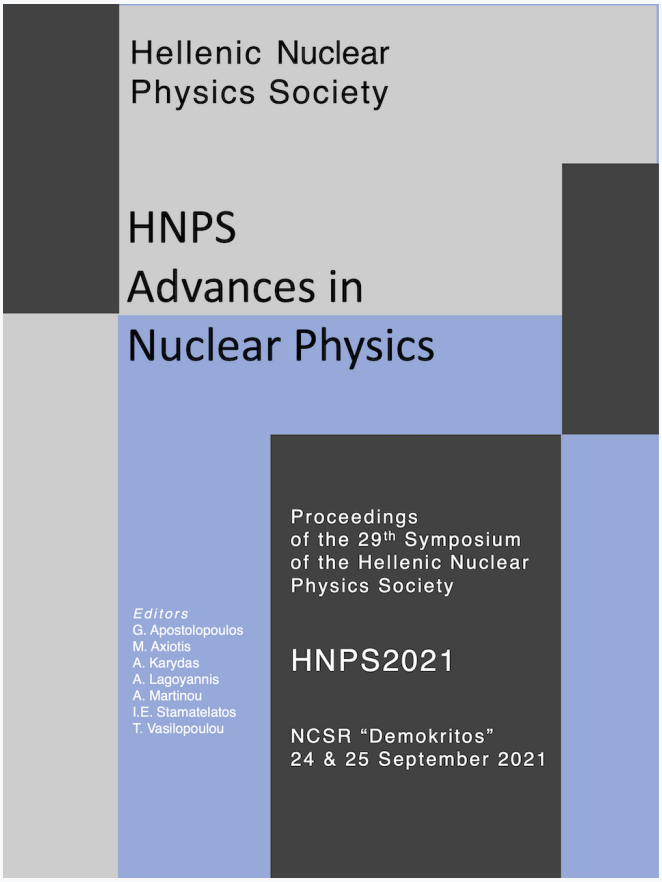
HNPS Advances in Nuclear Physics

Vol 28 (2021)

HNPS2021



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doi: 10.12681/hnps.3607

To cite this article:

Alafogiannis, I., Tugnoli, F., Mitsios, I., & Anagnostakis, M. (2022). Development of a computer code for the calculation of self-absorption correction factors in γ-spectrometry applications. *HNPS Advances in Nuclear Physics*, *28*, 98–103. https://doi.org/10.12681/hnps.3607

Development of a computer code for the calculation of self-absorption correction factors in γ-spectrometry applications

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Abstract In γ-spectroscopy applications, one of the main effects that needs to be considered is the self absorption of the photons – especially of low energy – within the photon source, which may be significantly different between the calibration standard and the sample analyzed. This effect is highly dependent on material composition, density and sample thickness. A common way of dealing with the self-absorption issue is by using Efficiency Correction Factors (ECF), to take into consideration the different absorbing properties between the calibration standard and the sample. This work presents the on-going development of a MATLAB code for ECF calculation. The code calculates ECF for a variety of material matrices and compositions, focusing on Naturally Occurring Radioactive Materials (NORM), which may have high density and contain high Z elements. The results of the code were compared with other methods of ECF calculation, such as Monte-Carlo simulation.

Keywords γ-spectrometry, self absorption, efficiency correction, NORM

INTRODUCTION

One of the the main methods for the identification and quantification of γ-emitting radionuclides in environmental samples is γ-spectroscopic analysis [1]. During γ-spectroscopic analysis, a series of correction factors may be required, in order to obtain sufficiently accurate and precise results.

In many cases the samples to be analyzed differ significantly, in terms of sample density and composition, from the standard that was used for the efficiency calibration of the sample-detector geometry. In these cases, a "corrected" efficiency other than the one obtained with the calibration standard should be used. This corrected efficiency may be calculated by using an efficiency correction factor (ECF), which takes into consideration the difference in the photon absorbing properties between calibration standard and sample material. Such efficiency correction factors may be calculated by Monte-Carlo simulation or experimental-numerical techniques [2].

