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APPLICATION OF DISCRETE ORDINATES AND MONTE CARLO METHODS TO TRANSPORT OF PHOTONS FROM ENVIRONMENTAL SOURCES

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ABSTRACT

Federal Guidance Report No. 12[1] tabulates dose coefficients for external exposure to photons and electrons emitted by radionuclides distributed in air, water, and soil. Although the dose coefficients of this report are based on previously developed dosimetric methodologies, they are derived from new, detailed calculations of the energy and angular distributions of the radiations incident upon the body and the transport of these radiations within the body. Particular effort was devoted to expanding the information available for the assessment of radiation dose from radionuclides distributed on or below the surface of the ground. A companion paper (External Exposure to Radionuclides in Air, Water, and Soil) discusses the significance of the new tabulations of coefficients and provides detailed comparisons to previously published values. This paper discusses the details of the photon transport calculations.

INTRODUCTION

Dose coefficients for external exposure relate the doses to organs and tissues of the body to the concentrations of radionuclides in environmental media. The modes considered here for external exposure are submersion in a contaminated atmospheric cloud, immersion in contaminated water, and exposure to contamination on or in the ground.

Since estimation of the dose to body tissues from radiations emitted by an arbitrary distribution of a radionuclide in an environmental medium is extremely difficult, it has become common practice to consider simplified and idealized exposure geometries. The radionuclide concentration in the medium, from the viewpoint of an exposed individual, is uniform and effectively infinite or semi-infinite in extent. If one assumes an infinite or semi-infinite source region with a uniform concentration $C(t)$ of a radionuclide at time t, the time-independent dose coefficient for external exposure of tissue T is

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$$h_T = \frac{H_T}{\int C(t)dt} \quad ,$$

where H_T is the dose equivalent in tissue T. The coefficient h_T represents the dose to tissue T of the body per unit time-integrated concentration, expressed in terms of the *time-integrated concentration of the radionuclide.* It incorporates the transport of emitted radiations in the environment, their subsequent transport in the body, and estimation of the deposition of ionizing energy in the tissues of the body.

ORGAN DOSES FROM MONOENERGETIC ENVIRONMENTAL PHOTON SOURCES

The calculation of organ doses from irradiation of the human body by photon emitters distributed in the environment requires the solution of a complex radiation transport problem. It is impractical to solve this problem for the precise spectrum of photons emitted by each radionuclide of interest. Therefore, organ doses were computed for monoenergetic photon sources at twelve energies from 0.01 to 5.0 MeV. The results of these calculations were then used to derive the dose coefficients for 825 radionuclides, taking into account the detailed photon spectrum of each radionuclide. This paper describes the methods used to compute organ dose coefficients for those monoenergetic sources.

Previous estimates of submersion dose[2-4] were based on Monte Carlo calculations with (1) poor statistics for some organ doses (due to the limitations of early computer systems) or (2) minor errors in sampling the radiation field.

The seminal work of Beck and de Planque[5] on dose due to contaminated soil, while accurately reflecting the radiation field, was limited to calculation of air dose for energies between 0.25 and 2.25 MeV. The next generation of calculations[4,6] produced useful dose estimates for many nuclides, but was limited by simplifying assumptions regarding the energy and angular dependence of the radiation field (assumed to be equivalent to that for submersion) and the use of the point kernel method for characterizing the field strength. More recent efforts[7-9] have used relatively sophisticated methods for analyzing the energy, angular, and spatial dependence of the radiation field and computing organ doses for both mathematical and CT-derived phantoms of various ages. These data are primarily for plane sources at or near the air-ground interface, or for naturally-occurring radionuclides distributed to effectively infinite depth in the soil. The calculations of Chen[10] include volume sources of many thicknesses as well as plane sources at the interface, but are only for effective dose equivalent based upon rotational normal beam exposure.

The computational methods used in this work were chosen to give an accurate characterization of the energy and angular dependence of the radiation field incident on the body, since dose to the body is very sensitive to the direction of incident radiation, and also to overcome other limitations of earlier calculations. Organ doses were computed for 25 organs in an adult hermaphrodite phantom,[11] modified to include the esophagus and to improve the modeling of the neck and thyroid.

