ACCURATE MODELING OF NUCLEAR-MEDICINE COLLIMATORS IN MONTE CARLO SIMULATION OF HIGH ENERGY PHOTONS

Scott J. Wilderman[1], Y. Dewaraja[2], and K.F. Koral[2]
[1]Dept of Nuclear Engineering and Radiologic Sciences
[2]Div. of Nuclear Medicine
University of Michigan

Abstract

Monte Carlo (MC) simulation of nuclear medicine imaging is more difficult for procedures employing ^{131}I than for those using ^{99m}Tc because penetration of the collimators by gammas emitted above the 364 keV photo peak (637 keV (6.5%) and 723 keV (1.7%)) must be considered. An accurate model of the imaging camera must include both scattering in the patient and transport in the collimator, a computationally intensive task. Most MC codes used in nuclear medicine either employ severe approximations of the collimator interactions or have not been extended to higher energies or to arbitrarily shaped collimator holes. The MC program SKEPTIC, which has previously been used to simulate slit aperture penetration of 511 keV gammas, has been modified to permit modeling of parallel hole collimators. We present here a comparison of measured and simulated detected energy spectra for ^{131}I for a hexagonal hole collimator, focusing on the spectra near the 364 keV photo peak. A point source 19 cm from the face of the collimator was modeled, and spectra were determined for both the full field of view and a limited region of interest near the source location.

I. Introduction

Quantification of ^{131}I emission may be carried out both by conjugate view imaging [1], and [2], and by SPECT [3], [4]. The latter is the preferred method when imaging tumors in the presence of significant activity in overlying tissue and for separating large, unresolved tumors into individual ones. Quantification is more difficult for studies employing ^{131}I than for those using more common nuclear medicine isotopes such as ^{99m}Tc due to the higher energy of the photo peak (364 keV) and the multiple gamma-ray emissions. The 637 and 722 keV photons are low in intensity but contribute significantly to the image, as these photons have relatively low attenuation in the patient and a higher probability of penetrating collimators which are optimized for 364 keV.

A Monte Carlo code capable of simulating ^{131}I imaging would be a powerful tool for investigating imaging characteristics and limitations of SPECT. Monte Carlo codes typically used in nuclear medicine do not model collimator scatter and penetration and photons entering the septa are assumed to be absorbed. This is a reasonable assumption for ^{99m}Tc since at 140 keV septal penetration in a standard low energy collimator is $<< 5\%$. For ^{131}I, modeling transport in the collimator is essential due to the higher penetration probability of both the 364 keV and higher energy gamma-rays. The significance of these interactions is demonstrated by our preliminary simulation results which predict that for a point source in air 52% - 55% of photons in a 20% photo peak at 364 keV have either penetrated or scattered in the collimator.

Literature on the simulation of ^{131}I collimator penetration is sparse. Bice has presented simulated results of the magnitude of collimator penetration and scatter when imaging a point source of ^{131}I in air [5]. The SimSPECT package (based on the Los Alamos code MCNP) developed by Yanch and Dobrzeniecki models the collimator in its physical entirety, and limited tests on its performance for ^{99m}Tc have been presented [6]. However, results of simulations of higher energy gamma-rays have not yet been reported. DeVries [7] has reported calculations of point spread functions taken over a 20% ^{123}I window (159 keV) for ^{51}Cr (320 keV) and ^{85}Sr (514 keV). They report good agreement with measurement for modeling the low energy point spread function, but do not present data on the higher energy parts of the absorbed energy spectra. We present below new work on modeling collimators for ^{131}I imaging.