For the determination of ECF at the Nuclear Engineering Laboratory of the National Technical University of Athens (NEL-NTUA), a numerical technique based on the double integral method introduced by [3] is applied for more than 25 years [4]. The ECF is calculated by a FORTRAN 77 program named "calceff" which is incorporated in the spectrum analysis software SPUNAL, for the typical cylindrical geometries used at NEL-NTUA, for photon energies below 200keV, calibration standard material 4M HCl and for a series of materials: water, black cement, fly ash, bottom ash, lignite and soil.

Based on the original program and the double integral method, in this work, a MATLAB code was developed [5] in order to extend the initial program's capabilities to perform ECF calculations for any cylindrical geometry and sample-detector configuration, for a wider photon energy range (30 to 2000 keV) and for various materials and densities, focusing on Naturally Occurring Radioactive Materials (NORM).

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PROGRAM DEVELOPMENT

Efficiency Correction Factor

The calculation of ECF can be carried out using different approaches. By using Monte Carlo Simulation, ECF can be calculated as the ratio of the full energy peak efficiency for the sample to be analyzed (eff_{sample}) to the full energy peak efficiency of the calibration standard ($eff_{standard}$). However, this method is time concuming and requires good knowledge of the material composition of the calibration standard and sample as well as the detector geometric characteristics. Another method to calculate ECF has been proposed by Cutshall [6], where the ECF for a specific energy-sample-geometry-detector configuration is calculated by performing measurements placing a radioactive source, that emits the photons of interest, on top of an empty container and afterwards on top of the same container filled with the sample material. However, this semi-experimental method provides reasonably accurate results when sample thickness is of the order of 2 cm and the density is not very high, but its use is questionable for thicker sample geometries and high density materials.

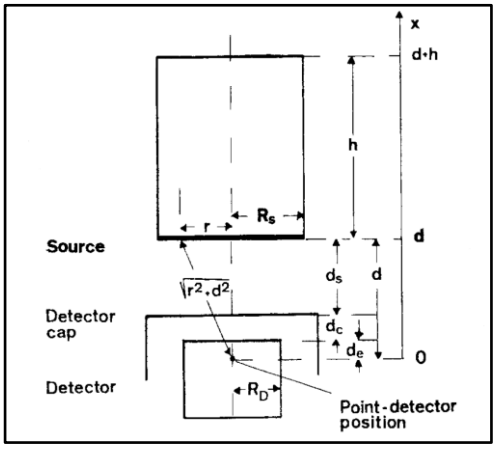

Fig.1. *Schematic drawing of a measuring Geometry with an extended source [4]*

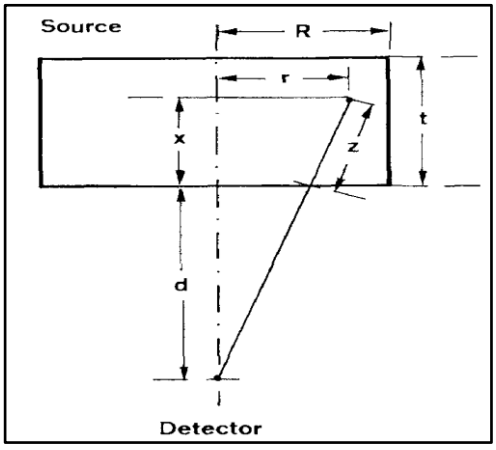

Fig.2. *Idealized measuring geometry and quantities used in the derivation of the integral in eq.(1)&(2) [4]*