GENERAL DESCRIPTION OF THE CALCULATIONS

Estimating organ dose in a human phantom exposed to radiation from an external source consists of calculating an effect of interest in a geometrically complex object located in an otherwise geometrically simple (one- or two-dimensional) system. This process is mathematically described by the time-independent neutral-particle Boltzmann transport equation, written here in operator notation:

$$\hat{H}\,\Phi(\bar{p}) = S(\bar{p}) \quad , \tag{2}$$

where $\bar{p}$ represents position, energy, and direction phase space, $\Phi(\bar{p})$ is the angular fluence, $\hat{H}$ is the Boltzmann transport operator, and $S(\bar{p})$ is the source. After the solution to Eq. (2) is obtained, the organ dose is computed from the following integral:

$$H_T = \int_{\bar{p}_T} \Phi(\bar{p})\,R(\bar{p})\,d\bar{p} \quad , \tag{3}$$

where H_T is the effect of interest, i.e.,the organ dose; $\bar{p}_T$ is the phase space of tissue or organ T; and $R(\bar{p})$ is the response function, i.e., the contribution to H_T due to unit angular fluence.

In principle, Eqs. (2) and (3) can be solved directly using Monte Carlo methods. However, this direct approach involves a combination of deep penetration (i.e., transport through many mean free paths of air and/or soil) and complex geometry (the human phantom). Calculations of this type require the use of sophisticated variance reduction techniques. Important regions of phase space are often undersampled, and the effect of interest is underestimated. To avoid these difficulties, the solution is broken into two steps: (1) the calculation of the radiation field incident on a cylindrical surface surrounding the human phantom model, and (2) the calculation of organ dose due to a surface source equivalent to the angular flow rate entering the cylinder surrounding the phantom. The phantom was removed from the calculation of the incident radiation field. This may be done since the presence of the phantom in the original problem does not significantly perturb the incoming angular flow rate across the bounding cylinder and is, at most, a second-order effect. The two steps of the calculation are illustrated in Figs. 1 and 2 for the case of a contaminated soil source (an isotropic plane source at depth d_S).

DESCRIPTION OF THE ENVIRONMENTAL SOURCES

The source for the submersion dose calculations is a semi-infinite cloud containing a uniformly-distributed monoenergetic photon emitter of unit strength (1 Bq m^{-3}) surrounding a human phantom standing on the soil at the air-ground interface. The air composition, given in Table 1, is for conditions of 40% relative humidity, a pressure of 760 mm Hg, a temperature of 20 °C, and a density of 1.2 kg m^{-3}.

The source for the contaminated soil calculations is an infinite isotropic plane source of monoenergetic photons of unit strength (1 Bq m^{-2}), located at the air-ground interface or at a specified depth in the soil. Again, a human phantom is standing on the soil at the air-ground interface. As noted later, the organ dose due to a source in the soil that is uniformly distributed from the surface to a specified depth may be readily computed from the doses due to a series of plane sources at different depths. The air composition is the same as for the submersion dose calculations (see Table 1). The assumed soil composition is given in Table 2, and is that for a typical silty soil containing 30% water and 20% air by volume.[7] The soil density was taken to be 1.6×10^3 kg m^{-3}.

It should be noted that the radiation field above the air-ground interface can, in some circumstances, be scaled to account for differences in soil density.[5,10] While the radiation field above the air-ground interface is relatively insensitive to soil composition for a plane surface source[5], this is not true for distributed sources within the soil.

The source for the water immersion calculations is an infinite pool of water containing a uniformly-distributed monoenergetic photon emitter of unit strength (1 Bq m^{-3}). A human phantom is assumed to be completely immersed in the pool. The water density is 1.0×10^3 kg m^{-3} and the composition is that of pure water.

