines for innovative research. In TOFPET, “position vector (PV)”, an image reconstruction method is applied where both energy and time of collinear γ-rays are taken into account. Those γ-rays are produced due to e+e− annihilation. The working principle of PV method is described in section 3 and can also be found elsewhere and references there in.

Monte Carlo Simulation (MCS) plays a vital role in designing the TOFPET system and modeling the image of a diagnostic object as many other branches of science. The MCS of TOFPET is executed with the aid of GEANT3.21. The main interests of MCS are: (i) crucial role played by GEANT3.21 in TOFPET, (ii) reconstruction of image of the diagnostic object using the newly established PV method instead of conventional image processing techniques, (iii) detection efficiencies and blurring effect in the presence of a brain phantom and (iv) validation of the PV method.

Phantom is a material that has physical properties similar to biological tissues and the human body. Biological tissue equivalent phantom was developed by Ito et al, in Chiba University, Japan which can be classified into two major categories: the high water content tissue such as muscle, brain and internal organs and low water content tissue such as fat and bone. Energy and time resolutions of Cerium-activated Lutetium Oxyorthosilicate (LSO), Cerium doped Yttrium Aluminum Perovskite (YAP), BriLanCe
213 (Cerium doped Lanthanum tri-Bromide, LaBr₃⁴) and Barium Fluoride (BaF₂⁵) have already been studied for different applications considering their good time and energy resolutions, γ-ray stopping powers, shorter decay times etc. However, systematic studies and comparison among LSO, LaBr₃ and BaF₂ are not yet accomplished for the purposes of TOFPET.

In this study a real TOFPET system with 48 LSO scintillation detector (each size is (3σ×3 cm³) and ring diameter of 80 cm is exhibited as proposed by earlier studies. Two close contact tumors are imaged by the PV method utilizing a tissue equivalent brain phantom conveying its validation.

**TOFPET Resolution**

A few definitions are given below. These are particularly creditable for subsequent discussions in characterizing TOFPET.

**Energy Resolution**

The energy resolution (ER) of a radiation detector emphasizes the precision with which the system can measure the energy of incident photons. In scintillation detectors the ER is a function of the relative light output of the scintillator and other associate electronics. ER is directly proportional to ΔE. To attain good image contrast it is essential to have better ER and this can be achieved by reducing the background and scattered events. Also fine tuning of detector, data acquisition system and data analysis techniques are required.

**Time Resolution**

The time resolution (TR) of a TOFPET is one of the crucial parameters for image reconstruction with least blurring effects (an effect dominated by random and scattered events). The full width at half maximum (fwhm) of a TOF distribution is often used as a measure of the overall timing uncertainty and is called the time resolution. However, the use of very fast scintillators such as CsF allows one to have a TR ≈ 400 ps⁶ and or BaF₂ ≈ 120 ps⁵.

**Spatial Resolution and Resolving power**

Spatial resolution (SR) or more accurately the resolving power (RP) is the other important parameter in TOFPET system. RP is the ability of the components of TOFPET to measure the minimum resolvable distance between distinguishable objects in an image. It determines the quality of the image, and depends on the image reconstruction, data analysis and data acquisition processes. The measurement technique of SR can be found elsewhere. RP can be expressed in the following form:

\[ \text{RP} = \left( \frac{\Delta \sigma}{\sigma_{or}} \right) \times 100\% \]  

Where, \( \sigma \) is the standard deviation of Gaussian distribution, \( \Delta \sigma \) = Average \( \sigma \) of reconstructed positions - average \( \sigma \) of original positions, and \( \sigma_{or} \) = average \( \sigma \) of the original positions. RP attributes the blurring effect of a reconstructed image and its brief discussions are available in the results section.

**Design of TOFPET**

The detection of two collinear photons depends upon the properties and geometry of the detectors. The type of detector chosen (scintillator as well as photomultiplier tube (PMT)) is a major part of the design of a TOFPET camera.