In this work, the Integral Method proposed in [3] was used to calculate ECF. One important prerequisite to use this method is good knowledge of the sample-detector geometry configuration – it is implied that the sample is mounted coaxially to the detector – as it can be seen in Figure 1. For this approach, the detector is approximated by a fictitious point detector inside the real detector, at a distance "d" from the sample. The depth of the fictitious point detector inside the real detector – named effective interaction depth (d_e) – needs to be experimentally determined. In this method, the full energy peak efficiency for a cylindrical sample geometry is considered approximately proportional to the integral:

$$J(\mu) = \int_0^R \int_0^t \frac{e^{-\mu \cdot z}}{r^2+(x+d)^2} \cdot r \cdot dx \cdot dr \quad (1)$$

where

$$z = x \cdot \sqrt{r^2 + (x+d)^2} \quad (2)$$

z represents the distance traveled by a photon inside the source before it is absorbed in the detector, d, d_s, d_c, d_e, R and t are as shown in Figures 1 and 2 and μ represents the linear attenuation coefficient of the source material.

By calculating the double integral of equation (1) for the sample to be analyzed as well as for the calibration standard, ECF can be calclulated by equation (3):

$$ECF = \frac{eff_{sample}}{eff_{standard}} = \frac{J(\mu_{sample})}{J(\mu_{standard})} \quad (3)$$

Code Developement

Focusing on NORM, the materials that were introduced in the code were: red mud, fly ash, shaft furnace slag, granulated slag, lead slag, phosphogypsum, soil and water. The composition of the selected materials are given in Table 1. For the determination of the mass attenuation coefficients μ_m required for ECF calculation, the code uses correlations of the form μ_m=f(E) that were produced for each material (Figure 3), and cover the desired energy region 30-2000 keV. To this end, the μ_m data used were calculated using Monte Carlo code PENELOPE [7]. This approach eliminates any inaccuracies introduced by the μ_m values used, when comparing ECF values calculated by the code with ECF values calculated by Monte-Carlo simulation with PENELOPE code. The μ values required in formula (1) are then calculated by multiplying the μ_m with the material density provided by the user, thus allowing for the study of the density effect on ECF.

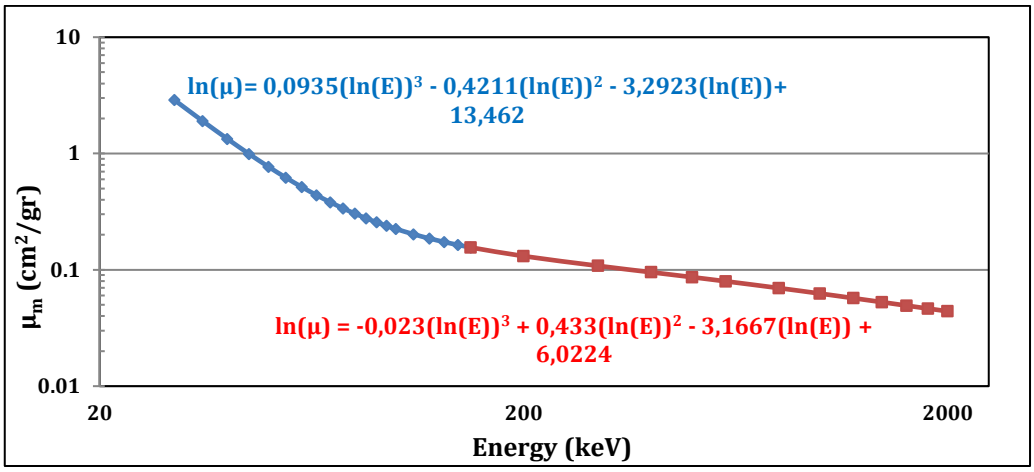

Fig. 3. *Mass attenuation coefficient μ_m for Lead Slag*

When running the code, the user selects the desired material from the list, as well as its density. At this initial stage of code development, for simplicity, the user then inputs distance "d" instead of d_s, d_c, d_e separately. For a typical Low Energy Germanium Detector of NEL-NTUA, "d" has been experimentally determined equal to 2 cm. Then the user, either selects a predefined sample geometry, or specifies the radius and thickness of a cylindrical sample geometry.

