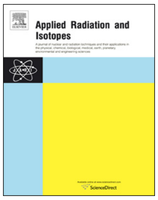
Applied Radiation and Isotopes 135 (2018) 78–82

Contents lists available at ScienceDirect

Applied Radiation and Isotopes

journal homepage: www.elsevier.com/locate/apradiso



ALPHACAL: A new user-friendly tool for the calibration of alpha-particle sources

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HIGHLIGHTS

- A new software for alpha source calibration is presented.
- It is based on AlfaMC code.
- It includes some additional tool for an advanced analysis.

ARTICLE INFO

Keywords:
Interaction of alpha particles
Monte Carlo Simulation
Alpha-particle spectrometry
AlfaMC code

ABSTRACT

In this work, we present and describe the program ALPHACAL, specifically developed for the calibration of alpha-particle sources. It is therefore more user-friendly and less time-consuming than multipurpose codes developed for a wide range of applications. The program is based on the recently developed code AlfaMC, which simulates specifically the transport of alpha particles. Both cylindrical and point sources mounted on the surface of polished backings can be simulated, as is the convention in experimental measurements of alpha-particle sources. In addition to the efficiency calculation and determination of the backscattering coefficient, some additional tools are available to the user, like the visualization of energy spectrum, use of energy cut-off or low-energy tail corrections. ALPHACAL has been implemented in C+ + language using QT library, so it is available for Windows, MacOs and Linux platforms. It is free and can be provided under request to the authors.

1. Introduction

Alpha-particle radioactive sources are often measured using detection systems with 2π counting geometry, in order to determine their activity with a very low deviation. However, the experimental ratio $C_{2\pi}/A$ (counting rate/activity) can deviate significantly from the theoretical value of 0.5, due to the self-absorption and scattering of alpha particles in the source substrate and in the backing material. Consequently, the experimental counting rate must be corrected taking into account these effects to determine the real activity for the source.

Traditionally, these corrections were evaluated theoretically using simplified scattering models, such as those of Crawford (1949), White (1970) or Lucas and Hutchinson (1976). These corrections can also be estimated experimentally for each particular backing and alpha-particle energy (Ballaux, 1985; Hutchinson et al., 1976; Jurado Vargas et al., 2004), but it would require the measurement of a great number of alpha-particle sources prepared with a wide range of thicknesses and using a substrate with a similar chemical composition to the source of interest. Moreover, the experimental evaluation of these corrections is often subject to large uncertainties, especially in the determination of the backscattering coefficient for sources with negligible thicknesses.

More recently, Monte Carlo methods have been used in this task by simulating the transport of alpha particles interacting into the source and backing material (Fernández Timón et al., 2014; Ferrero et al., 1990; Jurado Vargas and Fernández Timón, 2004; Jurado Vargas et al., 2015). Most of these computations were performed using the well-known code SRIM (Ziegler et al., 2010), and more recently, a new Monte Carlo code AlfaMC, developed by Peralta and Louro (2014). In spite of this effort, there is a lack of availability of MC tools specifically developed to determine the corrections to detection efficiency with low uncertainty, and consequently the activity of many alpha-particle sources.

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https://doi.org/10.1016/j.apradiso.2018.01.020
Received 31 October 2017; Received in revised form 8 January 2018; Accepted 12 January 2018

To solve this, in this work, we have developed the program ALPHACAL, particularly designed for the calibration of alpha-particle sources in a 2π counting geometry. It is therefore much more user-friendly and less time-consuming than multipurpose codes developed for a wide range of applications. The program considers both cylindrical and point sources mounted on the surface of polished backings, as it is commonly used in experimental measurements of alpha-particle sources. ALPHACAL is based on the code AlfaMC, and uses the information provided by this program for the main characteristics of alpha particles at each step of the track (as energy, position, or output direction after the last interaction with the source), to obtain the detection efficiency $C_{2\pi}/A$ as the rate between the detected and total emitted particles. In case of sources with null thickness, backscattering coefficients are also calculated. It also incorporates a post-simulation analysis for the treatment of the provided results. ALPHACAL is free and can be provided under request to the authors.

