Ancient TL

Short Communication

R scripts for dose rate calculation in trapped charge dating

Junjie Zhang[1*], Sumiko Tsukamoto[1,2]

[1]LIAG Institute for Applied Geophysics, Hannover, Germany
[2]Department of Geosciences, University of Tübingen, Tübingen, Germany

[*]Corresponding author: junjie.zhang@liag-institut.de

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Abstract

We present R scripts for environmental dose rate calculations for trapped charge dating, and this contribution introduces these scripts along with associated templates and provides instructions for their use. We also discuss issues related to radon loss and alpha dose rate calculation. In addition to the R scripts for quartz and feldspar, we have prepared R scripts to calculate dose rates of carbonate minerals in a homogeneous medium, and to model the time-dependent changes in dose rates resulting from U-series disequilibrium following carbonate crystallization. These R scripts are freely available on GitHub and Zenodo.

Keywords: Luminescence dating, ESR, Dose rate, R scripts, Radon loss, Alpha efficiency

1. Introduction

To date, a number of programs for dose rate calculation have been developed in trapped charge dating (OSL, TL, and ESR). These include, but are not limited to: ADELE (Degering and Degering, 2020), AGE (Grün, 2009), Carb (Nathan and Mauz, 2008; Mauz and Hoffmann, 2014) and RCarb (Kreutzer et al., 2019), DosiVox (Martin et al., 2015), DRAC (Durcan et al., 2015), DRc (Tsakalos et al., 2015), LDAC (Liang and Forman, 2019) and µRate (Tudyka et al., 2023).

In this short communication, we introduce an alternative approach for dose rate calculation, using code written in the R programming language (R Core Team, 2025). The code and associated files are organized within an R project named doserate_rProject.Rproj. The main R script used for quartz and feldspar (or polymineral material) is **doserate_main.R**. Two additional R scripts have been prepared for calculating dose rates of carbonate minerals, assuming an infinite homogeneous medium. They are called **doserate_carbonate_keff.R** and **doserate_carbonate_sa.R**. A total of twelve R functions have been developed to support the dose rate calculation process and are utilised by the main R scripts. Unlike some of the previous programs with 'encapsulated' code, these R scripts are more flexible and straightforward to modify, allowing users to easily customise them to suit their specific needs.

2. R scripts for quartz and feldspar

In case of quartz and feldspar (or polymineral material), **doserate_main.R** should be used for dose rate calculation. The flow chart of the calculations is shown in Fig. 1. The R scripts for the functions used for dose rate calculation are stored in the folder 'functions'. The information of the samples should be input into a comma-separated value (CSV) template file: **Template_input.csv**. In the 'mineral' column of the CSV template, either 'fsp' or 'qz' should be entered. The 'fsp' indicates feldspar or polymineral material, and the 'qz' indicates quartz. In the 'grainsize' column of the CSV template, enter either 'coarse' or 'fine'. Here, 'fine' refers to grains between 1 µm and 20 µm (the 4–11 µm fraction is typically used in dating), while 'coarse' encompasses sizes ranging from 20 µm to 1000 µm. The subdivision of 'fine' and 'coarse' is based on the fact that the grain size related parameters were fitted separately for grains smaller than 20 µm and larger than 20 µm, and different functional scripts for alpha and beta dose rate calculations are applied in the main script.

These grain size related parameters include alpha attenuation factors of U and Th, beta absorption factors of U, Th, K,

