INVESTIGATION OF RADIOLOGICAL PROPERTIES OF IMAGING AGENTS USED IN NUCLEAR MEDICINE WITH DIFFERENT METHODS AND GATE/GEANT4 SIMULATION PROGRAM

by

Turan SAHMARAN [1*] ***and Taylan TUGRUL*** [2]

[1] Kirikhan Vocational School, Hatay Mustafa Kemal University, Hatay, Turkey
[2] Department of Radiation Oncology, Faculty of Medicine, Van Yüzüncü Yil University, Van, Turkey

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This study aims to determine the radiological properties of various radiopharmaceuticals used in nuclear medicine. In the study, mass attenuation coefficient values in different energy ranges were obtained for six different radiopharmaceuticals dimercaptosuccinic acid, diethylenetriamine pentaacetate, mercaptoacetyltriglycine, hexamethylpropyleneamine oxime, methoxyisobutylisonitrile, methylene diphosphate by using GATE simulation program, XCOM and WinXCom programs. Using these values, effective atomic number and electron density values were calculated with the help of the direct method, interpolation method, Auto-Z_{eff} software, Phy-X/ZeXTra, XMuDat program, and Mayneourd's formula. In addition, the effective atomic number and electron density values obtained were compared for each radiopharmaceutical, both among themselves and between the methods. When radiopharmaceuticals were compared among themselves in low and high-energy regions, the highest effective atomic number values were obtained in dimercaptosuccinic acid, methylene diphosphate, and mercaptoacetyltriglycine. The mass attenuation coefficient values calculated using the GATE code indicate that it is a suitable method for determining the mass attenuation coefficient for imaging agents with no experimental values. This study indicates that the simulation geometry method is suitable to be used as an alternative method for the experiments. In addition, the values obtained for these molecules used as radiopharmaceuticals were examined for the first time.

Key words: radiopharmaceuticals, nuclear medicine, effective atomic number, Monte Carlo

INTRODUCTION

The increase in the use of radiation for diagnosis and treatment in fields such as radiology, nuclear medicine, and radiation oncology in recent years has increased the importance of many factors that play an important role in the interaction of radiation with matter. Knowing the physical quantities such as linear attenuation coefficient (μ), mass attenuation coefficient (μ/ρ_m, effective atomic number (Z_{eff}), effective electron density (N_{eff}), mass energy absorption coefficient (μ_{en}/ρ and total atomic cross section (σ_{ta}) and understanding the behavior of gamma and X-ray interactions are essential in medical imaging, radiation dosimetry, and health physics [1, 2]. The (μ/ρ_m is the basic quantity used to derive parameters such as energy storage, shielding effect, Z_{eff},and N_{eff} [2-10]. As with pure elements, in photon interactions of composite materials, atomic numbers in the entire energy range cannot be defined by a single number [11]. This number, which is used to characterize composite materials, is called Z_{eff} and has information about the material. The Z_{eff} depends on the incoming energy and the atomic number of the constitutive elements [12, 13]. At a given photon energy, the interaction cross-section is proportional to Zn. The n is expected to be between 4 and 5 for the photoelectric effect, 1 for Compton, and 2 for pair formation [14].

The energy range from 5 keV to about 1500 keV is widely utilized in medicine and biological applications [15]. In nuclear medicine departments, radionuclides are used for diagnosis and treatment in similar energy ranges. All of the radionuclides used in nuclear medicine are synthetic and there are many different production methods. Radioactive drugs containing radionuclides in their composition are defined as radiopharmaceuticals that can be used for diagnosis and treatment in nuclear medicine applications [16]. Radiopharmaceuticals consist of two structures. The first structure is the part that emits radiation, called the radionuclide, and the second structure is the part to which the radionuclide, called pharmaceutical, is attached. Radiopharmaceuticals collect in certain tissues or organs, depending on the properties of the drug. Thanks to the radiation emitted by the radionuclide to which it is attached, the structure and

* Corresponding author, e-mail: tsahmaran@gmail.com

function of the organs to be imaged can be examined or some tumors and inflammatory diseases can be treated [17]. More than 40 million nuclear medicine procedures are performed each year, and the demand for radionuclides is increasing at an annual rate of 5 % [18]. When radiopharmaceuticals are given for diagnosis or treatment in the nuclear medicine department, the patient is directly exposed to radiation. Therefore, examining the interaction of these pharmaceuticals with radiation gains importance. In the literature, there are many experimental and theoretical studies on effective atomic number, photon attenuation coefficients, electron density, molar attenuation coefficients, total and electronic cross-sections of some organic and inorganic substances, alloys, amino acids, polymers, glasses, various biological compounds [19-23]. However, theoretical studies on Z_{eff}, N_{eff}, and $(\mu/\rho)_m$ for radiopharmaceuticals in nuclear medicine in which diagnostic and therapeutic radiation are used are limited in the literature. Nuclear medicine applications increasing every year, and the demand for the radionuclides used and the limited studies on this subject have prompted us to do this study.

