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Computer Physics Communications 174 (2006) 391–395
Computer Physics Communications
www.elsevier.com/locate/cpc

PDSW: A program for the calculation of photon energy distribution resulting from radioactive elements in seawater ☆

D.S. Vlachos, T.E. Simos *

University of Peloponese, Department of Computer Science and Technology, 22100 Tripoli, Greece

Received 18 July 2005; received in revised form 29 September 2005; accepted 23 October 2005

Available online 15 December 2005

Abstract

Photons, when emitted from radioactive sources in seawater, are subsequent to multiple scattering mechanisms, namely the photoelectric effect, the Compton scattering and the pair production effect. Thus, the monoenergetic emission of photons in seawater will result in equilibrium in a distribution of photons with different energies. PDSW is a MATLAB program which calculates this distribution and can be found useful for the characterization of measured spectra obtained by gamma detectors such as NaI(Tl). PDSW has been developed as an autonomous MATLAB function in order to make possible to integrate it in other applications. All calculations are performed using a typical value for seawater salinity (3.5%).

Program summary

Title of program: PDSW
Catalogue identifier: ADWW
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADWW
Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland
Computer: x86
Operating systems: Windows
Programming language used: MATLAB
Memory required: 10 Mb
Number of bits in a word: 32
Number of processors used: 1
Vectorized or parallelized?: no
Number of bytes in distributed program, including test data, etc.: 16 378
Number of lines in distributed program, including test data, etc.: 3004
Distribution format: tar.gz
CPC Program Library subprograms used: none
Nature of physical problem: Calculation of photon energy distribution in seawater taking into account the photoelectric effect, the Compton scattering and the pair production effect.
Method of solution: Analytical calculation of the continuity equation for photon energy distribution in seawater and numerical integration of this equation in equilibrium.
Restrictions on the complexity of the program: Very small resolution results in large memory requirements and high execution time.
Typical running time: (Maximum energy-minimum resolution) 20 s
Unusual features of the program: none

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

* Corresponding author. Address: Prof. T.E. Simos, 26 Menelaou Street, GR-175 64 Athens, Greece. Fax: +30 210 94 20 091.
E-mail addresses: dvlachos@ncmr.gr (D.S. Vlachos), simos@uop.gr (T.E. Simos).

0010-4655/$ – see front matter
doi:10.1016/j.cpc.2005.10.010

PACS: 29.30.Kv; 29.40.Mc

Keywords: Photon distribution; Seawater

1. Introduction

In the last decades the systematic control of radioactive pollution of the seawater has been made an urgent matter. The marine environment may receive radioactive inputs via nuclear reactors or/and via nuclear accidents from neighboring countries. The natural radiation that can be measured in the seawater comprises the ^{40}K and the decay products of the ^{238}U and ^{232}Th series, most notably the ^{214}Bi, ^{214}Pb and ^{208}Tl isotopes. The measurable anthropogenic radioactivity in the seawater concerns mainly the following gamma emitters: ^{137}Cs, ^{134}Cs, ^{99m}Tc (from ^{99}Mo) and ^{60}Co [2].

The main problem encountered in radioactivity measurement in seawater (which is not faced in air), is the photon energy variation caused by the scattering of photons with the atoms in the seawater. Photons, after their emission and before they reach the detector, interact with seawater atoms and can change their energy due to Compton scattering or pair production, or disappear due to the photoelectric effect. The effect of the interaction of photons with the seawater can be formulated as follow. Let $S(E)$ be the source spectrum and $M(E)$ the measured one. In air,

$$M(E) = \int_0^\infty R(E, V) \cdot S(V)\,\mathrm{d}V, \tag{1}$$

where $R(E, V)$ is equal to the number of photons that will be recorded at energy E when one photon is emitted with energy V. The function $R(E, V)$ is known as the *transfer function* of the detector. In seawater, this relation is more complicated. If a photon with initial energy U is emitted, then there is a probability $P(V, U)$ that the photon will reach the detector surface with a final energy V. Thus, the measured spectrum now will be given by:

$$M(E) = \int_0^\infty R(E, V) \cdot \left(\int_0^\infty P(V, U) \cdot S(U)\,\mathrm{d}U \right) \mathrm{d}V. \tag{2}$$

Changing the order of integration in Eq. (2), the function

$$\hat{R}(E, U) = \int_0^\infty R(E, V) \cdot P(V, U)\,\mathrm{d}V \tag{3}$$

can be regarded now as the *modified transfer function* of the detector, for underwater operation. The measured spectrum of an underwater detector can now be expressed as:

$$M(E) = \int_0^\infty \hat{R}(E, V) \cdot S(V)\,\mathrm{d}V. \tag{4}$$

The motivation for the calculation of $P(V, U)$ is now clear. Knowing the modified transfer function of the detector, all the techniques applied to Eq. (1) for extracting information about the source spectrum, can be applied also to underwater spectra described by Eq. (4).