At this stage two cylindrical geometries often used at NEL-NTUA (geometry "2" and geometry "8") are predefined in the code. Finally, by inserting the desired photon energy in keV within the range of 30 to 2000keV and clicking the button "Calculate ECF", the code calculates ECF and the mass attenuation coefficient for the specific photon energy and the selected geometry-detector-material configuration. Currently, as calibration standard material a 4M HCl solution is used. The user interface at the current stage of development of the code is given in Fig. 4.

Table 1. *Selected materials composition [8-12]*

	Selected Materials Composition (w/w)							
Element	**4M HCL**	**Soil 3% Moisture**	**Red Mud**	**Fly Ash**	**Phospho-gypsum**	**Lead Slag**	**Gramulated Slag**	**Shaft Furnace Slag**
H	0.099	0.003	-	-	-	-	-	-
C	-	-	0.016	-	-	-	-	-
O	0.762	0.503	0.407	0.481	0.473	0.386	0.419	0.433
F	-	-	-	-	0.007	-	-	-
Na	-	-	0.023	-	-	0.026	0.007	0.006
Mg	-	-	0.010	0.009	0.005	0.031	0.039	0.040
Al	-	0.084	0.044	0.150	0.001	0.031	0.067	0.067
Si	-	0.284	0.095	0.260	0.023	0.159	0.184	0.208
P	-	-	-	-	0.007	-	-	-
S	-	-	-	0.003	0.216	0.027	-	-
Cl	0.139	-	-	-	-	-	-	-
K	-	0.037	0.008	0.008	-	0.018	0.022	0.021
Ca	-	0.037	0.265	0.032	0.267	0.076	0.173	0.084
Ti	-	-	0.038	0.007	-	-	0.004	0.004
Cr	-	-	-	-	-	0.004	-	-
Mn	-	-	-	-	-	-	0.002	0.002
Fe	-	0.052	0.093	0.048	0.001	0.241	0.083	0.135