This study aims to determine the radiological properties of various radiopharmaceuticals used in nuclear medicine. In the study, $(\mu/\rho)_m$ values in different energy ranges were obtained for six different radiopharmaceuticals: dimercaptosuccinicacid (DMSA), diethylenetriamine pentaacetate (DTPA), mercaptoacetyltriglycine (MAG3), hexamethylpropyleneamineoxime (HMPAO), methoxyisobutylisonitrile (MIBI), methylenediphosphate (MDP) by using GATE simulation program, XCOM and WinXCom programs [24, 25]. Using these values, Z_{eff} and N_{eff} values were calculated with the help of the direct method, interpolation method, Auto-Z_{eff} software [26], Phy-X/ZeXTra, Mayneourd's formula [27], and single-valued XMuDat program [28]. In addition, the Z_{eff} and N_{eff} values obtained were compared for each radiopharmaceutical, both among themselves and between the methods. This information is important clinically and dosimetrically. It is also believed that the results acquired may be useful in various applications (health physics, shielding, water equivalent material, nuclear medicine, radiology, *etc*.) where radiation is used. The mass attenuation coefficient is important in dosimetry to calculate the attenuation cross-section calculations. In addition, the values obtained for these molecules used as radiopharmaceuticals were examined for the first time. It is also thought to be important for this study.

MATERIAL AND METHODS

Selection of radiopharmaceuticals

In these methods, radiation is emitted from the patient's body thanks to the radiopharmaceuticals applied to the patient, and this emitted radiation is converted into numerical data by the devices used, processed, and an image is obtained. Thanks to these images obtained, functional abnormalities of organs and early imaging of tumors are detected and also useful for treatment planning. Considering all these, radiopharmaceuticals such as DMSA, DTPA, MAG3, HMPAO, MIBI, and MDP, which are frequently used in nuclear medicine, were included in this study. Table 1 shows the list of radiopharmaceuticals with their

Table 1. List of radiopharmaceuticals with their chemical formulas

Radiopharmaceutical	Chemical formula	Molar mass [gmol^{-1}]	Mean atomic number
DMSA	$C_4H_6O_4S_2$	182.22	6.30
DTPA	$C_{14}H_{23}N_3O_{10}$	393.35	4.16
MAG3	$C_8H_{13}N_3O_5S$	263.27	4.63
HMPAO	$C_{13}H_{28}N_4O_2$	272.39	3.19
MIBI	$C_6H_{11}NO$	113.16	3.26
MDP	$CH_6O_8P_2$	208.00	6.43

Table 2. Some commonly used radionuclides in nuclear medicine [29, 30]

Radionuclide	Physical half-life	Decay mode	Principal E [MeV]	Method of production
^{11}C	20.4 min	β^+	0.511	Cyclotron
^{18}F	109.8 min	β^+	0.511	Cyclotron
^{68}Ga	68 min	β^+, EC	0.511	Generator
^{67}Ga	3.3 d	EC	0.093, 0.185, 0.3	Cyclotron
^{99m}Tc	6.03 h	IT	0.14	Generator
^{111}In	2.8 d	EC	0.173, 0.247	Cyclotron
^{131}I	8.02 d	β^-	0.3645	Fission product
^{201}Tl	73 h	EC	0.07, 0.167	Cyclotron
^{177}Lu	6.65 d	β^-	0.208	Reactor
^{123}I	13.2 h	EC	0.159	Cyclotron
^{124}I	4.2 d	β^+, EC	0.511	Cyclotron

EC: electron capture; IT: isomeric transition; β: beta decay

chemical formulas. Some commonly used radionuclides in nuclear medicine are given in tab. 2.

Calculation of Z_{eff} by direct method

The following formula can be used to calculate the Z_{eff} of materials [31]

$$Z_{eff} \quad \frac{\sum_i f_i A_i \left(\frac{\mu}{\rho}\right)_i}{\sum_i f_i \frac{A_j}{Z_j} \left(\frac{\mu}{\rho}\right)_j} \tag{1}$$

where f_i, μ, ρ, $(\mu/\rho)_i$, A_i, and Z_j are the molar fraction, linear attenuation coefficient, density, mass attenuation coefficient, atomic weight, and atomic number, respectively. With the help of the XCOM program, the total (μ/ρ) of the elements in the materials were found.

