A SEMIEMPIRICAL FORMULA FOR THE ANGULAR DIFFERENTIAL NUMBER ALBEDO OF LOW-ENERGY PHOTONS

by

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Low-energy photon reflection from water, aluminium, and iron is simulated by the MCNP code and results are compared with similar Monte Carlo calculations. For the energy range from 60 to 150 keV and for the normal incidence of initial photons, a universal shape of the normalized angular differential number albedo is observed and after that fitted by the curve fitting procedure in form of a second order polynomial over the polar angle. Finally, a one-parametar formula for the angular differential number albedo is developed and verified for water through the comparison of results with the semiempirical formulae and Monte Carlo calculations of other authors.

Key words: photon reflection, angle differential number albedo, Monte Carlo method, semiempirical formula

INTRODUCTION

It has already been pointed out in radiation protection literature that X-ray diagnostic techniques irradiate the global population by more than 90% and that, from the point of view of radiation protection, there is plenty of room for a significant collective dose reduction in medical diagnostics. In order to establish a qualified estimation of individual and collective exposures and adequate radiation protection measures, there is a constant need for a good knowledge of the space, angle and energy distribution of reflected radiation. Apart from experimental investigations in this field, at least some of these studies are theoretical by nature, mostly those concerning the problem of low-energy photon reflection [1, 2].

In the past half a century, the interest of the scientific community has been mainly focused on the high energy domain of neutron and photon radiation in close agreement with the typical energy regions of radiation from nuclear power plants, different experimental nuclear facilities and facilities designated for specific military purposes. Therefore, the high energy domain has been the prime subject of analysis in a number of monographs [3-5], and earlier scientific papers [6, 7]. Interest in the photon energy domain below or around 100 keV may be regarded as a reliable sign of huge progress in nuclear medical practice. In theoretical studies, the Compton scattering for photons with energies below 100 keV may be treated with some simplification, for instance, in the Thomson form which allows the determination of reflected photons or photon albedo coefficients by analytical or semianalytical methods [8, 9]. In this manner, it was possible to determine differential or integral albedo coefficients by means of simple analytical functions. Moreover, some helpful redefinitions in the realm of theoretical studies of albedo coefficients were taken into account [10, 11].

In this paper, we propose a new semiempirical expression for the determination of the angular differential number albedo for low-energy photons. Instead of following a common albedo concept based on the combination of photon single scattering and multiple scattering components which leads to the two-parameter formula, we make use of the advantage that the normalized angular differential number albedo is a universal function for water, aluminium, and iron in the energy range from 60 to 150 keV, and derive an one-parameter analytical for-
PHOTON NUMBER ALBEDO

The photon albedo denotes the ratio of the flow rate of photons emitted from a small portion of the surface to the flow rate of the primary photons incident upon that surface \([5, 12]\); in this way, it articulates the reflecting features of a surface. It is obvious that reflection does not strictly suppose merely the surface scattering of photons, but presumes, primarily, photon penetration through the material and its interactions with nuclei and electrons. Instead of the exact deterministic or stochastic treatments of photon transport and reflection which comprise the spatial, energy and angular distribution of initial and backscattered photons, as well as the structural characteristics and geometry of the reflecting material, as a simplified technique, the albedo method is based on some quite correct assumptions:

- the distance between points of photon entry and photon emergence is neglected. This is an acceptable simplification for radiation shields with dimensions greater than a few mean free paths and for incident photons with a more or less constant intensity in lateral directions,
- reflecting materials are plane, homogeneous and infinite in thickness and laterally, i.e., they can be geometrically modeled as a half-space. If the finite thickness of the reflector is greater than two mean free paths, this assumption is fully adequate, and
- air-scattering may be neglected.

Basic definitions

The photon albedo is defined on the premise that a broad beam of parallel and monoenergetic initial photons, characterized by energy \(E_0\) and polar angle \(\theta_0\), impinge the boundary surface of the material, and that the reflected photons emerge from the surface with energy \(E\), and direction defined by the polar angles \(\theta\) and the azimuthal angle \(\phi\). Here, the incident polar angle \(\theta_0\) is measured in agreement to the surface inward normal, while the exit polar angle \(\theta\) is determined with respect to the outward normal. As for the value of the photon albedo, there is full equivalence between the two similar monoenergetic reflection problems: one induced by a broad parallel beam of the initial photons and the other produced by the initial monodirectional beam.

