

Determination of Radionuclide “S” values for any Voxel size, based on three-dimensional discrete Fourier Transform Convolution Method

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Abstract

The most widely extended method to determine the macroscopic non-uniform dose distribution at voxel level is the dose-point convolution method. The lack of tabulated S values for different combinations of voxel size used in SPECT and PET studies has limited the use of voxel S values as a method of choice for absorbed dose calculation at voxel level. The aim of this study was to describe and validate an approach for rapid determination of radionuclide S values for any voxel size used in SPECT or PET studies. An approach based on 3D Discrete Fourier Transform (3D-DFT) convolution method was used for generation of S values at voxel level from tabulated dose-point kernels. The method was verified by comparing our results with voxel S values derived from Monte Carlo EGS4 code radiation transport simulation and Monte Carlo volume integration methods. The method was validated by comparison of the mean dose calculation with those obtained from MCNP-4B Monte Carlo code for mathematical phantoms consisting of spheres of different size with uniform cumulated activity distribution. The voxel S values obtained by 3D-DFT convolution method shows good agreement with those derived from Monte Carlo EGS4 radiation transport simulation and Monte Carlo volume integration methods. The comparison of mean dose calculations shows an error less than 2% for selected mathematical phantoms. The voxel S values generated by 3D-DFT convolution method have a good accuracy and can be obtained in more computationally efficient manner than other published methods. The method can be used as method of choice to provide S values that correspond to any voxel geometry in SPECT or PET studies.

Key words: voxel S values, Discrete Fourier Transform, Monte Carlo method

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Introduction

Dose-point convolution method has been widely used for calculation of macroscopic non-uniform dose distribution from quantitative SPECT or PET imaging (1-5) provides more accurate dose estimates afforded by traditional methods assuming uniform activity within individual organs and is less demanding of computer time than the methods based on Monte Carlo radiation transport simulation.

Numerical methods based on Monte Carlo radiation transport simulation (6) on Monte Carlo volume integration of dose-point kernels (7) were described for the determination of radionuclide S values at voxel level. Another approach, based on voxel source kernel (8) has been used for voxel dosimetry. The voxel source kernel also has been generated using the Monte Carlo method for specific voxel size and was used to calculate patient-specific dosimetry based on the convolution method. The voxel source kernel approach is equivalent in concept to the voxel S values⁶. The voxel S values have been calculated only for a limited number of radionuclides and voxel dimensions (6,7,8).

The voxel S value is an accurate and computationally efficient tool for absorbed dose calculation from macroscopic non-uniform activity distribution⁶. The use of voxel S values as the method of choice for voxel dosimetry has been limited because of the lack of tabulated S values for different voxel dimensions and radionuclides.

Because it is impractical to create and to maintain a database with radionuclide voxel S values for all possible combinations of voxel dimensions used in PET and SPECT studies (7), it is convenient in routine clinical conditions to develop a computationally efficient method as accurate as the above described methods.

The purpose of this work is to describe and validate an approach based on the 3D Discrete Fourier Transform

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(DFT) convolution method for accurate determination of S values in a computationally efficient manner for any voxel size and radionuclides used in SPECT or PET studies.

Materials and Methods

All dosimetric calculations based on the 3D-DFT convolution method were performed on a PC based image processing station, IMAGAMMA (9). To validate the accuracy of voxel S values generated by the 3D-DFT convolution method for dose calculation a test was performed with mathematical phantoms consisting of spheres of different masses with uniform cumulated activity distribution. Convenient sphere masses were selected in order to obtain accurate spherical geometry represented by slices of a discrete set of voxels. The voxel size selected for generation of tomographic slices for spherical mathematical phantoms was a cubic voxel with size dimensions of 3 and 6 mm and density equal to 1 g/cm³. The test consisted of comparison of the calculation of the mean dose for selected spheres using voxel S values generated from the 3D-DFT convolution method and the MCNP-4B Monte Carlo radiation transport simulation code (10).

3D-DFT Convolution Method for Generation Voxel S Values

Radionuclide Kernel Representation for volume source.