Calculation of the attenuation cross-section

The following formula can be used to calculate the attenuation cross-section σ_a values of the compounds

$$\sigma_a \quad \frac{\left(\frac{\mu}{\rho}\right)_m}{N \sum_i \frac{W_i}{A_i}} \tag{2}$$

where $(\mu/\rho)_m$ is the mass attenuation coefficient of the material, N [g^{-1}] – the Avogadro's constant in atom, W_i – the weight fraction of the i-th element in a molecule of tissue substitute material, and A_i – the atomic weight of the i-th element in a molecule. The W_i and A_i are dimensionless. To calculate the Z_{eff}, the calculated attenuation cross-section values were interpolated for the elements produced at the desired energies in WinXCom using the logarithmic formula

$$Z_{eff} \quad \frac{Z_1(\log\sigma_2 \quad \log\sigma_a) \quad Z_2(\log\sigma_a \quad \log\sigma_1)}{\log\sigma_2 \quad \log\sigma_a} \tag{3}$$

where, σ_1 and σ_2 are the elemental cross-sections (barn per atom) in between which the atomic cross-section σ_a of the materials and Z_1 and Z_2 are atomic numbers of the elements corresponding to the cross-sections σ_1 and σ_2, respectively.

Calculation of Z_{eff} by XMuDat

The XMuDat computer program can produce a single value Z_{eff} for compounds [28]. The following formula can be used to calculate the Z_{eff} of materials for the XMuDat

$$Z_{eff,XMuDat} \quad \left(\sum_i \alpha_i Z_i^{m \ 1}\right)^{\frac{1}{m \ 1}} \tag{4}$$

where α_i is the fractional number of the electrons of the i-th element and m – the a constant between 3 and 5. It is preferred that m is set to 3.6 for materials with $Z_{eff} < 6$ and 4.1 for materials with $Z_{eff} > 6$ [32].

Calculation of Z_{eff} by Auto-Z_{eff}

The Auto-Z_{eff} program is used for rapid calculation of the energy-dependent effective atomic number, average atomic numbers, and spectral weighted average atomic numbers. The calculation of the coefficients for the materials is related to the linear addictiveness of the fractional components and is compared with the previously calculated matrix at the separate energies. Therefore, effective atomic numbers are obtained through interpolation of adjacent cross-section data [26, 33].

Calculation of Z_{eff} by Phy-X/ZeXTRa

The Phy-X/ZeXTRa is a new web program for calculating Z_{eff} values for photons, electrons, protons, alpha particles, and carbon ions [27]. For photons, this program uses the cross-section libraries from the WinXCom [25].

Calculation of electron density (N_{eff})

The following formula can be used to calculate the electron density [31]

$$N_{eff} \quad N_A \frac{Z_{eff} n}{\sum_i n_i A_i} \quad N_A \frac{Z_{eff}}{A} \text{(elektron } g^{\ 1}\text{)} \tag{5}$$

where $<A>$ is the average atomic mass of materials, N_A – the Avogadro's number, and Z_{eff} is the effective atomic number.

Calculation of Z_{eff} Mayneourd's formula

The effective atomic number Z_{eff} was first calculated using the Mayneord formula [34-36]

$$Z_{eff} \quad \left(\sum_i \alpha_i Z_i^{2.94}\right)^{1 \ 2.94} \tag{6}$$

where α_i is the relative electron fraction of the i-th element and Z_i – the atomic number of each element [37].

The GATE/Geant4 simulation program

The $(\mu/\rho)_m$ values were obtained using the GATE v8.1 simulation program at 10 keV, 50 keV, 100 keV, 140 keV, 364 keV, 511 keV, 1022 keV,

1250 keV, and 1500 keV energies and 10 m × 10 m field size with a source-surface distance of 100 cm. The main volume with 10 m × 10 m × 10 m size was filled with air. Then, the Fluence Actor was located in the defined volume at a 100 cm distance from the source to determine how many particles passed through it. The fraction weight of imaging agents and selected human organs and their concentration were classified inside the *Gatematerial list*. The number of histories for all simulations was 2×10^8 [10, 23].

