

Monte Carlo simulation of air kerma rate constants for different radionuclides

Simulação Monte Carlo de constantes de taxa de kerma no ar para diferentes radionuclídeos

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Abstract

The air kerma rate constant values for different radionuclides are often used in radiation shielding calculations, calibration of instruments, estimating the absorbed dose from brachytherapy sources, etc. Usually, air kerma rate constant values are calculated in a deterministic way. This work evaluates the possibility of air kerma rate constant estimation through Monte Carlo simulations. Ten different radionuclides were considered in this preliminary study, covering low and high-energy gamma spectra. Mean percentage differences of less than 10% relative to the results of reference works were found. Most of our results (C-11, O-15, F-18, Ga-67, Ga-68, I-131, and Tl-201 sources) present less than a 5% relative percentage difference considering the literature results. The air kerma rate constants calculated in this work agree with reference results, thus validating the methodology, the photon spectra database used, and the Monte Carlo simulations with EGSnrc. Future work can extend the calculation of air kerma rate constants for other radionuclides and study the influence of different sources of uncertainty in its results.

Keywords: air kerma rate constant; nuclear medicine; radiotherapy; radiation protection; radiation shielding; dosimetry.

Resumo

Os valores da constante de taxa de kerma no ar para diferentes radionuclídeos são frequentemente utilizados em cálculos de proteção radiológica, calibração de instrumentos, estimativa da dose absorvida de fontes de braquiterapia, etc. Geralmente, os valores da constante de taxa de kerma no ar são calculados de forma determinística. Este trabalho avalia a possibilidade de estimativa da constante de taxa de kerma no ar através de simulações Monte Carlo. Dez diferentes radionuclídeos foram considerados neste estudo preliminar, abrangendo espectros de raios gama de baixa e alta energia. Foram encontradas diferenças percentuais médias inferiores a 10% em relação aos resultados de trabalhos de referência. A maioria dos nossos resultados (fontes de C-11, O-15, F-18, Ga-67, Ga-68, I-131 e Tl-201) apresenta diferença percentual relativa inferior a 5% considerando os resultados da literatura. As constantes de taxa de kerma no ar calculadas neste trabalho estão de acordo com os resultados de referência, validando assim a metodologia aplicada, a base de dados de espectros de fótons utilizada e as simulações Monte Carlo com o código EGSnrc. Trabalhos futuros podem estender o cálculo das constantes de taxa de kerma no ar para outros radionuclídeos e estudar a influência de diferentes fontes de incerteza nos seus resultados.

Palavras-chave: constante de taxa de kerma no ar; medicina nuclear; radioterapia; proteção radiológica; blindagem; dosimetria.

1. Introduction

The air kerma rate constant of radionuclides is a dosimetric quantity that estimates the air kerma at various distances from radionuclide point sources of known activity. It is used in radiation shielding calculations, instrument calibration, estimating the absorbed dose from brachytherapy sources, etc. Historically, the air kerma rate constant (Γ) for radionuclides is calculated through the following equation:

$$\Gamma_{\delta} = ((K_{\delta}/t)d^2)/A \quad (1)$$

where d is the distance from a point source with activity A . K_{δ}/t is the air kerma rate. The subscript δ indicates that only photons with energy greater than δ are considered for the air kerma rate constant computation.

Wasserman and Groenewald (1988) compiled the air kerma rate constants for thirty radionuclides used in nuclear medicine and radiotherapy (1). The authors used exposure rate constant values available in the literature to obtain air kerma rate constants (in $\text{Gy m}^2 \text{Bq}^{-1} \text{s}^{-1}$). They considered $\delta = 20 \text{ keV}$ due to practical and clinical nuclear medicine reasons (1).

Ninkovic, Raicevic, and Adrovic (2005) argued that there was a strong disagreement regarding air kerma rate constants published and performed a reassessment of this quantity (2). The authors calculated the air kerma rate constant for thirty-five radionuclides using updated data for photon spectra and mass energy-transfer coefficients for air. Only photons with energy greater than 20 keV were considered, and the contribution of bremsstrahlung radiation from the source was omitted. They reported that the values for air kerma rate constants given in their paper were the most accurate available at the time. Also, according to the authors, the

bremsstrahlung contribution is small, and the major component of the standard error associated with the calculated values is the relative intensity measurements of the photon spectra.

Smith and Stabin (2012) compiled exposure rate constants that can be converted into air kerma rate constants for more than 1100 radionuclides (3). Their objective was to provide an updated and comprehensive list of exposure rate constants and factors to convert it into dose rate to tissue. They considered $\delta = 15$ keV and used updated photon spectra. Bremsstrahlung was also neglected. Good agreement with previous works was reported by the authors.