Table 1. Air Composition

Element	Mass Fraction
H	0.00064
C	0.00014
N	0.75086
O	0.23555
Ar	0.01281
Total	1.00000

Table 2. Soil Composition

Element	Mass Fraction
H	0.021
C	0.016
O	0.577
Al	0.050
Si	0.271
K	0.013
Ca	0.041
Fe	0.011
Total	1.000

RADIATION FIELDS FROM SEMI-INFINITE CLOUD AND INFINITE WATER SOURCES

The dose near the air-ground interface from a semi-infinite cloud source has been taken to be one-half that due to an infinite cloud source, following common practice.[2,4,12] Given this approximation, the radiation field may be computed as that due to an infinite cloud source of a monoenergetic photon emitter. In this case, the transport equation has no dependence on spatial position and angle, and may be written strictly as a function of energy. An updated version of the PHOFLUX computer program, developed by Dillman[12] to solve this Volterra-type integral transport equation, was used to compute the energy spectrum of scattered photons in an infinite cloud source as well as the intensity of uncollided photons. For an infinite water source, no approximation is necessary, since the energy-dependent integral transport equation is directly applicable. The PHOFLUX program was also used here to compute the energy spectrum of photons in an infinite water source. Since the methods used for these sources are not new, no further discussion is presented in this paper.

THE RADIATION FIELD FROM CONTAMINATED SOIL SOURCES

In this case, the solution to the transport equation (2) is a function of only one spatial and one angular variable. It can be seen from Eq. (2) that the transport equation is linear with respect to the source term $S(\bar{p})$. Therefore, the fluence $\Phi(\bar{p})$ due to an isotropic infinite source uniformly distributed over a finite depth in the soil may be determined by superposition of the fluence for a series of isotropic infinite plane sources in soil.

The radiation field due to isotropic infinite plane sources at twelve energies from 0.01 to 5.0 MeV was computed for source depths of 0, 0.04, 0.2, 1.0, 2.5, and 4.0 mean free paths in soil (specified at the source energy). These depths were chosen to facilitate an accurate integration during the determination of the dose coefficients for sources uniformly distributed over specified depths. The uncollided angular photon fluence was computed analytically. A spatial-, energy-, and angular-dependent first collision source was generated from the uncollided angular fluence and the cross sections for scattering from the source energy into a series of energy groups. The scattered photon fluence due to the first-collision source was computed using the one-dimensional multigroup discrete ordinates method. Seventy energy groups between 5.3 and 0.00865 MeV were used. The group boundaries were selected to satisfy two criteria: (1) a relatively narrow group was present about each source energy of interest, and (2) photons scattering from any group could scatter to at least two other groups. A subset of the 70 groups was used for each case. The highest energy group was just that group containing the source, and the lowest group was that containing the low-energy cutoff, determined by $\lambda_s + 14$, where λ_s is the Compton wavelength at the source energy. Since the maximum change in Compton wavelength is 2 for a single scatter, this cutoff ensures that a minimum of seven scatters is considered. The only exception to our use of the low-energy cutoff was for the 10 keV sources, in which case only 6 groups were used. At this energy, most photons are immediately absorbed, due to the high photoelectric cross section, and the scattered photon fluence decreases quite rapidly with decreasing energy.

In all calculations, the thickness of the air medium was three mean free paths (at the source energy). For the plane sources at depths of 0, 0.04, 0.2, and 1.0 mean free paths, the thickness of the soil medium was taken as three mean free paths (at the source energy). For the sources at depths of 2.5 and 4 mean free paths, the soil thicknesses were taken as 3.5 and 5 mean free paths, respectively. These thicknesses of air and water ensure that photons scattered beyond the problem boundaries would have to travel a minimum of six mean free paths from the source plane to reach the phantom location, and thus make no significant contribution to organ dose.