**Choice of Scintillation Crystals**

A thorough investigation over commercially available scintillators is necessary for achieving better TR, RP and detection efficiency. Recently a renewed interest in TOFPET was generated based on the fast decay time and better TR and SR of new type of scintillators, e.g., Lu₂SiO₅:Ce⁷ and LaBr₃:Ce, which offer high sensitivity, low dead time and a good time and energy resolutions. These lead to the reduction of random count rate (\( R_{nd2} = \frac{2N_{d1}N_{d2}}{N_{d2}} \), between two detectors) and scatter contribution.⁸

**Monte Carlo simulation of TOFPET**

**Array of detectors**

An extensive MCS study based on GEANT3.21 has been carried out to evaluate the design of a TOFPET. From among the commercially available scintillators, LSO of size 3φ×3 cm³ is optimized. A typical spectrum of TOFPET system is shown in Figure 1. There are 48 detectors in a single ring and face-to-face distance of each pair is 80 cm (diameter of the ring). A thin Al (0.1 cm) and a thick Pb (2 cm) shields are used outside the scintillator in order to reflect scintillation light and to stop Compton scattered γ-rays and natural backgrounds. An Al (3φ×0.1 cm³) disk is also used in front of the scintillator to prevent radiation

![Figure 1: A TOFPET spectrum is illustrated. It is obtained by MCS based on GEANT3.21. A brain-phantom is located at the center of the camera](image-url)
damage. Detectors are placed on the x-y plane perpendicular to the z-axis which is the direction of a patient movement. $E_n$ and $T_n$ are taken into account in the MCS.

The MCS can provide us not only the unique information of Compton scattered and full energy deposit of incident 511 keV γ-rays in the scintillator, but also the timing information. Therefore, image reconstruction of $e^+e^-$ annihilation points by selecting those true events and utilizing the Energy-Time (E-T) correlation[9] are very convenient. A high resolution brain PET scanner (G-PET) was developed by Karp et al.[10]

Table 1 comparisons among the various models of PET are shown.

**Brain Phantom and Positron Source**

Let us assume that a patient has been suffering from two brain tumors closely located and those are depicted in Figure 2. The aim of this study is to model a simplest physical tissue equivalent brain phantom and validate the PV image reconstruction method. The model should be anatomically accurate and realistic to have greater impact than simply-shaped phantoms. The model should be completely 3D to be essentially realistic.

The assumptions taken into account in the MCS based on GEANT3.21 are as follows:

i. One $e^+e^-$ annihilation event produces two collinear 511 keV photons. Those events are generated uniformly in $4\pi$ Gaussian distribution.

ii. Principal constituents of human head are: Skull, Brain and Water.

iii. Molecular Formula (MF) of human skull is $C_{20}H_{22}N_8O_5$. Assuming a 70 kg adult patient, volume of spherical skull (3D) is determined to be 234.99 cm$^3$ and density 10.3 g/cm$^3$.

iv. DNA (molecular weight (Mwt): 475.299 g/mol and MF: $C_{15}H_{26}O_{13}P_2$) and RNA (Mwt: 603.277 g/mol and MF: $C_{15}H_{26}O_{19}P_3$) are the main constituents of human brain and density of an adult brain is calculated to be 0.621 g/cm$^3$ (person to person it may vary). RNA and DNA are uniformly distributed in mass proportion inside the spherical skull.

v. A typical dose of FDG used in an oncological scan is 200 - 400 MBq for an adult human and very useful for brain tumor identification. Biochemical processes can be traced precisely and a patient can be diagnosed several times in a day due to its shorter half-life. The decay scheme of $^{18}$F and structural formula of FDG are given in Figure 3.

vi. The molecular mass of $C_6H_11FO_5$ is 182.15 g/mol and its density in the tumor site is 7.00 g/cm$^3$ and Poissionian distribution of $e^+$.

### PV Image Reconstruction Method in TOFPET

Instead of the conventional most likely position method[12] the PV method is applied for the image reconstruction. It is a new method of position reconstruction in TOFPET described elsewhere.[2] Position conversion factors (useful for reinstatement of $e^+e^-$ annihilation points) of this TOFPET system are determined (these values differ from system to system). General notions of image reconstruction equations in two dimensions (2D) are:[2]

\[
X = \sum_{i=1}^{n/2} [\cos(i-1)\theta - T_{i+1/2}\sin(i-1)\theta] x C / 2 / c] / (2m) \tag{2}
\]

and

\[
Y = \sum_{i=1}^{n/2} [\sin(i-1)\theta - T_{i+1/2}\cos(i-1)\theta] x C / 2 / c] / (2m) \tag{3}
\]