2. General structure of ALPHACAL

ALPHACAL has been implemented in C+ + language using the QT library (QT framework) and as such it is available for Windows, MacOs and Linux platforms. The program offers an easy and intuitive interface to input data for simulation. For instance, it allows the creation of energy files for the alpha particles and material files for the backing and substrate, or the creation of a series of simulations, which can be queued to be performed in a unique execution. However, its main improvement is related to the compilation of the text file that the code AlfaMC uses as input. This interface avoids ALPHACAL users to insert manually all the necessary data for the simulations, averting a task that is usually tricky and non-friendly for the user and a common source of error. In addition to the calculation of final efficiency values, some extra tools are available to the user, which include the visualization of the corresponding alpha-particle energy spectrum and the use of a given cut-off energy or low-energy tail corrections in the spectrum to evaluate the required corrections to the counting rate.

The basic structure of the ALPHACAL package is divided into three main folders, whose contents are separated each other, basing on their functionalities. The folder called Code houses all the files related to the interface implementation in C+ +. A second folder called Release is the site where user can find the application file and all the auxiliary files that the operative system needs to work. Finally, the folder MonteCarlo stores the two executable programs required by the ALPHACAL interface, which implement all the physical basis of the simulation process. In addition, this folder houses a set of auxiliary folders, where the different files provided and requested by the application are stored (energy and spectra files, among others).

AlfaExe is the executable file of the AlfaMC code, which is responsible for performing all the Monte Carlo calculations for each experience. It takes a text file as input, which includes all the mandatory data for AlfaMC to work. As results provided by each simulation, AlfaMC saves the main features of each particle emitted by the source (final position, direction and energy) in a particular file (used later for obtaining the spectrum by ALPHACAL), while a summary of this simulation is added to a compilation file shared with the remainder of the enquired experiences.

The other executable program in the MonteCarlo folder is MaterialGen. It generates the file that will contain the stopping-power data for a new material (required for the source substrate or the backing), if this material is not included in the ALPHACAL's database. This executable file works using data from the NIST/ASTAR (ASTAR) and SRIM databases (Ziegler et al., 2010) in the energy range between 0.001 and 1000 MeV, although AlfaMC is not designed to follow particles with energy higher than 12 MeV. This program computes the stopping-powers of the user-defined materials using the Bragg's rule.

3. Executing ALPHACAL

A general scheme about the execution flow of ALPHACAL is depictured in Fig. 1. The initial ALPHACAL window enquiries if the user needs to throw a new simulation or if he wants to re-analyse a saved one. This last option leads to a forthcoming window that the user will reach later after he has performed a new simulation, so we are going to describe the entire process starting at the beginning.

3.1. Input data and simulation

When the user requires a new simulation, the main ALPHACAL window is shown (see Fig. 2). In this window, the text needed for AlfaMC to work is inputted. This window is divided in three main blocks:

- The upper section contains the characteristics of the source substrate: geometry features (thickness and radius), number of alpha particles to simulate from random positions inside the substrate, source composition and energy of the alpha particles. These two last inputs must be provided by including two text files. ALPHACAL offers to the user the options to choose between existing files or creating new files, as aforementioned. On the other hand, as a variance reduction technique in the case of point sources, only the alpha particles emitted to the backing are generated and simulated.
- Next section is related to the backing features, where its geometric parameters and chemical composition have to be provided by the user.
- Finally, the last block is composed by other necessary data as the RNS (Random Number Seeds) or the number of repetitions for a same simulation (using the identical data for backing and source, although different seed for the generation of random numbers).

A help button can be found at each window during this process. In addition, if some required input data is wrong or blank, a warning message is thrown and the next stage cannot be reached until the problem is solved. As an example, Fig. 2 shows a snapshot of the input data for the simulation of a thick source of Barium Sulfate containing ^{226}Ra as alpha-particle emitter.

Once all input data have been provided, the simulation can start. When finished, a new window is displayed to the user containing a summary of the results obtained after the simulations, as seen in Fig. 3. The results for the detection efficiency $C_{2\pi}/A$ (counting rate/activity) for each individual simulation are shown (jointly to B coefficients in the case of non-thickness sources). In addition, simulations' results are also batch grouped (when they represent the same experiment changing only the random seed) showing its average value for detection efficiency (and the corresponding backscattering coefficient B, if source thickness is negligible).

3.2. Additional tools

In order to replicate as close as possible the experimental measurements, ALPHACAL includes some additional tools for obtaining the final values of efficiency and backscattering coefficient.