Therefore, the photon spectrum of a radioactive source plays an important role in the Γ calculation. Recently, efforts have been made to optimize the calculation of radiation shielding. For instance, the concept of the body dose rate constant has been investigated (4-6) using Monte Carlo (MC) modeling. Thus, in the context of MC simulations for shielding optimization, the radionuclide photon spectrum will directly affect the results. Since Monte Carlo simulation-derived results require validation (7-12), air kerma dose rate constant values can be reproduced to validate the photon spectra of radionuclides considered in the simulation scenario. Furthermore, the air kerma rate calculations using Monte Carlo simulations can be used to investigate sources of uncertainty and contribute to generating more accurate values. Although there are several sources of this radiologic quantity in the literature, the majority of published values have no uncertainties assigned (13).

Hence, the objective of this work is to calculate air kerma dose rate constant for different radionuclides using Monte Carlo simulations. The results can be used to demonstrate the validity of the used photon spectra database as well as the Monte Carlo code employed in the simulations.

2. Materials and Methods

Air kerma rate constant values were calculated for ten different radionuclides, covering low and high-energy gamma spectra: C-11, O-15, F-18, Ga-67, Ga-68, Tc-99m, I-123, I-131, Sm-153, and Tl-201.

2.1. Monte Carlo Simulations

The simulation scenario (Figure 1) proposed by Paixão and Fonseca (2023) was considered (14). A cubic universe of air ($\rho = 1.2048 \times 10^{-3}$ g/cm³) with an edge of 220 cm and centered at the origin was modeled. The isotropic point source was positioned at $z = 100$ cm. A circular scoring circle with a 25 cm radius was assumed and air kerma was tallied by the code.

The photon emission spectra were taken from the RADAR decay database (15) and a $\delta = 20$ keV was considered.

The MC simulations were performed using the EGSnrc code version number V4-r2-3-2 (16) with cavity usercode. The EGSnrc MC code is widely used and validated for medical physics research. The MC

transport parameters used were: electron and photon transport cutoff energy set to 10 keV. All other EGSnrc MC transport parameters were default. No variance reduction option was selected. The number of simulated particles was such that the statistical uncertainty for the calculated quantities was 1% or less. The simulations were performed in a computer with an Intel® Xeon® Quad CPU of 3.30 GHz with 4 GB RAM.

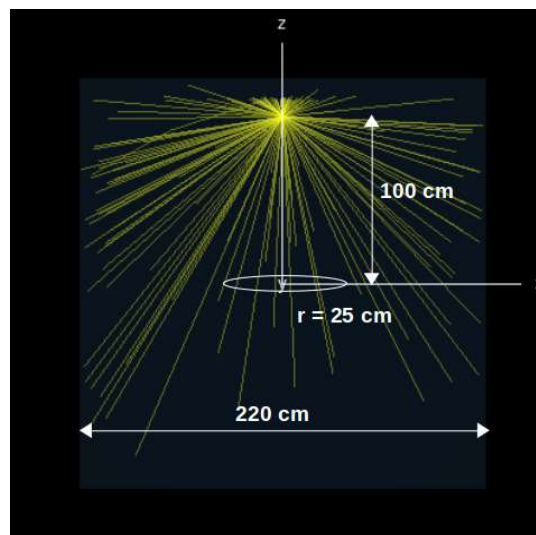


Figure 1. The scenario simulated in this work (not to scale).

The results were validated using the relative percentage difference ($\Delta\%$) between the values calculated in this work and those published in the literature. The relative percentage difference was calculated as follows:

$$\Delta\% = 100(q - q_0)(q_0)^{-1} \quad (2)$$

where q is the results calculated in this work, and q_0 is the reference results.

3. Results

Air kerma rate constant values were calculated for ten different radionuclides. The results are presented in Table 1. The Monte Carlo uncertainties (1σ) of all results are equal to or less than 0.12%. The results from references (1-3) are also presented as reference values.

Table 1. Air kerma rate constants ($\Gamma_{\delta=20\text{ keV}}$) calculated in this work ($\times 10^{-18}$ Gy m² Bq⁻¹ s⁻¹)

Source	This work	Ref. (1)	Ref. (2)	Ref. (3)
C-11	37.39	38.75	38.7	38.4
O-15	37.44	38.75	38.7	38.7
F-18	36.25	37.57	37.5	37.4
Ga-67	5.113	5.25	5.4	5.27
Ga-68	34.63	35.21	35.8	35.7
Tc-99m	3.956	3.93	3.92	5.23
I-123	10.25	10.03	10.0	11.8
I-131	14.05	14.16	14.5	14.5
Sm-153	2.960			3.17
Tl-201	2.817	2.95	2.84	2.96

Source: The authors (2024) and references (1-3).

The relative percentage differences ($\Delta\%$) from reference values were calculated and are presented in Figures 2 and 3.