The double angular-energy differential number albedo is given as a ratio between photon number flow rates

\[
a_N(E_0, \theta_0, \theta, \phi) = \frac{J_1(E, \theta, \phi)}{J_0} = \frac{\cos \theta \Phi (E, \theta, \phi)}{\cos \theta \Phi_0}
\]

In eq. (1), \(J_0\) and \(J_1\) stand for the incident and outgoing flow rates, while \(\Phi_0\) and \(\Phi_1\) denote the fluxes of the incident and reflected photons. The angular differential number albedo is defined as an integral of \(a_N(E_0, \theta_0; E, \theta, \phi)\) over all energies

\[
a_N(E_0, \theta_0, \theta, \phi) = \int_0^{E_0} a_N(E_0, \theta_0; E, \theta, \phi) dE
\]

Similarly, the total number albedo \(a_N(E_0, \theta_0)\) is defined as an integral of the angular differential number albedo \(a_N(E_0, \theta_0; \theta, \phi)\) over all reflected directions

\[
a_N(E_0, \theta_0) = \frac{2\pi}{\int_0^{\pi/2} a_N(E_0, \theta_0; \theta, \phi) \sin \theta d\theta}
\]

In the case of initial photon normal incidence, \(\theta_0 = 0^\circ\), albedo values do not depend on the azimuthal angle \(\phi\), i.e., the reflected photons are azimuthally independent. However, albedo values rely on the polar variable, initial photon energy and the physical nature of the reflector.

Calculation of the photon albedo by the Monte Carlo method

In order to analyze the photon albedo problem and establish a new expression for the angular differential number albedo, we have computed the double angular-energy differential photon albedo of a homogeneous semi-infinite medium separated from the void by a plane surface. We have considered water, aluminium, and iron materials and have applied the Monte Carlo simulation. The MCNP-4C code [13] is used with the standard photon nuclear data library MCPLIB2. The data for the reflected photons are collected in 9 angular and up to 20 energy groups for perpendicularly injected photons of the initial energy in the range from 40 to 1000 keV. Simulations have been realized with 10^8 or 10^9 photon histories, resulting in a statistical uncertainty of less than 1% for the total number albedo coefficient and less than 10% for each angular-energy interval. The number of energy groups for each simulation was chosen according to the initial photon energy, in order to en-
sure the required statistical uncertainty of the results. Here, we demonstrate a portion of the results concerning the angular differential number albedo and the total number albedo.

The angular differential number albedo for the three materials and perpendicularly injected photons of 60 keV initial energy is shown in fig. 1. Our results (solid symbols) are compared with the Monte Carlo calculations of other authors (open symbols) [3]. For water and aluminium, the agreement between the two Monte Carlo simulations is satisfactory, with a relative difference of around 10%, while the discrepancy for the iron material has proven to be greater (the relative difference being about 20%). This inconsistency should mainly be attributed to the uneven angular-energy intervals of the compared simulations and the modest statistics of the Monte Carlo techniques in [3].

For the same materials in the energy range of 20 keV up to 1000 keV, the total number albedo $a_{N}(E_0, \theta_0)$ is shown in fig. 2. Again, our results are presented by solid symbols, while the open symbols stand for water and iron data of the other authors [4]. The agreement between our simulations and the reference data is almost perfect. For example, in the case of water, the relative discrepancy of the results is around 2% for energies below 200 keV, and a few per mille for photon energies between 200 keV and 1000 keV. A similar conclusion is valid for iron, but with a slightly weaker congruence of results than for water.

A SEMIEMPIRICAL FORMULA FOR THE PHOTON ALBEDO

In order to derive a simple analytic expression for approximating the numerical values of the angular differential number albedo, we have to use the precise numerical data of the backscattered radiation for selected materials and specified energy ranges. For this purpose, we have applied only a part of our MCNP simulation data for water, aluminium, and iron materials, as well as a part from a more comprehensive set of data for the same materials acquired by the Monte Carlo simulation and for the three initial photon energies: 60 keV, 100 keV, and 150 keV [4]. Moreover, we have reduced our analysis to the case of normal incidence ($\theta_0 = 0^\circ$).

In fig. 3, the angular differential number albedo is presented in the form of full and dashed lines so as to emphasize the shape of the angular dependence of these functions. One can note a strong dependence of the angular differential number albedo on the type of material and initial photon energy. As a consequence of this common tendency, the semiempirical formulae previously obtained by fitting the corresponding set of albedo data [3-5, 7, 12], have suffered from the large numbers of energy and material dependent fitting parameters.