RESULT AND DISCUSSION

The $(\mu/\rho)_m$ values of DMSA, DTPA, MAG3, HMPAO, MIBI, and MDP for photon energies ranging from 1 keV to 100 MeV, fig. 1. Radiopharmaceuticals consist of elements with atomic numbers (Z) ranging from 1 to 16 (H:1, C:6, N:7, O:8, P:15, S:16). In fig. 1, it was observed that the $(\mu/\rho)_m$ values of all radiopharmaceuticals were maximum at 1 keV energy, and the $(\mu/\rho)_m$ values decreased rapidly with increasing photon energy over the range of 0.01 to 0.1 MeV. Up to 10 MeV $(\mu/\rho)_m$ values continue to decrease. However, since radiopharmaceuticals such as MDP, DMSA, and MAG3 contain elements with high atomic numbers such as 16S and 15P, their decay rate is slower than others. These elements have a sudden jump in $(\mu/\rho)_m$ values, around 3 keV, due to *K*-edge absorption. The sharp decrease up to 0.1 MeV can be explained by the fact that photoelectric absorption is more dominant at lower energies, especially for elements with high atomic numbers. In the energy range where photoelectric absorption is dominant, the photon interaction cross-section depends on Z^{4-5} and E^3 [38-40].

Figure 1 shows the variation of radiofarmaceuticals with $(\mu\rho)_m$ for various photon energy. The Z_{eff} calculated by various methods in the 10 keV to 1 GeV photon energy region are shown in fig. 2. Z_{eff} below 10 keV energy were not compared due to uncertainty (25 %) in Auto-Z_{eff} [26]. It has been found that Auto-Z_{eff}, Phy-X/ZeXTRa, direct and interpolation methods are in harmony with the Z_{eff} calculation in the 50 keV and 20 MeV energy regions where the component interaction process is dominant. While the effective atomic number was found to be constant in the medium energy photon region, significant differences were found in the low (<30 keV) and high (>20 MeV) photon regions. The $(\mu/\rho)_m$ obtained with XCOM and GATE are given in tab. 3 $(\mu/\rho)_m$ for imaging agents were obtained using GATE and different methods and are presented in tab. 4.

The $(\mu/\rho)_m$ of selected human organs were found using the GATE simulation program to validate the measurement geometry and functioning before the results were obtained. These results were compared with values obtained from XCOM. It was found that the $(\mu/\rho)_m$ values for the selected human organs were very close to theoretical XCOM data results. The $(\mu/\rho)_m$ values of imaging agents were obtained using GATE at various photon energies and compared with different methods. Thus, it has been observed that the GATE simulation program provides photon interaction parameters for imaging agents. The $(\mu/\rho)_m$ values obtained using the GATE simulation program were in good agreement with the results obtained by different methods, tab. 3.

The Z_{eff} values calculated by Phy-X/ZeXTra and the direct method were higher in the photoelectric absorption and pair formation regions when compared to the Z_{eff} values calculated by the Auto-Z_{eff} and interpolation method. In the energy region where pair formation is dominant, the difference between Z_{eff} values is less than in the photoelectric absorption region. Büyükyildiz stated in his study [41] that the differences between the Z_{eff} obtained by direct and interpolation methods in the energy region where the photoelectric effect is dominant are large and not uniform. It is thought to be due to the non-uniform variation of $(\mu/\rho)_m$ in this energy region. Similar results were obtained in our study. In addition, since the Z_{eff} has more than one value for the direct and interpolation method at the *K* absorption edge, which corresponds to the high *Z* element in radiopharmaceuticals, the two methods do not give compatible results with each other. In

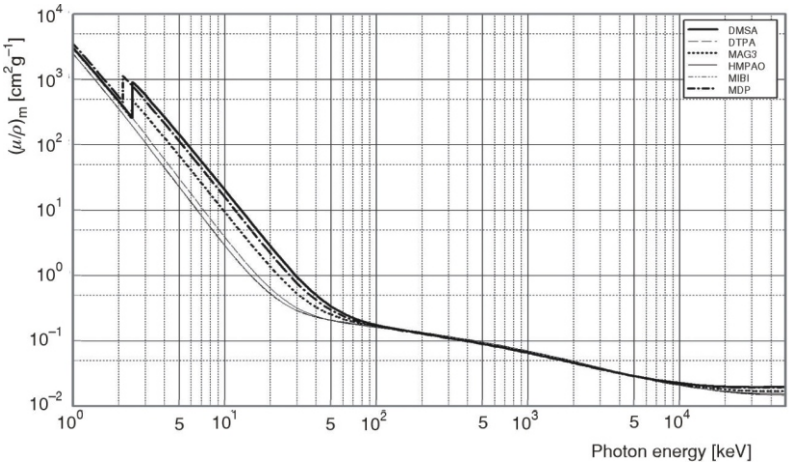

Figure 1. Variation of $(\mu/\rho)_m$ with photon energy for various radiopharmaceuticals