A first step is to visualize the energy spectrum of the alpha particles just after leaving the source, i.e., the energy spectrum. This modal window is available from the initial ALPHACAL window if the option of non-simulation is chosen (see Fig. 1). ALPHACAL allows the user to load a spectrum previously stored in the *spectra* folder or to create a new spectrum. This new spectrum can be obtained from an individual simulation or from the sum of two or more experiments. The option to change the histogram's gain and the maximum and minimum energy is offered to the user for modelling the spectrum, which can be saved for a later analysis. The spectrum is shown jointly with the original efficiency value obtained (see Fig. 4).

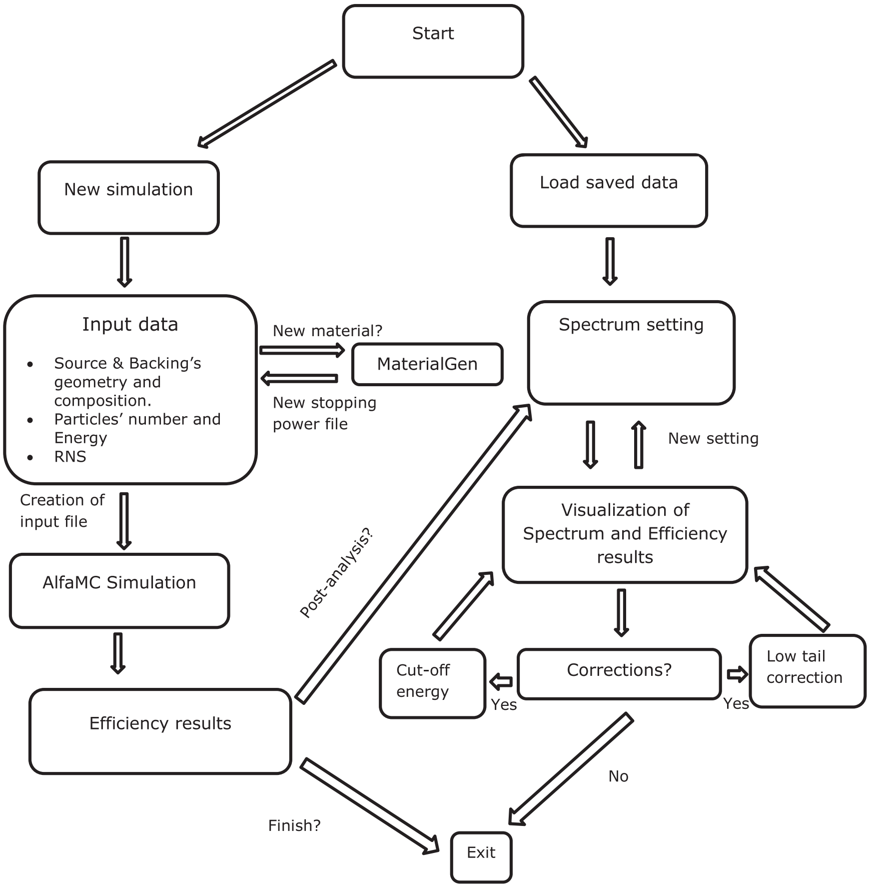
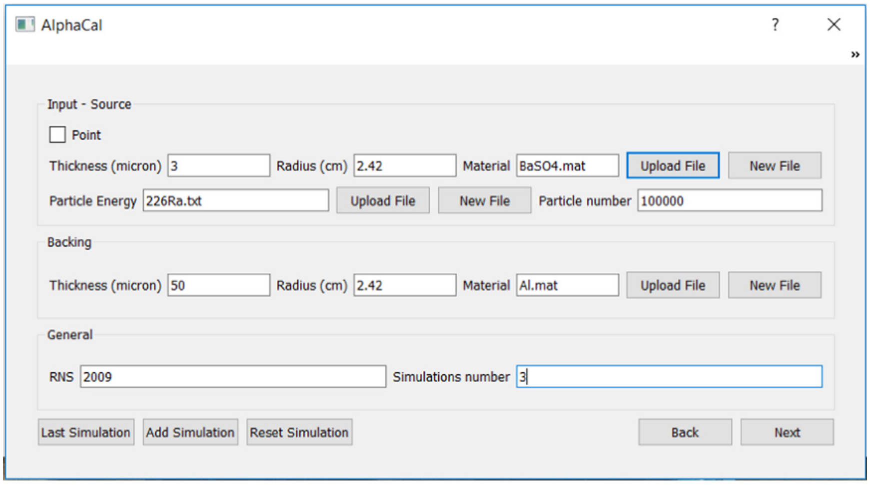


Fig. 1. Flow diagram of ALPHACAL execution.