Therefore, we propose a more simplified technique based on the universal form of the normalized albedo function, instead of the albedo function itself.
The normalized angular differential number albedo

If the data on the angular differential number albedo obtained by the Monte Carlo simulations are normalized to the unit value of the photons reflected perpendicularly backward, which corresponds to the zero value of the polar angle \( (\theta_0 = 0^\circ) \), albedo functions assume an almost universal form. For example, the three distinct curves describing photon reflection from water (previously, fig. 3), coalesce almost entirely, if drawn in the normalized form (fig. 4). Except for the polar angle \( \theta \approx 90^\circ \), when the differential angular number albedo has the lowest values anyway, the differences between the curves in fig. 4 are around 1-2%, or less.

Similarly, the normalized angular differential number albedo for all three materials studied here, and for the same initial photon energy of 60 keV, are presented in fig. 5. In contrast to the emphasized differences between the three corresponding curves in fig. 3, it is, once again, evident that the three curves in fig. 5 are very close to each other. However, as the albedo value is predominately influenced by the structure of relevant materials, the relative differences among the curves are more pronounced than in fig. 4. If one takes the normalized angular differential number albedo of aluminium as an acceptable reference value, the relative differences of water data fall within 3% and the data for iron within the interval of 6%.

In addition, it has been verified that the relative differences of normalized albedo functions for water, aluminium, and iron do not change essentially within the range of selected initial photon energies. Therefore, the same universal form of a normalized function may be proposed for all three materials and energy ranges from 60 to 150 keV.
Formula for the angular differential number albedo

Supposing the universal form of the normalized angular differential number albedo for the perpendicular incidence of the initial photons, we can express \( a_N(E_0, \theta_0 = 0^\circ; \theta) \) as a product of two functions with the energy variable \( E_0 \) separated from the angular variable \( \theta \)

\[
a_N(E_0, \theta_0 = 0^\circ; \theta) = A(E_0) f(\theta)
\] (4)

Here, we assume that the angular component \( f(\theta) \) is a polynomial of the second order over \( \theta \)

\[
f(\theta) = \sum_{k=0}^{2} a_k \theta^k
\] (5)

In eq. (5), the polar variable \( \theta \) is measured in radians and coefficients \( a_k \) have the values of \( a_0 = 1.0072 \), \( a_1 = -0.05953 \) and \( a_2 = -0.38169 \). These coefficients are determined by dealing with the normalized Monte Carlo simulation data for aluminium, and 100 keV initial photons [3], while applying the least square curve fitting procedure.

From eqs. (3) and (4), it is easy to derive the energy dependent coefficient \( A(E_0) \) by using the total number albedo \( a_N(E_0, \theta_0 = 0^\circ) \)

\[
A(E_0) = \frac{a_N(E_0, \theta_0 = 0^\circ)}{2\pi [a_0 + a_1 + (\pi - 2)a_2]} = \frac{a_N(E_0, \theta_0 = 0^\circ)}{3.2165}
\] (6)

In tab. 1, for photon energies of 60 keV up to 200 keV regarding all three materials, the numerical values of the total number albedo \( a_N(E_0, \theta_0 = 0^\circ) \) determined by the MCNP-4C code are given, as well as the calculated coefficients \( A(E_0) \).

Comparison of results

We compare our result, eqs. (4-6), with some semiempirical expressions already well known [3, 4]. These expressions are derived assuming that the photon reflection, on the whole, should be given by a linear combination of the terms for single-scattered and many-scattered photons. One of the most straightforward formulae for the angular differential number albedo is

\[
a_N(E_0, \theta_0; \theta, \varphi) = \frac{\cos \theta}{\cos \theta + \cos \theta_0}.
\]

\[
[C_N K_{E}(E_0, \theta_s) \cdot 10^{26} + C'_N]
\] (7)

where \( K_{E}(E_0, \theta_s) \) is the Klein-Nishina energy scattering cross-section for photons and \( \theta_s \) is the scattering angle which is defined by \( \cos \theta_s = -\cos \theta \) for the normal incidence of initial photons. The two parameters \( C_N \) and \( C'_N \), which come from a fit of the formula (7) to experimental or Monte Carlo data, are tabulated for different materials and various initial photon energies [3].

A more efficient variant of formula (7) has also been provided in literature [4]

\[
a_N(E_0, \theta_0; \theta, \varphi) = \frac{\cos \theta}{\cos \theta + \cos \theta_0} \sqrt{1 + \frac{E_0}{0.511} (1 - \cos \theta_s) + [A_N K_{E}(E_0, \theta_s) \cdot 10^{26} + B_N (H_p(\cos \theta_s) H_p(\cos \theta) - 1)]}
\] (8)

In eq. (8), \( K_{E}(E_0, \theta_s) \) is the Klein-Nishina number scattering cross-section, \( H_p \) is the Chandrasekhar function tabulated precisely for the different values of \( \cos \theta \) and parameter \( p \) (p is the ratio of the photon scattering cross-section and the photon total cross-section). For selected values of \( E_0 \) and for a number of common materials, the values of \( A_N \) and \( B_N \) fitting coefficients can be found in tables [4].