In conformity with MIRD convention (11) for volume sources of beta particles, the absorbed dose may be written in the form

$$D(r) = C \cdot (r) \quad \text{Eq. 1}$$

where (r) is the absorbed fraction for beta particles, C is the mean cumulated activity per unit of mass ($\frac{MBq \cdot s}{g}$) and is the mean energy emitted per unit of cumulated activity ($\frac{mGy \cdot g}{MBq \cdot s}$).

For a spherical volume source, the absorbed dose per unit of cumulated activity in a sphere of radius **a** by a point source of activity at the center of the sphere and having a dose-point kernel, $\kappa(r)$, may be obtained by integration of the dose-point kernel over the sphere volume by the mass of sphere as follow:

$$D(a) = \frac{4}{m} \int_0^a r^2 \kappa(r) dr \quad \text{Eq. 2}$$

where $r^2 \kappa(r)$ is the dose point-kernel in $\frac{mGy \cdot cm^2}{MBq \cdot s}$; $\frac{g}{cm^3}$ is the medium density in $\frac{g}{cm^3}$ and r the distance in cm from point source and m is the sphere mass in g.

According to the reciprocity theorem, the absorbed dose at the center of a sphere containing uniform activity distribution is equal to the absorbed dose due to a point source of the same activity located at center of this sphere (12).

The absorbed dose per unit of cumulated activity at a point P outside of sphere of radius **a**, located at distance **b** from the center of this sphere can be defined as follows

$$D(b) = \frac{4}{m} \int_{a-b}^{a+b} r^2 \kappa(r) (r) dr \quad \text{Eq. 3}$$

where (r) is the geometry reduction factor for a point P outside the sphere and is defined as:

$$(r) = \begin{cases} 0 & 0 < r < b - a \\ \frac{[a^2 - (b - r)^2]}{4rb} & b - a < r < b + a \\ 0 & r > b + a \end{cases} \quad \text{Eq. 4}$$

Applying equations 2 and 3 it is possible to obtain the absorbed dose distribution per unit of cumulated activity at any target point located at the center and around of spherical volume source in an infinite homogeneous medium from known dose-point kernels (13).

Consider a voxel array of SPECT or PET images. In this array, each voxel was divided into subvoxels, and dimension of each subvoxel was equals to the original image voxel size divided by an odd integer number. At the center of this subvoxels array was located a spherical source of radius **a**. It is assumed that the sphere volume is equals to the defined subvoxels volume. Each target point was determined as distance **b** from the center of the sphere to the center of each target subvoxel. For this geometry, a discrete dose kernel representation as function of distance from the center of the sphere to each target point was computed applying the equations 2 and 3 using the dose point-kernels tabulated by Cross (14). In these calculations, it was assumed that the cumulated activity is uniformly distributed within the sphere and that the spherical source is inside an absorber of the same density and composition.

Generation of Voxel S Values

Consider a volume source with uniform cumulated activity distribution and size equals to the size of the SPECT or PET images voxel located at the center of the previously defined array of target points. This spatial distribution of cumulated activity was convolved with the dose kernel representation obtained from spherical volume source described above using the 3D-DFT convolution method to yield the dose distribution around the central voxel volume source in the array.

Once the spatial dose distribution is obtained, a volume of interest (VOI) is created over the voxel volume source and the mean dose per unit of cumulated activity was determined as the total absorbed dose divided by the number of sub-voxels contained in the VOI. The VOI is then moved to source-to-target center to center distance according to size of the original SPECT or PET images voxel and the mean dose per unit of cumulated activity was determined in a similar way. This process is repeated only in the positive octant of cube. The S values for other octant may be obtained applying the symmetrical properties of cube. Through this way, a set of S values can be generated for image voxel of any size.

Monte Carlo Transport MCNP-4B Code

The MCNP-4B Monte Carlo code was used for simulations of radiation transport and energy deposition of electrons. The ³²P and ⁹⁰Y radionuclides were assumed to be uniformly distributed in the spheres. For these selected radionuclides,