In transport problems involving an isotropic plane source, the angular fluence has a singularity at the source plane for directions parallel to the plane which cannot be accommodated by the discrete ordinates formulation. To avoid the numerical problems associated with the singularity, the uncollided angular fluence is computed analytically. Then, a first-collision source; i.e., a distributed source based on the spatial, energy, and angular distribution of photons produced by the first collision of source photons, is calculated from the analytic uncollided angular fluence. In photon transport, a collision which leads to secondary photons can include pair production as well as Compton scatter. The first-collision source, averaged over the spatial mesh cells of the discrete ordinates formulation, is taken to be the source term in the transport equation, which is solved for the angular fluence of scattered photons. Cell-averaged angular first-collision sources have no singularities, even in cells adjacent to the source plane. It should also be noted that the scattered angular fluence has a singular component at the source plane, and, at short distances from the source, will have components of large magnitude in directions nearly parallel to the plane. It has been demonstrated[12] that discrete ordinates calculations for the scattered fluence due to a first-collision source must use an angular mesh which has several directions nearly parallel to the source plane. Failure to do so will give rise to scalar fluences that are depressed or enhanced in a physically unrealistic manner in regions near the source. Since, for plane geometries, the fluence near an interface is better represented when the angular quadrature directions are chosen from a double-P_N Gauss quadrature set, a DP_{15} quadrature set with 32 directions was selected for these calculations.

A discrete ordinates solution of the transport equation in which the cross sections are represented by truncated Legendre polynomial expansions can give rise to physically unrealistic negative angular fluences, due to the negative oscillations in the cross section expansions. This problem is worse for highly anisotropic sources, narrow energy groups, and highly anisotropic scatter, e.g., Compton scatter of photons. It has been demonstrated[13,14] that this problem may be eliminated by the use of the exact-kernel cross section representation, i.e., use of a discrete scattering matrix rather than a polynomial representation. In this work, a one-dimensional multigroup discrete ordinates code that uses the exact-kernel representation of group-to-group transfer cross sections,[13] was used to perform the radiation field calculations.

The accuracy of the solutions was checked by comparing the energy and angular dependence of the air kerma (i.e., *dose to air*) 1 m above a 1.25 MeV plane source at the air-ground interface with the calculations of Beck and de Planque[5] and with the calculations and measurements given in the Shielding Benchmark Problems report.[15] Excellent agreement was found in both cases. The angular dependence of the air kerma one meter above the air-ground interface is shown in Figs. 3 and 4 for 100 keV sources. The ninety-degree angle corresponds to radiation incident from the horizon.

ORGAN DOSE FROM EXTERNAL FIELDS

The organ doses due to the external radiation fields were computed using the continuous energy Monte Carlo photon transport code ALGAMP.[16] For air submersion and water immersion, calculations were performed for twelve monoenergetic sources ranging from 0.01 to 5.0 MeV, sampled from a cosine current source, which corresponds to an isotropic fluence; and sampled uniformly on the curved and end surfaces of a cylinder surrounding the phantom. For contaminated soil, the uncollided and scattered angular fluences from an isotropic plane source of radiation were computed as a function of energy, angle, and height above the air-ground interface as described earlier. These fluence data were used to construct an angular current source on a cylinder surrounding the phantom as a function of position, energy, and polar angle. Ten million histories were sampled for each calculation. The organ doses from the monoenergetic sources incident on the phantom were folded with the spectra generated by the PHOFLUX code for the air submersion and water immersion sources and normalized to unit source strength to produce the final organ dose coefficients for monoenergetic sources in contaminated air and water. For submersion and immersion, the dose coefficients are inversely proportional to the density of the source medium, so scaling to a different density is straightforward. Since the discrete ordinates calculations were performed for a first-collision source derived from a unit strength plane source, the organ dose coefficients are computed directly by the Monte Carlo calculations; no further normalization is needed.