In fig. 6, we compare the values of the angular differential number albedo obtained by the Monte Carlo simulations and by different semiempirical formulae for water and initial photon energy of 60 keV. Full lines represent our semiempirical result, eqs.

<table>
<thead>
<tr>
<th>( E ) [keV]</th>
<th>Water ( a_N(E_0, \theta_0 = 0^\circ) )</th>
<th>Water ( A(E_0) )</th>
<th>Aluminium ( a_N(E_0, \theta_0 = 0^\circ) )</th>
<th>Aluminium ( A(E_0) )</th>
<th>Iron ( a_N(E_0, \theta_0 = 0^\circ) )</th>
<th>Iron ( A(E_0) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>0.4182</td>
<td>0.1300</td>
<td>0.2907</td>
<td>0.0904</td>
<td>0.1092</td>
<td>0.0339</td>
</tr>
<tr>
<td>100</td>
<td>0.4001</td>
<td>0.1244</td>
<td>0.2163</td>
<td>0.0672</td>
<td>0.0444</td>
<td>0.0138</td>
</tr>
<tr>
<td>80</td>
<td>0.3734</td>
<td>0.1161</td>
<td>0.1731</td>
<td>0.0538</td>
<td>0.0302</td>
<td>0.0094</td>
</tr>
<tr>
<td>60</td>
<td>0.3192</td>
<td>0.0992</td>
<td>0.1141</td>
<td>0.0355</td>
<td>0.0162</td>
<td>0.0050</td>
</tr>
</tbody>
</table>
(4–6), and solid circles stand for our simulations done by the MCNP code. The results of the Monte Carlo simulations [3] are given by the open circles, and the two other semiempirical expressions, eqs. (7–8), which come from references [3] and [4], are presented by the cross and star symbols, respectively. It is evident that, for water and 60 keV initial photons, our formula (4) is in full agreement with the Monte Carlo simulation [3], in spite of the fact that the normalized universal function f(θ) has been obtained by fitting the Monte Carlo simulation data [3] for aluminium at 150 keV. Unexpectedly, the agreement between this simulation data and the values obtained by the referent formula (7) is rather poor, especially for the small reflection angle θ = 0. It should be emphasized that the formula (7) has also been obtained by fitting the same set of data [3].

However, our MCNP simulations agree quite well with the more sophisticated referent expression (8) and differ for about 10% from the old Monte Carlo simulations [3]. We have already explained that the disagreement between the two Monte Carlo simulations comes from the different preset angular-energy intervals, as well as the modest statistics related to the older one. Moreover, our simulation seems approved by the results of the advanced expression (8) and this analysis points to the conclusion that our albedo formula should be based on our new MCNP simulation data, rather than on the older data obtained from literature.

CONCLUSION

Contrary to the already existing two-parameter formulae, eqs. (7, 8), the semiempirical formula (4) derived in this paper is a one-parameter function. It provides a clear analytical means for calculating the angular differential number albedo precisely enough for most engineering purposes. Compared to formula (7), it is more simple and more accurate, while in relation to expression (8), it is more self-sufficient, depending entirely on the A(E₀) parameter given in tab.1. However, formula (4) is restricted to a normal incidence of initial photons and the limited energy range from 60 to 150 keV. To remove these restrictions as much as possible, we need to investigate a more general reflection problem related to the oblique photon incidence in the larger energy interval by means of the Monte Carlo simulation.

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ЈЕДНА СЕМИЕМПРИЈСКА ФОРМУЛА ЗА ДИФЕРЕНЦИЈАЛНИ БРОЈНИ АЛБЕДО НИСКОЕНЕРГЕТСКИХ ФОТОНА

Помоћу МСНР програма симулирана је рефлексија нискоенергетских фотона од воде, алуминијума и гвожђа и резултати су упоређени са вредностима Монте Карло прорачуна. У енергетском подручју од 60 до 150 keV и за нормални упад иницијалних фотона, уочен је заједнички облик нормираног диференцијалног бројног албеда коме је фитовањем дато формулума другог реда по поларном углу. Потом је изведена једнопараметарска формулума за диференцијални бројни албедо која је за рефлексију фотона од воде потврђена поредењем резултата са семиепријским формулама и резултатима Монте Карло прорачуна других автора.

Кључне речи: рефлексија фотона, диференцијални бројни албедо, Монте Карло метода, семиепријска формула