Radionuclide	Distances (cm)	3D-DFT	EGS4	Difference (%)
32P	0.000	1.69E+0	1.65E+0	-2.4
	0.300	2.38E-1	2.32E-1	-2.6
	0.424	6.14E-2	6.20E-2	1.0
	0.519	1.96E-2	2.12E-2	7.54
	0.600	5.48E-3	6.78E-3	19.2
	0.670	2.01E-3	2.88E-3	30.2
	0.734	7.23E-4	1.24E-3	41.7
	90Y	0.000	1.64E+0	1.61E+0
90Y	0.300	2.81E-1	2.76E-1	-1.8
	0.424	9.85E-2	9.76E-2	-0.9
	0.519	4.51E-2	4.53E-2	0.4
	0.600	2.18E-2	2.26E-2	3.5
	0.670	1.19E-2	1.28E-2	7.0
	0.734	6.55E-3	7.38E-3	11.2
	0.848	1.93E-3	2.47E-3	21.9
	0.900	1.04E-3	1.41E-3	26.5
	0.948	5.10E-4	7.65E-4	33.3
	0.995	2.60E-4	4.25E-4	38.8

Table-1. Voxel S values (mGy/MBq.s) calculated from 3D-DFT convolution method and Monte Carlo EGS4 radiation transport simulation (Ref. 6) for P-32 and Y-90 within 3 mm voxel size.

Radionuclide	Distances (cm)	3D-DFT	EGS4	Difference (%)
32P	0.000	3.28E-1	3.19E-1	-2.8
	0.600	2.49E-2	2.53E-2	1.6
	0.849	2.87E-3	3.13E-3	8.3
	1.039	3.75E-4	4.64E-4	19.4
90Y	0.000	3.55E-1	3.46E-1	-2.6
	0.600	3.91E-2	3.95E-2	1.0
	0.849	7.20E-3	7.57E-3	4.9
	1.039	1.54E-3	1.74E-3	11.5
	1.200	1.40E-4	2.13E-4	34.3

Table-2. Voxel S values (mGy/MBq.s) calculated from 3D-DFT convolution method and Monte Carlo EGS4 radiation transport simulation (Ref. 6) for P-32 and Y-90 within 6 mm voxel size.

the average electron energies were used. The water composition inside and outside of spheres was considered for calculations. The provided option of MCNP-4B code for energy deposition tally was used. The calculated mean dose in mGy/MBq.s for spheres of different size using the MCNP-4B code were deduced from the energy deposition for electrons in a cell, in MeV per particle. The generation of secondary photons was considered in the present calculations. One hundred thousand electron histories were run, resulting in a relative error of mean dose calculations for selected spheres less than 0.01% for electron transport. Dose distribution using Monte Carlo calculations were performed using MCNP-4B code (9) in a Dell 8100 computer workstation.

Results

Tables 1 and 2 shows the voxel S values calculated by 3D-DFT convolution method compared with those obtained by

Bolch, et al (6). The comparison shows very good agreement between both methods at distances less than Combined Continuous Slowing Down Approximation (CSDA) range of beta particles. At larger distances, beyond CSDA range, the differences are larger. However, these differences are small when compared in magnitude with the source voxel S value.

A very good agreement was obtained when our results were compared with those reported by Franquiz, et al (7) for all distances from source voxel. These results are shown on Tables 3 and 4.

The results of calculation of the mean dose for selected mathematical phantoms using the voxel S values generated from the 3D-DFT convolution method and the MCNP-4B Monte Carlo code are shown in Tables 5 and 6 for P-32 and Y-90 radionuclides within voxel sizes of 3 and 6 mm respectively. The comparison of the mean dose calculations for both methods shows a relative difference of less than 2% for P-32 and Y-90.

Radionuclide	Distances (cm)	3D-DFT	Volume integration	Difference (%)
32P	0.000	1.69E+0	1.64E+0	-3.0
	0.300	2.38E-1	2.39E-1	<1.0
	0.424	6.14E-2	6.10E-2	<-1.0
	0.519	1.96E-2	1.96E-2	0
	0.600	5.48E-3	5.50E-3	<1.0
	0.670	2.01E-3	2.00E-3	<-1.0
	0.734	7.23E-4	7.00E-4	-3.3
90Y	0.000	1.64E+0	1.62E+0	-1.2
	0.300	2.81E-1	2.82E-1	<1.0
	0.424	9.85E-2	9.88E-2	<1.0
	0.519	4.51E-2	4.50E-2	<-1.0
	0.600	2.18E-2	2.18E-2	0
	0.670	1.19E-2	1.18E-2	<-1.0
	0.734	6.55E-3	6.50E-3	<-1.0
	0.848	1.93E-3	1.90E-3	-1.6
	0.900	1.04E-3	1.00E-3	-4.0
	0.948	5.10E-4	5.00E-4	-2.0
	0.995	2.60E-4	3.00E-4	13.3