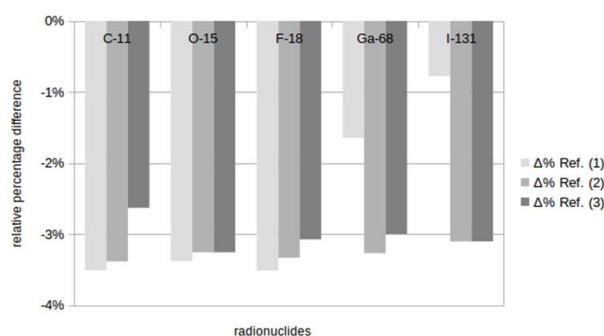


Figure 2. Relative percentage differences from reference values for high energy gamma emission radionuclides.

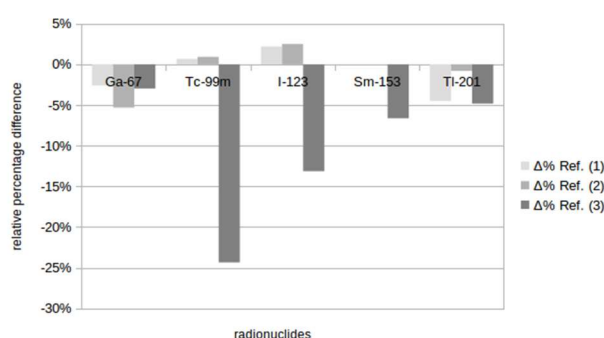


Figure 3. Relative percentage differences from reference values for low energy gamma emission radionuclides.

4. Discussion

The air kerma rate constants calculated for the radionuclides considered in this work present good agreement with the results from the literature. Mean percentage differences of 3%, 3%, and 7% were found relative to the works of Wasserman and Groenewald (1988) (1), Ninkovic, Raicevic, and Adrovic (2005) (2), and Smith and Stabin (2012) (3), respectively. The majority of our results (C-11, O-15, F-18, Ga-67, Ga-68, I-131, and Tl-201 sources) present less than a 5% relative percentage difference considering all three references works.

As presented in Table 1, the results of this work are more precise. However, it is worth noting that the uncertainty is only related to the Monte Carlo simulation and was estimated by the code.

Figures 2 and 3 show that our results are generally lower than the reference values. The exceptions are for Tc-99m and I-123 sources in comparison with (1) and (2) (Figure 3). These same sources were the only ones that presented $\Delta\% > \pm 10\%$. In comparison with Smith and Stabin (2012) (3), the differences were equal to -24% for Tc-99m and -13% for I-123. We believe that the use by Smith and Stabin (2012) of a lower energy limit ($\delta = 15$ keV) in the radionuclide photon spectrum would not be the only responsible for these differences. For $\delta = 15$ keV, this would include two x-ray photons in the Tc-99m spectrum (18.3 keV and 18.4 keV, both with relatively low emission probability in comparison with the main gamma photon) and no photon in the

I-123 spectrum. However, Smith and Stabin (2012) considered a different source for radionuclide spectra, the ICRP publication 107 (17). Considering this emission photon spectrum reference and $\delta = 15$ keV for Tc-99m and I-123 sources, we obtain air kerma rate constants equal to 4.861×10^{-18} $\text{Gym}^2\text{Bq}^{-1}\text{s}^{-1}$ and 10.28×10^{-18} $\text{Gym}^2\text{Bq}^{-1}\text{s}^{-1}$, respectively. Such results represent relative percentage differences of 7% for Tc-99m and 12.6% for I-123, relative to the results from Smith and Stabin (2012). The Tc-99m spectrum from ICRP 107 is considerably different, presenting a mean energy of 0.131 MeV against 0.139 MeV for the spectrum considered in this work. For the I-123 photon spectrum, the difference was not relevant (1 keV mean energy difference). Therefore, the discrepancies found are due to differences in the methodology. Nevertheless, our results agree quite well for Tc-99m ($\Delta\% = 1\%$) and I-123 ($\Delta\% \leq 3\%$), considering references (1) and (2). Furthermore, in the context of radiation shielding, our results are conservative since the photon spectra are more penetrating due to their higher mean energy.

Consequently, the air kerma rate constants calculated in this work agree with reference results, thus validating the methodology, the photon spectra database used, and the Monte Carlo simulations with EGSnrc. Future work can extend the calculation of air kerma rate constants for other radionuclides. More importantly, it can focus on studying the influence of different sources of uncertainty in the air kerma rate constant results, contributing to minimizing the error in various applications that rely on this radiation quantity.

5. Conclusions

Usually, air kerma rate constant values are calculated deterministically. This work evaluated the possibility of air kerma rate constant estimation through Monte Carlo simulations. Since the photon spectrum of a radioactive source plays an important role, air kerma rate constant values were estimated for ten different radionuclides, covering low and high-energy gamma spectra. The results of this work are more precise, and most of our results present less than a 5% relative percentage difference considering the literature results, thus validating the methodology, the photon spectra database, and the Monte Carlo simulations with EGSnrc. Future work can extend the calculation of air kerma rate constants for other radionuclides and focus on studying the influence of different sources of uncertainty in the air kerma rate constant results.

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