2. Theoretical background

Although a large number of possible interaction mechanisms are known for gamma rays in matter, only three major types play an important role in radiation measurement: *photoelectric absorption*, *Compton scattering* and *pair production*. All these processes lead to the partial or complete transfer of the gamma ray photon energy to electron energy. They result in sudden and abrupt changes in the gamma-ray photon history, in that the photon either disappears entirely or is scattered through a significant angle.

In the photoelectric absorption process, a photon undergoes an interaction with an absorber atom in which the photon completely disappears. In its place, an energetic *photoelectron* is ejected by the atom from one of its bound shells. The interaction is with the atom as a whole and cannot take place with free electrons. Suppose now that in a material medium, there is a uniform in space distribution of photons. Let $n(\alpha, t)$ be the concentration of photons with energy α at time t. Each photon, undergoes a photoelectric absorption process with probability $P(\alpha)$ (P is a function of photon energy) and consequently the number of photons with energy α that disappear is $n(\alpha, t) \cdot P(\alpha)$. Thus:

$$\frac{\partial n(\alpha, t)}{\partial t} \propto -n(\alpha, t) \cdot P(\alpha). \tag{5}$$

The interaction process of Compton scattering takes place between the incident gamma ray photon and an electron in the absorbing material. In this mechanism, the incoming photon is deflected through an angle θ with respect to its original direction. The photon transfers a portion of its energy to the electron which is then known as a *recoil electron*. Because all angles are possible, the energy transferred to the recoil electron can vary from zero to a large fraction of the photon energy. Again, we can assign a probability $C(\alpha, \alpha')$ for a photon with initial energy α that undergoes a Compton scattering process, leaving the photon finally with energy α'. Note here that $C(\alpha, \alpha')$ is zero if $\alpha < \alpha'$ since the photon cannot gain energy. The total number of photons with initial energy α that alter their energy through the Compton scattering mechanism is $\int_0^\alpha n(\alpha, t) \cdot C(\alpha, v)\,\mathrm{d}v$. On the other hand, the total number of photons that result in energy α through the same mechanism is $\int_\alpha^\infty n(v, t) \cdot C(v, \alpha)\,\mathrm{d}v$. Consequently

$$\frac{\partial n(\alpha, t)}{\partial t} \propto \int_\alpha^\infty n(v, t) \cdot C(v, \alpha)\,\mathrm{d}v - \int_0^\alpha n(\alpha, t) \cdot C(\alpha, v)\,\mathrm{d}v. \tag{6}$$

Finally, the interaction process of pair production occurs in the field of a nucleus of the absorbing material and corresponds to the creation of an electron–positron pair at the point of complete disappearance of the incident photon. Because an energy of $2m_0c^2$ (m_0 is the electron rest mass and c the speed of light) is required to create the electron–positron pair, a minimum gamma ray energy of 1.022 MeV is required to make the process energetically possible. The excess photon energy appears in the form of kinetic energy shared by the electron–positron pair. Once the positron's kinetic energy becomes very low, it will annihilate or combine with a normal electron in the absorbing medium. At this point, both disappear, and they are replaced by two annihilation photons of energy m_0c^2 (0.511 MeV). Again we can assign a probability $R(\alpha)$ that a photon with energy α disappears due to the pair production interaction. Thus, the total number of photons that disappear is $n(\alpha,t)\cdot R(\alpha)$. On the other hand, a number of photons with energy m_0c^2 will be created. Using a dimensionless representation for the energy ($\alpha = \text{Photon energy}/m_0c^2$), the number of photons that are created is $2\delta(\alpha-1)\cdot\int_2^\infty n(v,t)\cdot R(v)\,\mathrm{d}v$ where δ is the Dirac delta function with the properties:

$$\delta(x)=0, \qquad x\neq 0,$$

$$\int_{-\epsilon}^{\epsilon}\delta(x)\,\mathrm{d}x=1, \quad \epsilon>0.$$

Consequently:

$$\frac{\partial n(\alpha,t)}{\partial t}\propto 2\delta(\alpha-1)\cdot\int_2^\infty n(v,t)\cdot R(v)\,\mathrm{d}v - n(\alpha,t)\cdot R(\alpha). \tag{7}$$