II. Methods

The Monte Carlo program SKEPTIC [8] has been modified to model penetration of parallel hole collimators for ^{131}I imaging. SKEPTIC has been employed and tested extensively in numerous medical imaging applications [9], [10], including simulation of Compton scatter cameras [11], [12], [13], [14]

The program employs a cross section data set similar to that used in TIGER, the photon simulation programs developed and supported by Los Alamos National Laboratories [15]. Photoelectric cross sections are treated on a subshell by subshell basis through 10 eV or the N shell (which is averaged) whichever is lower in energy, using the expanded parameterization of Biggs and Lighthill [16]. Carter and Cashwell [17] have suggested that the total photoelectric cross section can be resolved into individual subshell cross sections by assuming that the ratio between the cross sections for the n^{th} and $n^{th}+1$ levels is constant at all energies greater than E_n and is given by their ratio at E_n, and this scheme is employed throughout the entire energy range. Compton scattering is treated using a modification of the standard Klein-Nishina formula, taking into account the population of electrons in the atom and the probability that the electron will be ejected after having absorbed the photon momentum. This is done by multiplying σ_{KN} by the incoherent scattering function $S(Z,q)$, where q is related to the momentum transfer and is given by $q = 2\pi\sin(\theta/2)/\lambdabar$ if $\lambdabar$ is the reduced photon wavelength. Form factors for this work are taken from Hubbell *et al*[18]. Coherent scattering, here meant to include only elastic (Rayleigh) scattering from the bound atomic electrons is also treated, and the cross section is given as the classically derived Thomson formula for the elastic scattering of a photon by a particle at rest times the square of the atomic form factor $F(Z,q)$. The form factors, like the scattering functions, are taken from tabulated data of Hubbell *et al*. Characteristic x-rays are generated (and subsequently tracked) on a subshell basis also, with all transitions from M shell inward treated explicitly, subject to the condition that the emitted x-ray have energy greater than the code cut-off (generally set to 1 keV). Data for the possible de-excitation transitions (energies and probabilities) is derived from that presented by Halbleib and Morel [19] and used in the P-codes (extended relaxation) of the ITS series. Doppler broadening of the Compton scattered gamma spectrum, which has recently been found to be a limiting factor in the resolution performance of Compton cameras [20], is modeled using the tabulated data of Biggs [21].

SKEPTIC was originally designed for modeling the transport of low energy electrons on an event by event basis on vector supercomputers. As that problem is always CPU limited, SKEPTIC was optimized for speed. It employs exclusively fast sampling schemes applied to pre-calculated and tabulated cross section and distribution data, and has two geometry tracking versions(one for exclusively rectangular problems, and one for general quadratic surfaces), both of which take advantage of regularities in system geometry to preclude computationally expensive cell searches after boundary crossings.

III. Results and Discussion

The performance of SKEPTIC for ^{131}I simulation was tested by comparison with experimental data obtained using a Picker Prism XP3000 3-headed SPECT camera with high energy general purpose parallel hole (HEGAPP) collimators. Energy spectra for the entire field of view (FOV) and a specific 3x3 pixel ROI were generated utilizing the prototype Picker multi-window acquisition software. Thirty two adjacent windows of 5.1 keV width were used in four acquisitions to cover the energy range 283 - 442 keV. A point source (6 mm diameter filter-paper punch soaked with 200 mCi of ^{131}I solution) was placed at a distance of 19.2 cm from the collimator face of one of the heads. At the source was secured using a Styrofoam tower and hence can be considered to be in air. Acquisitions were performed both with the source and then with no source to generate the background spectrum which was subtracted from the source spectrum. Acquisitions were planar and the grid size was 128x128. Each source acquisition was 15 min while the background was acquired over 4 hours.

Three basic measurements were both performed and simulated:

- radial profile for a 6 mm disk source at 19 cm
- Full field of view (FOV) energy spectrum for various size disk sources at 6 cm
- Energy spectra for a 3x3 pixel region of interest (ROI), taken near the disk source location distances

The collimator was modeled as a square hole collimator, as proposed by DeVries [7]. DeVries suggested that the dimensions of the simulated collimator be chosen by fixing the lead septa thickness, and adjusting the area of the hole to retain a constant lead to hole area ratio. Such a geometry should preserve the radially averaged thickness of lead traversed by photons passing though the collimator, and so correctly model the scatter and penetration components of the detected spectra. DeVries notes that the area of the simulated square holes is, however, 15% greater than the hexagonal hole area, leading to an overestimation of geometric component of the spectra in the pixels near the source. Conversely, choosing the dimensions of the simulated collimator by fixing the area of the hole and lead septa thickness provides accurate modeling of the geometric component of the transmitted gammas, but underestimates the penetration component, as the model contains more lead per area than the actual collimator. A third possibility lies in modeling the collimator by fixing the hole area and the lead to hole area ratio, and adjusting both the hole dimension and lead septa thickness accordingly. All three schemes have been explored here. While the magnitudes of the geometric and the penetration and scatter components determined for the schemes varied as expected (see table 1), the choice of model was found to have almost no impact on the shape of radial point spread functions or energy spectra.