Input - Source

☐ Point

Thickness (micron) 3
Radius (cm) 2.42
Material BaSO4.mat
Particle Energy 226Ra.txt
Particle number 100000

Backing

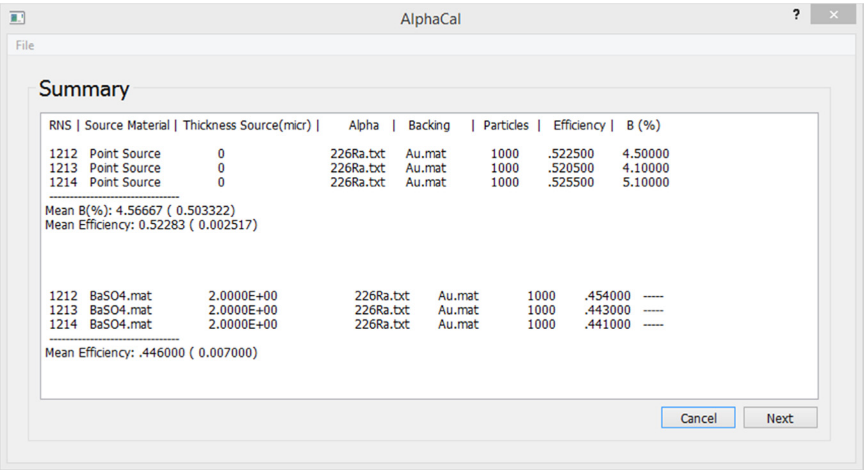
Thickness (micron) 50
Radius (cm) 2.42
Material Al.mat

General

RNS 2009
Simulations number 3

Fig. 2. Main ALPHACAL's window for starting a new simulation.

Due to the nature of the multiple scattering processes, the energy distribution of the detected particles shows a marked peak or maximum in the low-energy part of the spectrum, as observed in Fig. 4. This maximum has already been studied by us in a previous work (Jurado Vargas and Fernández Timón, 2004), and constitutes a significant factor to take into account in the calibration of alpha-particle sources, especially in the cases of backings with high atomic numbers and thick sources. In addition, in experimental measurements, the alpha particles in the low-energy zone of the spectrum cannot be distinguished from pulses due to recoiling daughters (≈ 100 keV). Moreover, the low energy part of the spectrum is also affected by electronic noise. Therefore, only pulses above a given energy cut-off are considered in the measurements (Jurado Vargas and Fernández Timón, 2015). However, an extrapolation to zero energy is usually carried out to include the total alpha-particle count rate from the whole experimental spectrum. Consequently, this zero energy extrapolation must be also performed in the corresponding simulated spectrum to determine the efficiency. Two options are therefore offered to the user in the spectrum window. If the user decides to add a cut-off value, an energy range will be enquired by ALPHACAL. Only the selected zone will be depicted in the spectrum and considered for the determination of the efficiency. If, as usual, the user decides to perform a zero energy extrapolation in the simulated



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RNS | Source Material | Thickness Source(micr) |     Alpha   |  Backing    | Particles |  Efficiency |  B (%)

1212  Point Source          0                  226Ra.txt   Au.mat        1000     .522500     4.50000
1213  Point Source          0                  226Ra.txt   Au.mat        1000     .520500     4.10000
1214  Point Source          0                  226Ra.txt   Au.mat        1000     .525500     5.10000
 ---------------------------------
Mean B(%): 4.56667 ( 0.503322)
Mean Efficiency: 0.52283 ( 0.002517)