Table 1: Comparison among the various models

| Properties                      | G-PET | PET Simens/CTI | Mondal TOFPET |
|---------------------------------|-------|---------------|---------------|
| Ring diameter [cm]              | 42    | 82            | 80            |
| Number of ring(s)               | 8     | 24            | 1             |
| Number of detectors per ring    | 36    | 784           | 48            |
| Crystal dimension [cm$^3$]      | 0.4x0.4x1 | 0.29x0.59x3   | 3x3           |
| Type of Crystal                 | GSO   | BGO           | LSO           |
| Spatial resolution [cm]         | 0.4   | 0.4           | <1            |
| Time resolution [ps]            | ---   | ---           | 886           |

![Figure 2: Drawing of a human brain with positions of two tumors](image)

![Figure 3: Decay scheme of $^{18}$F (a), and molecular formula of FDG ($C_2H_2F_6$) (b).[11]](image)
Where, $T_i$ and $T_{i+\Delta t}$: TOF of collinear photons, $\theta = 2\pi/n$: angle between the neighboring detectors, $n$: even number of detectors (here $n=48$, see figure 1), $C$: speed of light, $c$ and $m$ respectively are intercept and slope of the fitted line of the spectrum where reconstructed versus real positions are plotted.

**Results and Discussion**

**Spatial Resolution and Detection Efficiency**

To procure realistic MCS, the simulated energy distribution of 511 keV photons was considered Gaussian. Time and energy resolutions of different scintillators incorporated in this study are shown in table 2. Equal number of annihilation events ($1 \times 10^6$) are generated in each case. $S_R$s with statistical errors (estimated from the fitting parameters) along the x-axis and detection efficiencies ($D_e$) of each scintillator are estimated without TOF window and brain phantom settings. Those results are shown respectively in columns 4 and 5 in table 2 and outcomes are obtained considering the point source distribution of $e^+e^-$ and from the detected 511 keV events in coincidence.

Similarly the effect of TOF window setting (1 ns) on $D_e$s and $S_R$s of different scintillators can be noted easily from the Table 3 where similar $T_R$ and $E_R$ of table 2 are applied and coincidence events are selected using the energy-time (E-T) correlation $^{[9]}$ (cut of energy conservation: $950 \leq (E_1 + E_2) \leq 1050$ keV and lower energy cut of $\gamma$-rays is 10 keV).

It can be perceived from Tables 2 and 3 that $D_e$s and $S_R$s respectively are decreased and improved about three times. Although $T_R$ and $E_R$ of LSO are inferior and the $S_R$s are changed significantly among the scintillators of the same order but $D_e$s of LSO increased about five and three times than those of LaBr$_3$ and BaF$_2$ respectively. The orders remain almost the same when time window is considered. There seems to be better execution in LSO due to its excellent photon yield (32 photons/keV) and best stopping power of $\gamma$-rays (because of the highest atomic density, 7.4 g/cm$^3$). The number of detectors may be increased by adding more rings on both sides of the present TOFPET system [Figure 1] for the improvement of $D_e$. It is also observed that coincidence $D_e$s increases 8–10 times by increasing the crystal size from $19 \times 3 \times 3$ cm$^3$ to $39 \times 3 \times 3$ cm$^3$. At the same time, $S_R$s degrades about three times. Results of MCS infer that E-T correlation technique is an essential tool for the improvement of $S_R$ as well as $R_P$. The timing uncertainty of a TOFPET detector preludes blurring effects in the image reconstruction process of X and Y.

**Determination of $R_p$ in TOFPET**

To determine $R_p$ and observe image resolution of this system in one dimension, let us assume two identical sources of $e^+$ which are sitting 4 cm ($2,0,0$ and $-2,0,0$) apart from each other. Annihilation positions along the X-axis are reconstructed by using equation (2). A typical image is depicted in Figure 4.

The data is fitted with two Gaussians and convoluted using the fitting parameters after normalizing with the real spectra. Face-to-face long distance among the detectors and a few time windows make it possible to run down the blurring effects. $R_p$s of different scintillators of this TOFPET system are determined by equation (1) and results are arranged in column 5 of Table 4. $R_p$s of LSO attributes less blurring effects than those of other two.