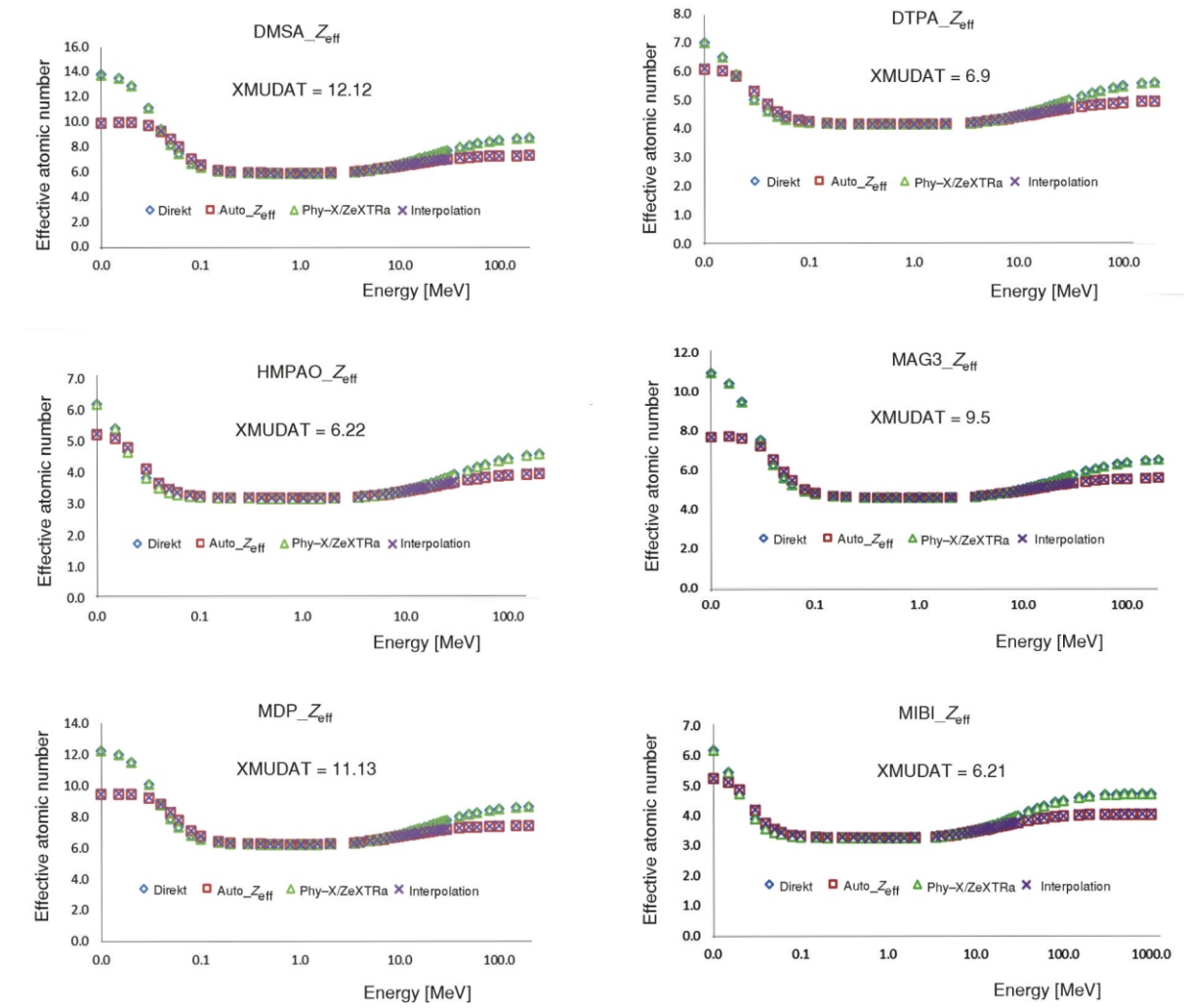

Figure 2. The Z_{eff} of radiopharmaceuticals calculated by different methods

direct and interpolation methods, different weights are given to individual atomic numbers when calculating the weighted average [42]. It can be said that these differences are because the absorption processes depend on the atomic number and energy. The Z_{eff} calculated using the XMuDat program of DMSA, DTPA, MAG3, HMPAO, MIBI, and MDP were found as 12.12, 6.90, 9.50, 6.22, 6.21, 11.13, respectively. The single-valued Z_{eff} and N_{eff} have been calculated for radiopharmaceuticals using the XMuDat program. It was seen that significant differences occur between the single-valued Z_{eff} and the Z_{eff} obtained for different energies, fig. 2. It is recommended that the XMuDat program can be used with safety at low photon energies up to 0.01 MeV where photoelectric absorption predominates for calculation of Z_{eff} and N_{eff} since it gives values close to the ones obtained with the energy-dependent Mayneourd's formula. Similar results were obtained in Kurudirek 's study [34]. Since the radiation energy used in nuclear medicine is for diagnostic purposes, their energies are quite low. Therefore, lower energies are preferred in tabs. 5 and 6.

As in other literature studies [3, 12, 27, 39], it was found that the Z_{eff} values calculated by all four methods in the Compton scattering region and the calculation methods used were compatible, but there was a difference between the Z_{eff} values in the photoelectric and pair formation regions.

CONCLUSIONS