1212  BaSO4.mat        2.0000E+00          226Ra.txt    Au.mat        1000     .454000   -----
1213  BaSO4.mat        2.0000E+00          226Ra.txt    Au.mat        1000     .443000   -----
1214  BaSO4.mat        2.0000E+00          226Ra.txt    Au.mat        1000     .441000   -----
 ---------------------------------
Mean Efficiency: .446000 ( 0.007000)
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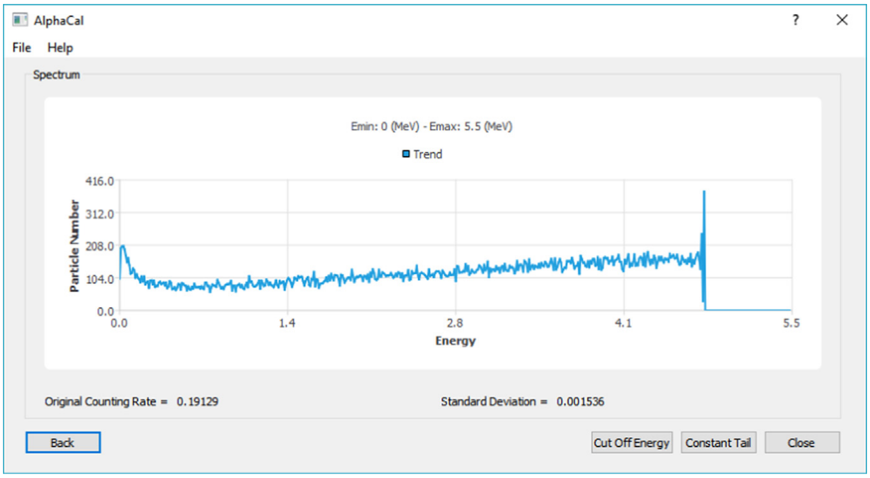
Fig. 3. ALPHACAL's window showing a summary of the provided results.



Original Counting Rate = 0.19129

Standard Deviation = 0.001536

Fig. 4. Energy distribution of alpha particles for the case of a 20 µm thickness source of Barium Sulfate containing ^{226}Ra.

spectrum, a constant tail correction is carried out following the basic procedure described in the work of Martín Sánchez et al. (1992). To do this, two energy intervals must be provided. A first interval including the spectrum range below the energy cut-off value established in the corresponding experimental spectrum. The second interval must include an energy range above the cut-off energy, which can be taken as a reference interval for performing the required constant tail correction. After this correction, the corresponding efficiency value taking into account the zero energy extrapolation will be shown at the window.

Finally, it must be noted that the code AlfaMC includes the option of choosing two different models for the energy straggling of alpha particles: a first model given by a Gaussian distribution, and a second one by assuming the Landau and Vavilov's theory (Vavilov, 1957), more appropriate for cases in which the number of collisions is very small. As observed by us, there were no significant differences in the energy distributions obtained for alpha-particle sources, depending on the model considered. Therefore, we implemented in ALPHACAL the simplest model given by a Gaussian distribution for the energy straggling.

4. Some applications

It must be noted that ALPHACAL is based on the code AlfaMC, which has already been checked by us as suitable to evaluate backscattering corrections for null-thickness sources (Jurado Vargas and Fernández Timón, 2015) and also to determine the scattering and self-absorption corrections for thick alpha-particle sources (Jurado Vargas et al., 2015). In order to see the functionality of the code ALPHACAL, we briefly present here some applications in alpha-particle spectrometry, including point sources mounted on several backings, radioactive sources with a given substrate and several thicknesses.

4.1. Backscattering coefficients

As an example of the application of ALPHACAL to the point sources case, we include here the simulation of several point sources of ^{238}U deposited onto different backings with a wide range of mass numbers (from Be to Au). Each source, for a particular backing, was simulated three times, including a total of 100,000 alpha particles for each individual simulation.

The values obtained for the backscattering coefficients, and their uncertainties, are shown in Fig. 5 versus the mass number of each backing. These coefficients show, for a fixed alpha particle's energy, an increasing relationship for backscattering effect with the mass number of the support material. This behavior is in agreement with those previously obtained by SRIM (Fernández Timón and Jurado Vargas, 2007).