**Validation of PV Method**

One of the usages of validation is that it is a process of

![Figure 4: (a) Reconstructed position distribution, (b) Convoluted and real (smaller sigma) position distributions](image)

**Table 2: Comparisons of Scintillators without Setting Time Window**

| Name of Scintillators | $T_R$ (ps) | $E_R$ (at 511 keV) | $S_R\pm$ error along x-axis (cm) | $D_e$ (%) |
|-----------------------|------------|-------------------|----------------------------------|---------|
| LSO(3x3x3 cm$^3$)    | 886 [4]    | 9.1%              | 3.63±0.08                        | 0.65    |
| LaBr$_3$(3x3x3 cm$^3$)| 576 [4]    | 3.9%              | 4.59±0.33                        | 0.15    |
| BaF$_2$(3x3x3 cm$^3$) | 120 [5]    | 4.3%              | 3.07±0.10                        | 0.20    |

**Table 3: Comparisons of Scintillators with Setting of Time Window**

| Name of Scintillators | Generated events | Coincidence 511 keV | $S_R\pm$ error along x-axis (cm) | $D_e$ (%) |
|-----------------------|------------------|---------------------|----------------------------------|---------|
| LSO(3x3x3 cm$^3$)    | $1\times 10^6$   | 2012                | 1.32±0.02                        | 0.201   |
| LaBr$_3$(3x3x3 cm$^3$)| $1\times 10^6$   | 405                 | 1.45±0.06                        | 0.041   |
| BaF$_2$(3x3x3 cm$^3$) | $1\times 10^6$   | 647                 | 1.35±0.04                        | 0.065   |

**Table 4: Resolving Power of Different Scintillators in TOFPET**

| Name of Scintillators | $\sigma_{tumor}$ of tumor, x-axis (cm) | $\sigma_{tumor}$ of tumor, x-axis (cm) | Difference of $\sigma$ (cm) (%) |
|-----------------------|-----------------------------------------|----------------------------------------|--------------------------------|
| LSO(3x3x3 cm$^3$)    | 0.567075                                 | 0.163874                               | 0.4033201 2.46                  |
| LaBr$_3$(3x3x3 cm$^3$)| 0.798145                                 | 0.164270                               | 0.633875 3.86                     |
| BaF$_2$(3x3x3 cm$^3$) | 0.654930                                 | 0.164270                               | 0.490660 3.00                     |
checking if something satisfies a certain criterion. In order to understand the validation of PV method [Figure 1] in 2D, two identical tumors at (2,-2,0 and -2,2,0) are considered in a brain phantom (stated before) and MCS is performed with backgrounds. Using equations (2) and (3) 2D images of those tumors are reconstructed and those are depicted in Figure 5. Reconstructed scattered (a) and its surface (c) plots show how cleanly backgrounds are suppressed by the PV method. Their original 2D scattered and corresponding surface plots [Figure 2] are shown respectively in spectra (b) and (d).

Detection efficiencies of TOFPET system in presence of a brain phantom with FDG and in absence of them are 0.11% and 0.65% respectively in the case of LSO. Blurring effect increases slightly. Results attribute that $\gamma$-rays are absorbed, scattered in different directions and attenuated in the presence of brain phantom. Perhaps the differences in results will increase when positron implantation depth, ortho-positronium and para-positronium formation effects are taken into account (none of this effects are considered here), but quality of the image might be improved. It would be very interesting if phantom model could be compared with a real data. In this method, position conversion factors are important ingredients for positioning the reconstructed position very close to its original. PV is an on-line image reconstruction method and requires a few minutes and MBq source for data acquisition, and image processing with a few Mb memories.

**Conclusion**

A 2D image reconstruction of tumors in a brain phantom, performed by MCS, validates the PV method. Detection efficiencies, spatial resolutions and resolving powers of LSO, BaF$_2$, and LaBr$_3$ scintillators are verified. In every aspect LSÚ shows better performance than the other two. Proper setting of time window improves spatial resolution and resolves powers significantly. It is important to achieve better energy and time resolution of scintillation detectors to confine real number of coincidence events which has less blurring effects on the image. It may be concluded that the excellent performance of PV method shows its beauty over any conventional iterative image reconstruction technique by saving huge computational time and memory.

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