In the energy region between 1 keV and 100 GeV, Z_{eff} and N_{eff} values for DMSA, DTPA, MAG3, HMPAO, MIBI, and MDP used in nuclear medicine were calculated using four different methods. While the Z_{eff} values obtained depend on the chemical compound of the material at low and high energies, it is observed that this dependence weakens in the middle energy region. The values obtained as a result of the Neff calculation are closely related to Z_{eff} and N_{eff}'s tendency towards energy was found to be similar to Z_{eff}'s for all samples. While these four methods give good results in the Compton scattering region for the new

Table 3. Comparison of (μ/ρ_m [cm^{2}g^{-1}] in energies commonly used in nuclear medicine with XCOM and GATE results

Materials	Energy [keV]							
	140		364		511		1022	
	XCOM	GATE	XCOM	GATE	XCOM	GATE	XCOM	GATE
[a]Water	0.1531	0.1528	0.1102	0.1095	0.0956	0.0953	0.0692	0.0679
[a]Soft tissue	0.1524	0.1515	0.1093	0.1094	0.0944	0.0941	0.0691	0.0677
[a]Muscle	0.1521	0.1502	0.1094	0.1087	0.0953	0.0943	0.0697	0.0685
[a]Bone	0.1526	0.1534	0.1103	0.1089	0.0917	0.0920	0.0664	0.0671
[a]Brain	0.1534	0.1517	0.1095	0.1087	0.0952	0.0947	0.0696	0.0673
[a]Breast	0.1527	0.1524	0.1097	0.1081	0.0954	0.0946	0.0695	0.0692
[a]Testis	0.1535	0.1512	0.1099	0.1083	0.0954	0.0962	0.0695	0.0689
[a]Eye	0.1516	0.1501	0.1083	0.1087	0.0946	0.0942	0.0689	0.0681
[a]Adipose	0.1517	0.1516	0.1084	0.1097	0.0946	0.0944	0.0689	0.0677
[a]Lung	0.1523	0.1527	0.1091	0.1076	0.0951	0.0952	0.0693	0.0682
[a]Blood	0.1524	0.1505	0.1092	0.1085	0.0951	0.0951	0.0693	0.0682
DMSA	0.1491	0.1485	0.1034	0.1026	0.0891	0.0887	0.0652	0.0638
DTPA	0.1464	0.1417	0.1055	0.1039	0.0914	0.0904	0.0661	0.0645
MAG3	0.1473	0.1468	0.1047	0.1037	0.0905	0.0912	0.0665	0.0647
HMPAO	0.1515	0.1489	0.1096	0.1068	0.0952	0.0945	0.0694	0.0678
MIBI	0.1502	0.1517	0.1087	0.1068	0.0943	0.0927	0.0697	0.0681
MDP	0.1451	0.1441	0.1013	0.1021	0.0881	0.0878	0.0643	0.0642

[a]ICRU Report 44, Tissue Substitutes in Radiation Dosimetry and Measurement, Bethesda (MD), USA, 2023

Table 4. Comparison of the (μ/ρ_m [cm^{2}g^{-1}]obtained for some energies with the different methods