Table-3. Voxel S values (mGy/MBq.s) calculated from 3D-DFT convolution method and Monte

Radionuclide	Distances (cm)	3D-DFT	Volume integration	Difference (%)
32P	0.000	3.28E-1	3.19E-1	-2.8
	0.600	2.49E-2	2.51E-2	<1.0
	0.849	2.87E-3	2.9E-3	<1.0
	1.039	3.75E-4	4.00E-4	6.2
90Y	0.000	3.55E-1	3.50E-1	-1.4
	0.600	3.91E-2	3.93E-2	<1.0
	0.849	7.20E-3	7.20E-3	0
	1.039	1.54E-3	1.50E-3	<-1.0

Table 4. Voxel S values (mGy/MBq.s) calculated from 3D-DFT convolution method and Monte Carlo volume integration (Ref. 7) for P-32 and Y-90 within 6 mm voxel size.

Radionuclide	Sphere mass	Voxels	3D-DFT	MCNP-4B	Difference
32P	999	4625	1.08E-4	1.09E-4	<1%
	1980.9	9171	5.49E-5	5.53E-5	<1%
90Y	999	4625	1.43E-4	1.45E-4	1.4%
	1980.9	9171	7.29E-5	7.39E-5	1.4%

Table-5. Comparison of the mean dose (mGy/MBq.s) for selected spherical masses in g using voxel S values calculated by 3D-DFT convolution and Monte Carlo MCNP-4B code for P-32 and Y-90 within 6 mm voxel size.

Radionuclide	Sphere mass	Voxels	3D-DFT	MCNP-4B	Difference
32P	1002.3	31121	1.08E-04	1.09E-4	<1%
	2001.4	74125	5.43E-05	5.47E-5	<1%
90Y	1002.3	31121	1.43E-4	1.45E-4	1.4%
	2001.4	74125	7.20E-5	7.32E-5	1.6%

Table 6. Comparison of the mean dose (mGy/MBq.s) for selected spherical masses in g using voxel S values calculated by 3D-DFT convolution and Monte Carlo MCNP-4B code for P-32 and Y-90 within 3 mm voxel size.

Discussion

The larger differences observed at distances beyond CSDA range of beta particles between the voxel S values generated by 3D-DFT convolution method with those of Bolch et al (6) may be explained by the use of the dose-point kernel tabulated by Cross et al (2) which does not take into account the contribution of bremsstrahlung photons to radiation dose beyond beta range. This explains the underestimation of voxel S values at largest distances when compared with EGS4 Monte Carlo code (6). However, it was found experimentally that contribution of bremsstrahlung photons to the total dose is less than 2% (14). In addition, the absolute value of dose at largest distances is very small when compared in magnitude to the source S value (6).

A very good agreement was obtained for all distances from source voxel when our results were compared with those reported by Franquiz, et al (7). As was expected, these results should be similar because both methods use the same tabulated dose-point kernels for voxel S values calculation.

The results of mean dose calculation using voxel S values generated by 3D-DFT convolution method and MCNP-4B Monte Carlo method for selected mathematical phantoms shows a relative difference less than 2% for P-32 and Y-90 (Tables 5 and 6). These results reflect that existing inaccuracies at largest distances don't have any impact on dose calculation for beta emitter radionuclides and its contribution to the absorbed dose may be considered negligible. The proposed approach for generation of S values for any voxel size is as accurate as MCNP-4B Monte Carlo code for dose calculations which validate the accuracy of voxel S values reported in this paper.

The methodology presented here for the determination of voxel S values is valid for any voxel size used in SPECT or PET studies and could be obtained in less than 5 minutes which represents a significant advancement over other published methods (6,7,8).

The proposed method could be used as a method of choice to provide S values that correspond to the voxel geometry of imaging data in routine clinical practice. Therefore, the voxel S values generated from the 3D-DFT convolution method can be used for patient-specific voxel dosimetry based on MIRD methodology for clinical applications of targeting therapy with beta emitting radiopharmaceuticals.

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