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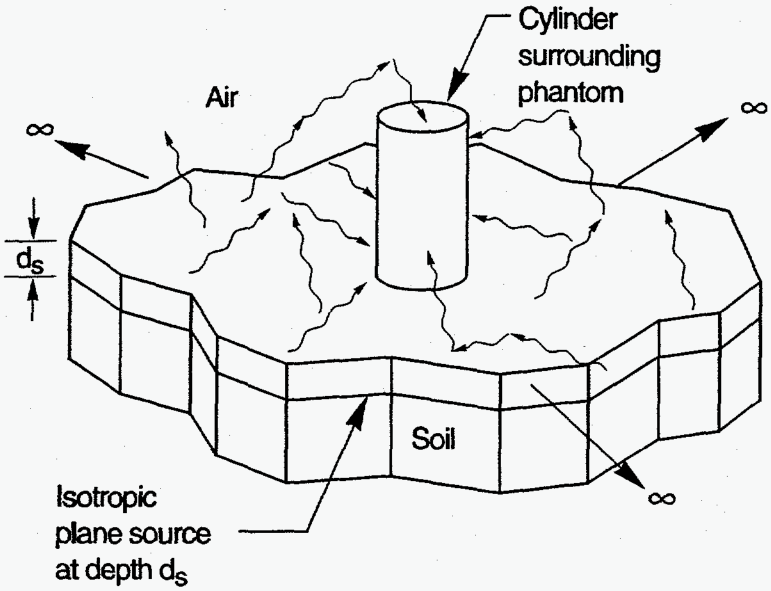

Fig. 1. Calculation of radiation field due to a contaminated ground plane.

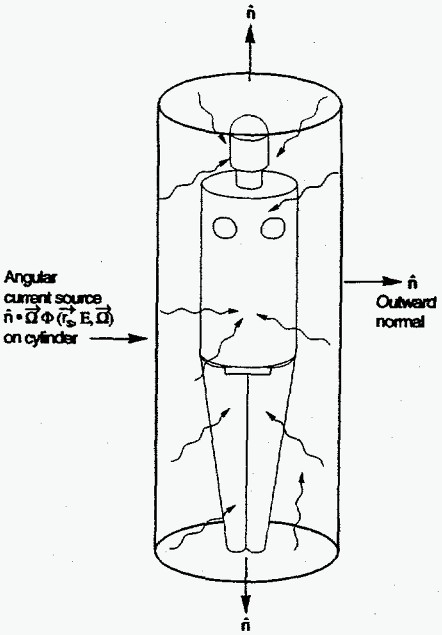

Fig. 2. Calculation of organ dose from an angular current source on the cylinder.

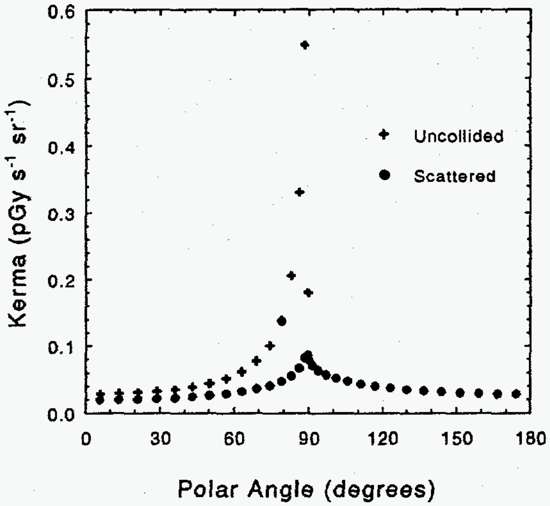

Fig. 3. Angular dependence of air kerma for a 1 Bq m^{-2} isotropic plane surface source.

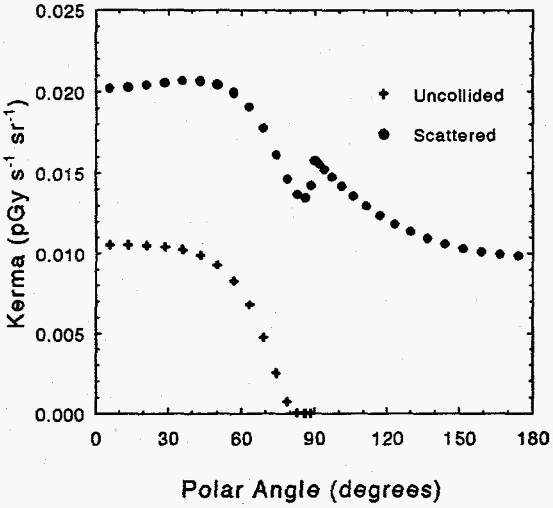

Fig. 4. Angular dependence of air kerma for a 1 Bq m^{-2} 100 keV isotropic plane source 1 mean free path deep.