In equilibrium, $n(\alpha,t)$ is independent on time. Combining Eqs. (5), (6) and (7), the photon energy distribution can be described by the following equation:

$$0=\sum_i G^i\delta(\alpha-\alpha_0^i)+\int_0^\infty n(v)C(v,\alpha)\,\mathrm{d}v + 2\delta(\alpha-1)\int_0^\infty n(v)R(v)\,\mathrm{d}v - n(\alpha)S(\alpha), \tag{8}$$

where: $G^i\delta(\alpha-\alpha_0^i)$ is the generation of photons at energy α, when G^i photons per second are generated with energy α_0^i. This term is necessary to account for the radioactive sources. The term $S(\alpha)$ collects all the mechanisms that alter the energy of a photon and is given by:

$$S(\alpha)=P(\alpha)+R(\alpha)+\int_0^\alpha C(\alpha,v)\,\mathrm{d}v. \tag{9}$$

Eq. (8) is linear in the sense that if n_1 is the photon energy distribution caused by a source that emits photons with energy α_0^1 and n_2 is the photon energy distribution caused by a source that emits photons with energy α_0^2, then if both sources are present, the photon energy distribution will be n_1+n_2. Consequently, it is adequate to solve Eq. (8) for a single source that emits at energy α_0, G photons per unit time and unit volume.

Due to the existence of the delta functions in Eq. (8), the solution can be written as:

$$n(\alpha)=\lambda(\alpha)+k\cdot\delta(\alpha-\alpha_0)+m\cdot\delta(\alpha-1), \tag{10}$$

where $\lambda(\alpha)$ is a smooth function in energy α with $\lambda(\alpha)=0$ when $\alpha\geqslant\alpha_0$. Substituting the expression for $n(\alpha)$ in Eq. (8), we can calculate the coefficients k and m as follow:

$$k=\frac{G}{S(\alpha_0)}, \tag{11}$$

$$m=2\cdot\frac{k\cdot R(\alpha_0)+\int_0^\infty\lambda(v)R(v)\,\mathrm{d}v}{S(1)}. \tag{12}$$

Substituting the results from Eqs. (10), (11) and (12) in Eq. (8), the delta functions are eliminated and the resulting equation for $\lambda(\alpha)$ is:

$$\frac{G\cdot C(\alpha_0,\alpha)}{S(\alpha_0)}+2\cdot\frac{\frac{G}{S(\alpha_0)}R(\alpha_0)+\int_0^\infty\lambda(v)R(v)\,\mathrm{d}v}{S(1)}C(1,\alpha) + \int_0^\infty\lambda(v)C(v,\alpha)\,\mathrm{d}v-\lambda(\alpha)S(\alpha)=0. \tag{13}$$

For the numerical solution, the functions $R(v)$ and $S(\alpha)$ are calculated from XCOM software [1]. The function $C(v,\alpha)$ is calculated from the Klein–Nishina formula [3] which gives for the angular distribution of scattered photons:

$$p(\theta)=C_M\pi r_0^2\left(\frac{v}{\alpha}\right)^2\left(\frac{v}{\alpha}+\frac{\alpha}{v}-\sin^2\theta\right),$$
$$v=\frac{\alpha}{v+\alpha(1-\cos\theta)}, \tag{14}$$

where α is the initial photon energy, v the resulting photon energy after the scattering, r_0 the classical electron radius and C_M is a constant that depends on the absorbing medium and is related to the density of scattering centres. Changing now the variable from θ to v we get

$$C(\alpha,v)=C_M\pi r_0^2\frac{1}{\alpha^2}\left[\frac{v}{\alpha}+\frac{\alpha}{v}-1+\left(1-\frac{1}{v}+\frac{1}{\alpha}\right)^2\right] \times\left[u\left(v-\frac{\alpha}{v+2\alpha}\right)-u(v-\alpha)\right], \tag{15}$$

where u is the step function, whose role is to ensure that the scattered photon can neither increases its energy nor results in an energy lower than the Compton edge.