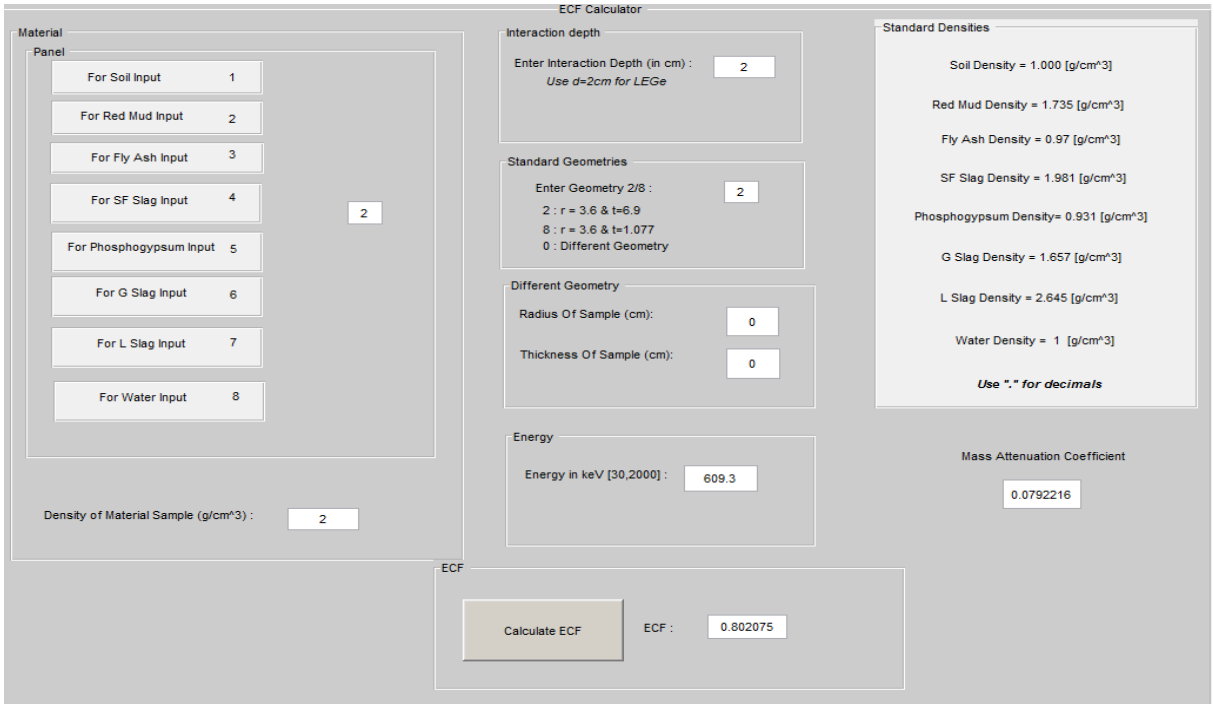

Fig.4. *User interface of ECF calculator code*

RESULTS AND DISCUSSION

By running the code and calculating ECF values for selected energies within the specified energy range and for all of the selected materials, the results show that as the photon energy increases, ECF tends to a constant value. However, for low density materials this constant value is greater than 1 while for high density materials is lower than 1, indicating that significant corrections are required for this energy region. Figures 5 and 6 present the ECF results for geometries “2” and “8”, for all the selected materials and the standard densities as presented in Figure 4. As expected for heavier materials, lower photon energies and thicker samples, the need for efficiency corrections is greater. It

is of great importance to observe that for high density materials like lead slag, the use of ECF may be required even for high energy photons, like those emitted by ^{40}K (1460keV) and the short lived radon daughters ^{214}Pb and ^{214}Bi.

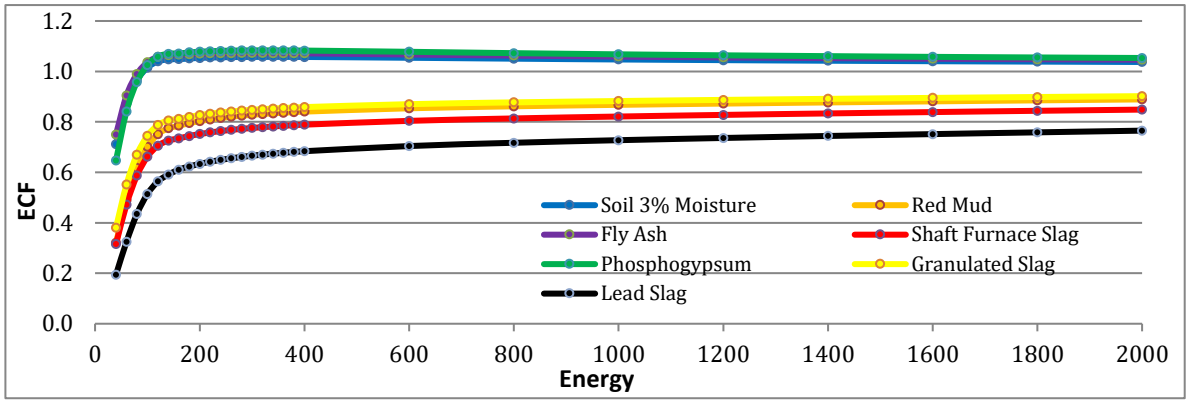

Fig. 5. *ECF calculation for selected materials, typical densities and geometry "2" (thickness 69mm)*