Materials	Method	Energy [MeV]				
		0.01	0.05	0.10	1.25	1.50
DMSA	XCOM	20.371	0.341	0.175	0.058	0.053
	Phy-X/ZeXTRa	20.404	0.341	0.175	0.065	0.054
	XMuDat	20.373	0.337	0.168	0.066	0.054
	GATE	20.072	0.338	0.165	0.058	0.056
DTPA	XCOM	3.873	0.207	0.161	0.060	0.054
	Phy-X/ZeXTRa	3.872	0.207	0.161	0.063	0.054
	XMuDat	3.851	0.204	0.168	0.059	0.055
	GATE	3.867	0.206	0,163	0.061	0.057
MAG3	XCOM	9.418	0.252	0.166	0.059	0.054
	Phy X/ZeXTRa	9.418	0.252	0.167	0.059	0.054
	XMuDat	9.405	0.246	0.167	0.058	0.053
	GATE	9.407	0.249	0.164	0.055	0.055
HMPAO	XCOM	2.897	0.207	0.166	0.062	0.057
	PhyX/ZeXTRa	2.897	0.208	0.165	0.063	0.057
	XMuDat	2.883	0.216	0.158	0.064	0.054
	GATE	2.889	0.205	0.155	0.063	0.052
MIBI	XCOM	2.871	0.206	0.166	0.062	0.056
	Phy-X/ZeXTRa	2.870	0.206	0.165	0.062	0.056
	XMuDat	2.856	0.215	0.158	0.061	0.055
	GATE	2.868	0.220	0.163	0.063	0.056
MDP	XCOM	15.831	0.298	0.168	0.058	0.052
	Phy-X/ZeXTRa	15.831	0.297	0.168	0.057	0.052
	XMuDat	5.828	0.307	0.161	0.058	0.053
	GATE	15.819	0.299	0.170	0.059	0.055

materials to be Z_{eff} calculated, they give different Z_{eff} values in the low and high-energy regions. Therefore, Z_{eff} values need more experimental accuracy, especially in high and low-energy regions. When radiopharmaceuticals were compared among themselves in low and high-energy regions, the highest Z_{eff} values were obtained in DMSA, MDP, and MAG3, respectively. The lowest Z_{eff} value was obtained in DTPA, MIBI, and HMPAO. The Monte Carlo simulated (μ/ρ_m for the imaging agents in some photon energies were found to be very close to the theoretical XCOM values and GATE simulation program. This study indicates that the simulation geometry method is suitable to be used as an alternative method for the ex-

Table 5. The Z_{eff} of radiopharmaceuticals calculated by the Auto-Z_{eff}, Phy-X/ZeXTRa, direct, interpolation, XMuDat, and Mayneourd's formula

Radiopharmaceuticals	Method	Energy [MeV]					
		0.01	0.05	0.1	1.25	XMuDat	Mayneourd
DMSA	Direct	13.75	8.21	6.33	5.87		
	Interpolation	9.90	8.62	6.57	5.89	12.12	11.71
	Auto-Z_{eff}	9.88	8.60	6.55	5.88		
	Phy-X/ZeXTRa	13.75	8.20	6.33	5.88		
DTPA	Direct	6.99	4.42	4.21	4.16		
	Interpolation	6.10	4.59	4.26	4.17	6.90	6.82
	Auto-Z_{eff}	6.07	4.58	4.24	4.16		
	Phy-X/ZeXTRa	7.00	4.42	4.20	4.16		
MAG3	Direct	10.96	5.62	4.80	4.63		
	Interpolation	7.70	5.94	4.86	4.61	9.50	9.04
	Auto-Z_{eff}	7.69	5.93	4.85	4.60		
	Phy-X/ZeXTRa	10.95	5.59	4.77	4.61		
HMPAO	Direct	6.19	3.37	3.23	3.19		
	Interpolation	5.24	3.49	3.26	3.18	6.22	6.13
	Auto-Z_{eff}	5.21	3.47	3.24	3.19		
	Phy-X/ZeXTRa	6.18	3.37	3.23	3.19		
MIBI	Direct	6.20	3.45	3.29	3.26		
	Interpolation	5.26	3.56	3.34	3.27	6.21	6.12
	Auto-Z_{eff}	5.24	3.54	3.31	3.26		
	Phy-X/ZeXTRa	6.19	3.44	3.30	3.26		
MDP	Direct	12.24	7.91	6.56	6.24		
	Interpolation	9.46	8.32	6.75	6.25	11.13	10.81
	Auto-Z_{eff}	9.44	8.30	6.74	6.23		
	Phy-X/ZeXTRa	12.24	7.90	6.56	6.23		

Table 6. The N_{eff} (10^{23} g^{-1}) of radiopharmaceuticals calculated by the Auto-Z_{eff}, Phy-X/ZeXTRa, direct, interpolation, XMuDat, and Mayneourd's formula