Geometry Model	Total γ's	Penetration & Scatter	Geometry
Fixed Hole, Septa	19596	10303	9293
Fixed Area Ratio, Septa	22253	11803	10450
Fixed Area Ratio, Hole	20560	11241	9319

Table 1
Number of counted gammas in 20% window at 364 keV, (50M initial particles)

Finite energy resolution in the NaI was simulated by applying a Gaussian blur to the calculated energy deposition for each particle, with an energy dependent $FWHM$ given by

$$FWHM = 2.6132 \times E^{0.4414},$$

where the constants were determined by fit to measurement at the 364 and 637 keV photo peaks. SPECT position measurement was simulated by performing a centroid computation for all detector hits for each particle, and then sampling from a radial distribution about the simulated centroid, using 5 mm $FWHM$ resolution. Backscattering from the PM tube and other camera head components was simulated by inserting a 6 cm thick block of SiO_2 behind the collimator.

Figure 1 shows excellent agreement between the simulated and and measured spectra. The ratio of the intensities of the 364 and 637 keV photo peaks as well as the $FWHM$ of both peaks agree within a few percent. The only discrepancy between the Monte Carlo results and the experiments lies in the underestimation by the simulation of the count rate just below the 364 and the 284 keV photo peaks. We postulate that this difference is caused by the approximation of using square holes, in that gammas which scatter off the collimator walls at low angle and are more likely to be re-absorbed in the walls of a square hole than in a hexagonal hole.

In figure 2 we present a comparison of simulated and measured radially point spread function in a 40% energy window about the 364 keV photo peak. Agreement is excellent for the first 5 pixels (1.8 cm), after which the simulated results underestimate the number of counts significantly. We believe that the error is due to either incomplete modeling of scatter into the NaI from components not modeled in the simulation.

Next we examined the spectra near 364 keV photo peak for the full field of view and for the a 3x3 pixel region of interest near the source location. Initial agreement was only fair. As the simulation consistently overestimated the count rate in the ROI, and as the actual source was comparable in size to the area of the hole, we performed further computations with the source in slightly different locations, and

Fig. 1 FOV Energy Spectra for the 6 mm disk source

determined that there was a sensitivity. Results for several source locations, one centered directly over a hole, and one directly over a corner where septa meet are shown in figure 3. Agreement between simulated and measured results is much better for the case in which the center of the source was deemed to be over septa rather than directly over a hole.

IV. Conclusions

Penetration by ^{131}I gammas of a hexagonal hole collimator has been calculated by Monte Carlo simulation. Excellent good agreement with experiment is found for most cases, but several areas of discrepancy between simulated and experimental results for second order effects have been identified. Future work should include more detailed modeling of the camera head and simulation of hexagonal holes.

V. References

[1] D.J. Macey, E.J. Grant, J.E. Bayouth, H.B. Giap, S.J. Danna, R. Sirisriro, and D.A. PodoloffDA, *Med. Phys.*, vol. 33, 1995 pp. 1637-1643.

[2] K.R. Pollard, A.N. Bice, J.F. Eary, L.D. Durack, and T.K. Lewellen, *J. Nucl. Medicine*, vol. 33, 1192 pp. 771-776.

[3] K.F. Koral, K.R. Zasadny, M.L. Kessler, J-Q Lou, S.F. Buchbinder, M.S. Kaminski, I. Francis,and R.L. Wahl, *J. Nucl. Medicine*, vol. 35, 1994 pp. 1714-1720.