Eq. (13) can be rewritten in the form

$$\lambda(a)=B(a_0,a)+\int_0^\infty D(a,v)\lambda(v)\,\mathrm{d}v, \tag{16}$$

Table 1

Function [e,l,k,m] = pdsw(e0,res)	
IN	
e0	the energy at which photons are generated in seawater in MeV
res	the desired energy resolution in MeV. If zero or negative value passed, the default resolution 0.004088 MeV is used
OUT	
e	a vector containing the energy values in MeV at which the photon concentration is calculated
l	a vector containing the photon concentration at energies given in e
k	the peak height at e0
m	the peak height at 0.511 MeV due to pair production

where

$$B(a_0,a)=\frac{GC(a_0,a)S(1)+2GR(a_0)C(1,a)}{S(1)S(a)S(a_0)},$$

$$D(a,v)=2\frac{C(1,a)}{S(1)S(a)}R(v)+\frac{C(v,a)}{S(a)}.$$

Since $\lambda(a)=0$ when $a>a_0$ and $D(a,v)=0$ when $v<a$ we can get

$$f(t)=g(t)+\int_0^t K(t,s)f(s)\,\mathrm{d}s, \tag{17}$$

where

$$f(t)=\lambda(a_0-t),\qquad g(t)=B(a_0,a_0-t),$$

$$K(t,s)=D(a_0-t,a_0-s).$$

Eq. (17) can be solved by the extended trapezoidal rule considering a mesh of uniform spacing:

$$t_i=ih,\quad i=0,1,\ldots,N,\quad h=\frac{a_0}{N}. \tag{18}$$

The function f is calculated on points t_i by solving the linear system

$$\left(1-\frac{1}{2}hK_{ii}\right)f_i=g_i+h\sum_{j=1}^{i-1}K_{ij}f_j,\quad i=1,2,\ldots,N, \tag{19}$$

where

$$f_i=f(ih),\qquad g_i=g(ih),\qquad K_{ij}=K(ih,jh).$$

3. Description of the program

The calculation of the photon energy distribution in seawater is performed by the MATLAB function *pdsw* contained in the m-file *pdsw.m*. The definition of this function is as follows (see Table 1).

The function pdsw uses three internal functions, namely C(a,v), R(a) and S(a). C(a,v) implements Eq. (15) for the calculation of the probability for a photon with initial energy a to change its energy to v due to Compton scattering. R(a) calculates the probability for a photon with initial energy a to produce an electron–positron pair. The positron is considered to interact with an electron an thus producing two photons with energy 0.511 MeV. S(a) calculates the probability for a photon with energy a to alter its energy due to all scattering mechanisms. Internal functions R(a) and S(a) use the vectors RR(a) and SS(a) which contain the corresponding probabilities for energies up to 3.066 MeV with a step of 0.004088 MeV. These probabilities have been calculated by the XCOM software [1] for seawater of 3.5% salinity [4]. The calculation at intermediate energies is performed by interpolation.

Finally, function pdsw solves the linear system (19) and calculates constants k and m by Eqs. (11) and (12). The function returns two vectors e and l which contain the energies and the corresponding photon concentrations and the two constants k and m.

Appendix A. Test Run for ^{137}Cs

^{137}Cs emits at 0.667 MeV. The MATLAB call to produce the photon energy distribution is (default resolution is used):

```
>[e,l,k,m]=pdsw(0.667,0);
```

The results are plotted in Fig. 1.