Radiopharmaceuticals	Method	Energy [MeV]					
		0.01	0.05	0.1	1.25	XMuDat	Mayneourd
DMSA	Direct	7.27	4.33	3.35	3.11		
	Interpolation	5.23	4.56	3.47	3.12	3.11	3.51
	Auto-Z_{eff}	7.26	4.54	3.46	3.11		
	Phy-X/ZeXTRa	5.24	4.34	3.34	3.11		
DTPA	Direct	5.35	3.38	3.22	3.18		
	Interpolation	4.66	3.52	3.25	3.19	3.18	3.11
	Auto-Z_{eff}	4.65	3.51	3.24	3.19		
	Phy-X/ZeXTRa	5.34	3.39	3.24	3.18		
MAG3	Direct	7.52	3.86	3.30	3.18		
	Interpolation	5.28	4.07	3.33	3.16	3.16	3.52
	Auto-Z_{eff}	7.51	3.83	3.32	3.15		
	Phy-X/ZeXTRa	5.28	4.05	3.28	3.16		
HMPAO	Direct	6.43	3.51	3.35	3.32		
	Interpolation	5.42	3.60	3.37	3.30	3.32	3.14
	Auto-Z_{eff}	6.42	3.59	3.37	3.31		
	Phy-X/ZeXTRa	5.43	3.50	3.35	3.32		
MIBI	Direct	6.26	3.48	3.33	3.30		
	Interpolation	5.30	3.58	3.35	3.30	3.30	3.13
	Auto-Z_{eff}	5.29	3.58	3.35	3.31		
	Phy-X/ZeXTRa	6.26	3.49	3.36	3.30		
MDP	Direct	6.02	3.89	3.22	3.06		
	Interpolation	4.65	4.08	3.32	3.07	3.07	3.29
	Auto-Z_{eff}	6.64	4.08	3.31	3.06		
	Phy-X/ZeXTRa	6.03	3.89	3.23	3.07		

periments. It is thought that it would be beneficial to use μ/ρ Z_{eff}, and N_{eff} values obtained by different methods in various applications such as health physics, engineering, and medical dosimetry.

AUTHORS' CONTRIBUTIONS

T. Sahmaran: Conceptualization, methodology, formal analysis, calculations, and analyses – writing the original draft. T. Tugrul: Conceptualization, methodology, original draft, writing – review and editing.

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Туран ШАХМАРАН, Тајлан ТУГРУЛ

ИСТРАЖИВАЊЕ РАЗЛИЧИТИМ МЕТОДАМА И GATE/GEANT4 ПРОГРАМОМ СИМУЛАЦИЈЕ РАДИОЛОШКИХ СВОЈСТВА АГЕНАСА СЛИКЕ КОЈИ СЕ КОРИСТЕ У НУКЛЕАРНОЈ МЕДИЦИНИ

Циљ рада је да се утврде радиолошка својства различитих радиофармацеутика који се користе у нуклеарној медицини. Коришћењем GATE програма за симулацију, XCOM и WinXCom програма, добијене су вредности масених коефицијената слабљења у различитим енергетским опсезима за шест различитих радиофармацеутика: димеркаптосукцинске киселине, диетилентриамин пента-ацетата, меркапто-ацетил триглицина, хексаметилпропиленамин оксима, метокси-изобутил-изонитрила и метилен дифосфата. Користећи ове вредности, израчунати су ефективни атомски број и вредност густине електрона уз помоћ директне методе, методе интерполације, Auto-Z_{eff} софтвера, Phy-X/ZeXTra и XMuDat програма и Мајнардове формуле. Поред тога, добијене вредности ефективног атомског броја и густине електрона упоређене су за сваки радиофармацеутик, како између њих, тако и између метода. Када су радиофармацеутици међусобно упоређивани у регионима ниске и високе енергије, највеће ефективне вредности атомског броја добијене су у димеркаптосукцинској киселини, метилен дифосфату и меркапто-ацетил триглицину. Вредности масених коефицијената слабљења израчунате коришћењем GATE програма указују на то да је то примерена метода за одређивање масених коефицијената слабљења агенаса за снимање без експерименталних вредности. Рад показује да је метода геометријске симулације погодна за примену као алтернативна метода експериментима. Поред тога, по први пут испитане су вредности добијене за ове молекуле који се користе као радиофармацеутици.

Кључне речи: фармацеутик, нуклеарна медицина, ефективни атомски број, Монте Карло метода