4.2. Mass attenuation curves

We also applied ALPHACAL to the determination of the mass attenuation curves in 2π counting systems. As an example, we considered a set of sources with different substrate thicknesses of $BaSO_4$,

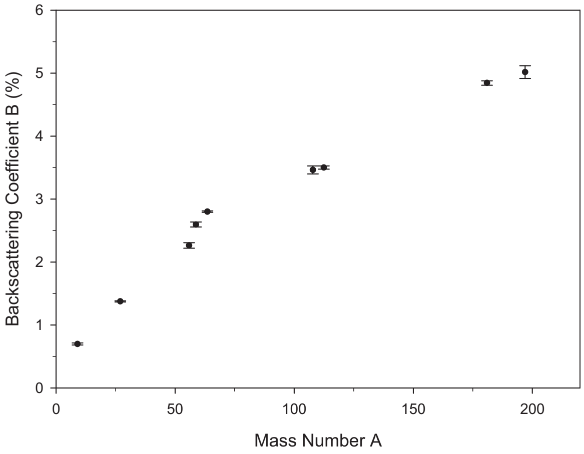


Fig. 5. Backscattering coefficients obtained by ALPHACAL for ^{238}U alpha particles in various backing materials versus mass number. Uncertainties correspond to one standard deviation.

containing ^{226}Ra as alpha-particle emitter and a backing of aluminium. Source thicknesses from 1 up to 50 µm were considered, in order to include thin and thick sources. Each source with a given thickness was simulated three times, each including 100,000 alpha particles, with a mean calculation time of about 1.25 min for each individual simulation. The corresponding efficiency values, and their uncertainties, are depicted in Fig. 6 versus the source thickness. As established in a previous work (Jurado Vargas et al., 2015), a simple theoretical model based on a more detailed model developed by Semkow et al. (2005) can describe the dependence of the detection efficiency on the source thickness.

In particular, the dependence of alpha efficiency *Eff* on the source thickness *T* can be described by:

$$Eff\,(T) = a - b^{*}T,\ when \quad T \leq R \tag{1}$$

$$Eff\,(T) = \frac{c}{T} \quad ,\ when \quad T \geq R \tag{2}$$

being R = 15.2 µm the mean range of ^{226}Ra alpha particles in the substrate of $BaSO_4$, and *T* denotes the substrate thickness.

For both zones, a good agreement with the model was found, as can be corroborated by the reduced chi-squared coefficient obtained for each one (0.3199 and 0.6476 respectively). This indicates the suitability of the code ALPHACAL to obtain in a short time the mass attenuation curves usually required in the calibration of alpha-particle sources measured in 2π counting geometry.

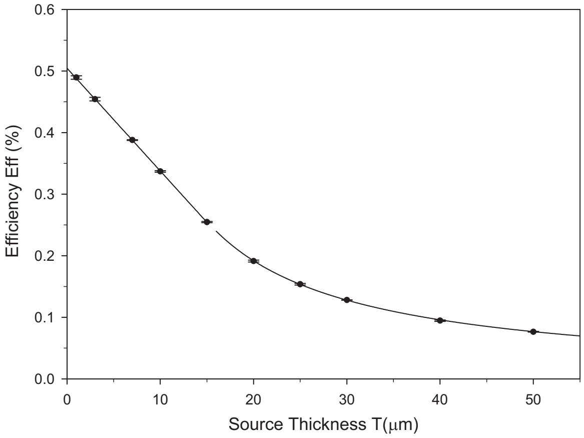


Fig. 6. Efficiency values obtained with ALPHACAL for ^{226}Ra alpha-particle sources with a $BaSO_4$ substrate mounted onto an aluminium backing. The plot shows the dependence of efficiency on substrate thickness.

5. Conclusions

There is a lack of available MC tools specifically designed to evaluate the required corrections needed in the calibration of alpha-particle sources. To solve this, we developed the program ALPHACAL, specifically developed for this particular task, taking into account the self-absorption and scattering of alpha particles in the source and the backing material. It is therefore much more user-friendly and less time-consuming than multipurpose codes that are intended for a wide range of applications. It is based on the code AlfaMC, and uses its information for the main characteristics of alpha particles at each step of the track (as energy, position, or output direction after the last interaction) to obtain the rate between the detected particles and the total emitted ones. In case of sources with null thickness, backscattering coefficients are also provided. ALPHACAL considers both cylindrical and point sources mounted on polished backings. It has been implemented in C++ language using the QT library and as such it is available for Windows, MacOs and Linux platforms. ALPHACAL is free and can be provided under request to the authors.

Acknowledgements

Thanks are due to the Junta de Extremadura (project GR15103) and the Ministerio de Economía y Competitividad (project TIN2015-65460-C2-2-P) for financial support.

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