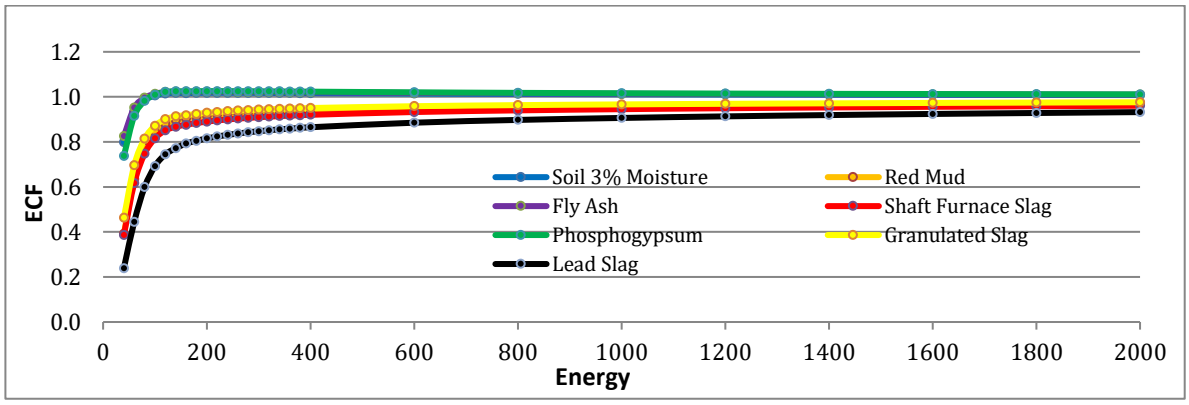

Fig. 6. *ECF calculation for selected materials, typical densities and geometry "8" (thickness 10mm)*

In Figure 7, the ECF values calculated using Monte Carlo simulation and the MATLAB code are compared. As it can be seen in Figure 7, for low density materials such as fly ash and soil there are small differences for energies higher than 100keV. For all materials, the MATLAB code provides lower ECF values than the simulation. These differences are below 5% in most cases, with the exception of very low photon energies and very dense materials, where difference may be as much as 20%.

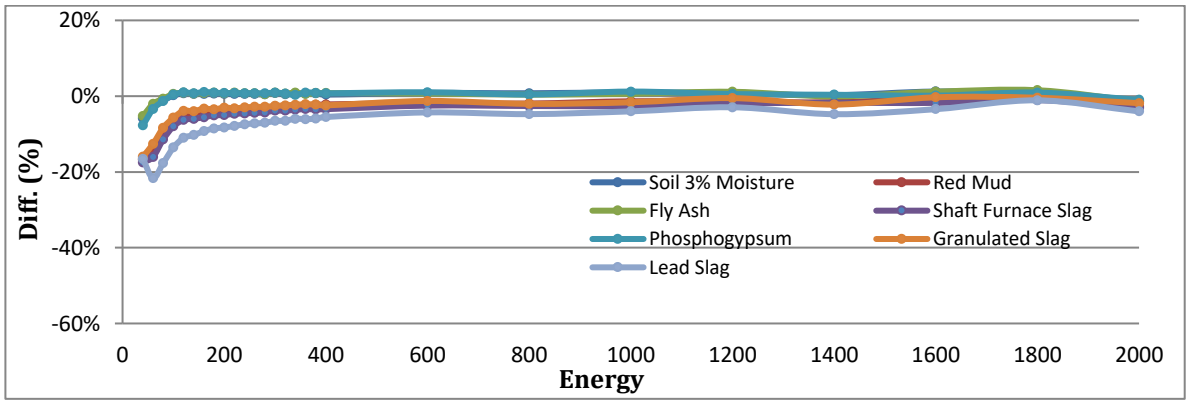

Fig. 7. Comparison of values obtained from simulation and the MATLAB code for geometry "8"

CONCLUSIONS

In this work, the on-going development of a standalone computer code for the calculation of ECF is presented. The code provides flexibility in geometry, material composition and material density selection, as well as sample-to-detector distance. Furthermore, from the acquired results, it is concluded that the use of ECF is important even for energies higher than 200keV, especially for high density materials. The code results were compared with results obtained with Monte-Carlo simulation. The code provides fairly good results with the exception of very low energy photons and very dense materials, where the results are not as satisfactory.

Future steps will include investigation of the influence of the effective interaction depth on ECF calculation, in order to improve code accuracy for low photon energies and high-density, high-Z materials. Furthermore an improved interface that will provide more flexibility to the user, to select different materials and detection geometries is foreseen. The improved code will allow for the investigation of the effect of various parameters, such as material composition, density, geometrical chatacteristics and effective interaction depth on the ECF calculation.

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