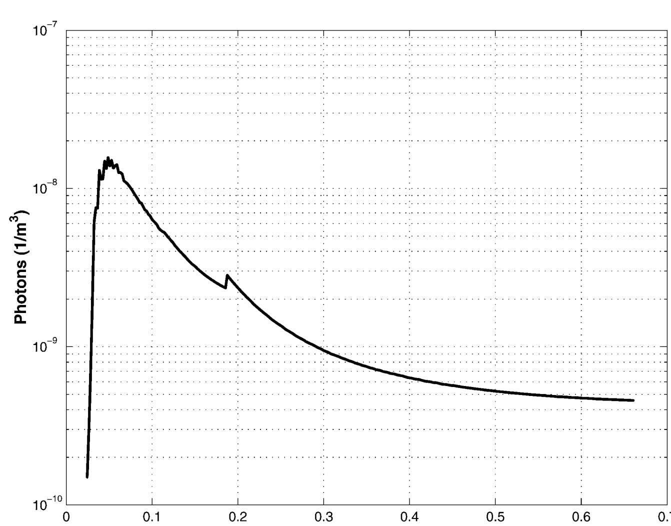

Fig. 1. Photon energy distribution for ^{137}Cs.

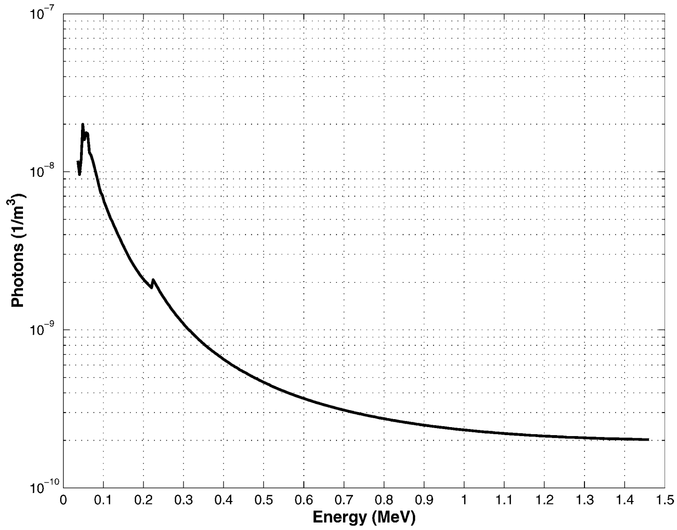

Fig. 2. Photon energy distribution for ^{40}K.

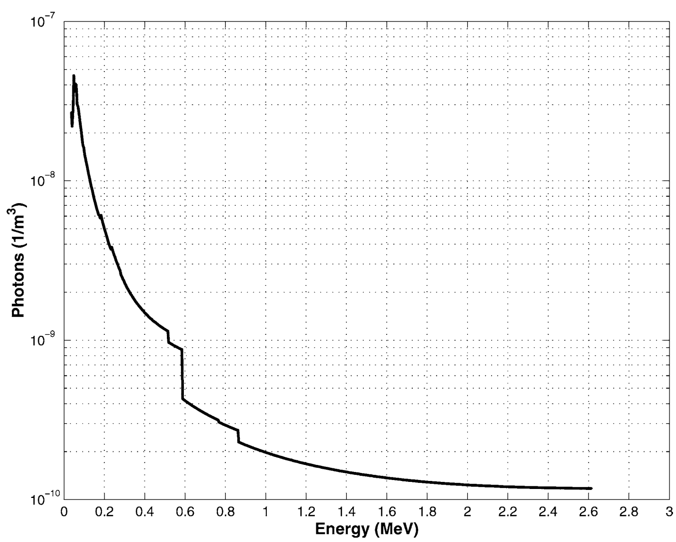

Fig. 3. Photon energy distribution for ^{208}Tl.

Appendix B. Test Run for ^{40}K

^{40}K emits at 1.461 MeV. The MATLAB call to produce the photon energy distribution is (default resolution is used):

```
>[e,l,k,m]=pdsw(1.461,0);
```

The results are plotted in Fig. 2.

Appendix C. Test Run for ^{208}Tl

^{208}Tl emits at energies 0.277, 0.511, 0.583, 0.763, 0.861 and 2.615 MeV with corresponding intensities 0.06, 0.22, 0.84, 0.002, 0.12 and 1. The MATLAB call to produce the photon energy distribution is (default resolution is used):

```
>e0=[0.277,0.511,0.583,0.763,0.861,2.615];
>inten=[0.06,0.22,0.84,0.02,0.12,1];
>[e,l,k,m]=pdsw(2.615,0);
>for i=1:5
    [et,lt,kt,mt]=pdsw(e0(i),0);
    for j=1:max(size(et))
        l(j)=l(j)+inten(i)*lt(j);
    end
end
```

The results are plotted in Fig. 3.

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