[4] A.J. Green, S.E. Dewhurst, R.H.J. Begent, K.D. Bagshawe, and S.J. Riggs, *Eur. J. Nucl. Medicine*, vol. 16, 1990 pp. 361-365.

[5] A.N. Bice, L.D. Durack, K.R. Pollard, and J.F. Eary, *J. Nucl. Medicine*, vol. 32, 1991 pp. P1058.

[6] J.C. Yanch, A.B. Dobrzeniecki, *Conference Record*

Fig. 2 Radial Profile of 6 mm disk source

Fig. 3 Energy Spectra for FOV and ROI near the 364 keV photo peak, 6 mm disk source in several locations

of the IEEE Nucl. Sci. Sym., vol. 3, 1991 pp. 1809.

[7] D.J. DeVries, S.C. Moore, R.E. Zimmerman, S.P. Mueller, B. Friedland, R.C. Lanza, *IEEE Trans. Med. Imag.*, vol. 9, 1990 pp. 430-438.

[8] S.J. Wilderman, "Vectorized algorithms for the Monte Carlo simulation of kilovolt electron and photon transport," *University of Michigan, Ann Arbor, MI, Ph.D. dissertation, 1990.*

[9] M.J. Flynn, S.M. Hames, S.J. Wilderman, and J.J. Ciarelli, *IEEE Trans. Nucl. Sci.*, vol. 43, 1996 pp. 2320-2325.

[10] M.C. Wrobel, N.H. Clinthorne, J.A. Fessler, Y. Zhang, S.J. Wilderman, and W.L. Rogers, *IEEE Trans. Nucl. Sci.*, vol. 44, 1997 pp. 1564-1570.

[11] N.H. Clinthorne, C-y Ng, C-h. Hua, J.E. Gormley, J.W. LeBlanc, D.K. Wehe, S.J. Wilderman, and W.L. Rogers, *Conference Record of the IEEE Nucl. Sci. Sym.*, vol. 2, 1996 pp. 788-792.

[12] J.W. LeBlanc, N.H. Clinthorne, C-h. Hua, E. Nygard, W.L. Rogers, D.K. Wehe, P. Weilhammer, S.J. Wilderman, "C-Sprint: A prototype Compton camera system for low energy gamma ray imaging", presented at *IEEE Nucl. Sci. Sym. and Med. Imaging Conf., Albuquerque, N.M., 1997.*

[13] A. Uritani, N.H. Clinthorne, J.E. Gormley, J.W.LeBlanc, W.L. Rogers, D.K. Wehe, and S.J. Wilderman, *IEEE Trans. Nucl. Sci.*, vol. 44, 1997 pp. 894-898.

[14] S.J. Wilderman, W.L. Rogers, G.F. Knoll and J.C. Engdahl, *IEEE Trans. Nucl. Sci.*, vol. 42, 1997 pp. 250.

[15] J.A. Halbleib Sr. and T.A. Mehlhorn, "ITS: The integrated TIGER series of coupled electron/Photon Monte Carlo transport codes," Sandia National Laboratories Report SAND84-0573 1984.

[16] F. Biggs and R. Lighthill, "Analytical approximations of x-ray cross sections II," SC-RR-710507, 1971.

[17] L.L. Carter and E.D. Cashwell, "Particle transport simulation with the Monte Carlo method," TID-26607, 1975.

[18] J. H. Hubbell, W. J. Veigle, E. A. Briggs, R. T. Brown, D. T. Cromer and R. J. Howerton, *J. Phys. Chem. Ref. Data*, vol. 4, 471-538 pp. 1975.

[19] J.A. Halbleib Sr. and J.E. Morel, "Improved Atomic Shell Excitation and Relaxation in the Tiger Series Codes," Sandia Laboratory Report SAND-78-0580, 1978.

[20] C. Ordonez, A. Bolozdynya, and W. Chang, "Energy uncertainties in Compton scatter Cameras," presented at *IEEE Nucl. Sci. Sym. and Med. Imaging Conf, Albuquerque, N.M., 1997.*

[21] F. Biggs, L.B. Mendelsohn, and J.B. Mann, *At. Data Nuc. Data Tables*, vol. 16, 1975 pp. 201-309.