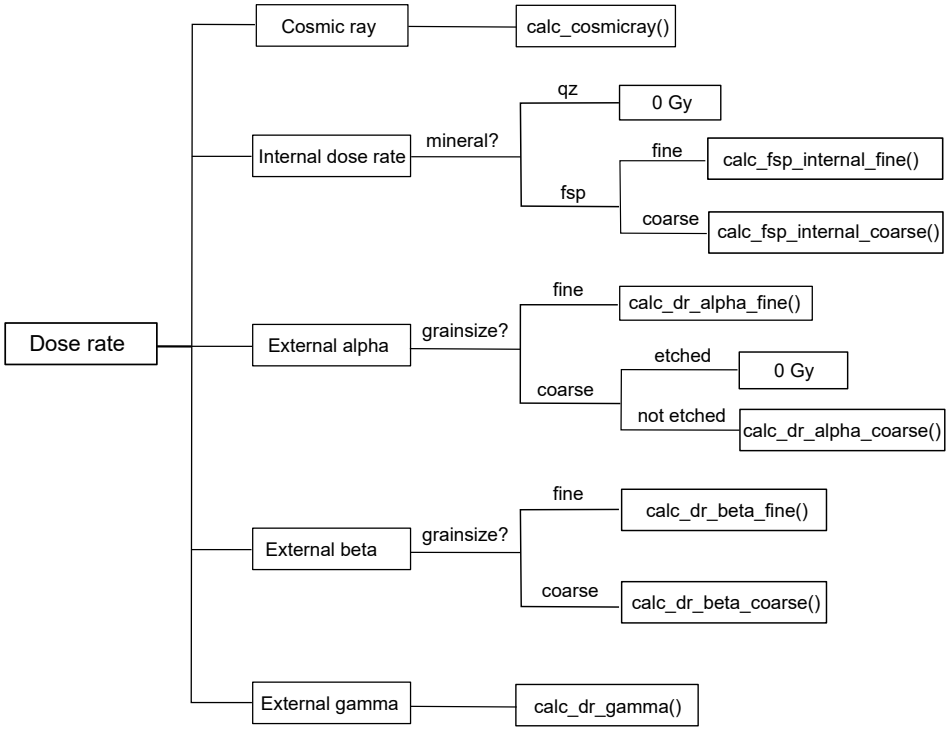

Figure 1: Flowchart of dose rate calculation using the **doserate_main.R** script with defined 'calc_' functional scripts. The parameters 'mineral' and 'grainsize' are entered in the CSV template. For the 'mineral', 'qz' means quartz and 'fsp' means feldspar or polymineral material. For the 'grainsize', 'fine' refers to grains between 1 µm and 20 µm, while 'coarse' refers to grain sizes between 20 µm and 1000 µm.

as well as ^{87}Rb. The alpha attenuation factors used by our R scripts are based on Brennan et al. (1991). The beta absorption factors of U, Th, K are based on Guérin et al. (2012) for grain sizes between 20 µm and 1000 µm, and Brennan (2003) for grain sizes between 1 µm and 20 µm. The absorbed dose for ^{87}Rb beta particles for calculating the internal dose rate of feldspar is based on Readhead (2002). The dose rate contribution of Rb from the external environment is not considered, as it is negligible (e.g., 0.0358 Gy ka^{-1} for 100 µg g^{-1} Rb in a homogeneous medium). The R scripts will calculate these parameters based on the mean grain size, deduced from the 'grain_min' and 'grain_max' values (unit: µm) provided in the CSV file. DRAC applies a smoothed spline function to fit these parameters with the grain size (Durcan et al., 2015). In our R scripts, we use linear and exponential functions for the fitting (see Tables S1–S3 in the Supplementary Materials). Though with different functions, the calculated attenuation or absorption factors from the fittings are always very close to the reported values.

The CSV template includes an 'etch_depth_um' parameter (in µm), which represents the etched thickness, i.e., reduction in grain radius due to HF etching for coarse grains. For fine grains (1–20 µm), the value of zero should always be entered for this parameter. For coarse grains, when the entered value is zero, alpha dose rates will be calculated. When it is greater than zero, alpha dose rates are set to zero with the assumption that the HF etching has sufficiently removed the outer rim affected by alpha irradiation. The entered value will also be used to calculate the etching factor for the beta absorption factor, following the data reported in Brennan (2003) (raw data in the Supplementary Materials of Durcan et al. (2015)). For etched coarse grains, a value of 10 µm is suggested for the 'etch_depth_um' parameter, as reported in previous studies (Bell and Zimmerman, 1978; Porat et al., 2015; Duval et al., 2018).

Other information in the CSV template include: alpha efficiency (a_value), radon loss (Rn_loss), latitude, longitude, altitude (m), burial depth (m), water content (%), U concentration (µg g^{-1}), Th concentration (µg g^{-1}) and K concentration (%), as well as the corresponding errors. Cosmic-ray dose rates are calculated following Prescott and Hutton (1988, 1994). Latitude values should be negative for locations in the southern hemisphere, and longitude values should be negative for locations in the western hemisphere. The default a-value is set to 0.04 ± 0.01 for quartz (e.g., Rees-Jones, 1995; Rees-Jones and Tite, 1997; Lai et al., 2008), and 0.09 ± 0.02 for the pIRIR signal of feldspar (e.g., Kreutzer et al., 2014; Schmidt et al., 2018). For internal dose rate calculation of feldspar, an internal K concentration of 12.5 ± 0.5 % (Huntley and Baril, 1997; Zhao and Li, 2005) and an internal Rb concentration of 400 ± 100 µg g^{-1} (Huntley and Hancock, 2001) are used. These default values can be changed in the 'calc_fsp_internal_coarse' and 'calc_fsp_internal_fine' functional R scripts. Internal dose rates of quartz samples are assumed to be zero. Three sets of conversion coefficients are stored as CSV files in the 'con-

version_data' folder, which are from Guérin et al. (2011), Liritzis et al. (2013) and Cresswell et al. (2018), respectively. Users can choose the conversion coefficients they wish to use by specifying it in the code line of 'conversion <- read.csv()' inside the script **doserate_main.R**. The calculated dose rate results will be saved in the CSV file **Doserate_output.csv**.

2.1. Radon loss

In the gas phase, ^{222}Rn from the ^{238}U decay chain may escape from the sediment matrix, causing disequilibrium in the ^{238}U decay chain (Krbetschek et al., 1994; Olley et al., 1996, 1997). In this case, the dose rates calculated assuming the U series in secular equilibrium will be overestimated. In the R scripts, the ^{238}U decay chain is divided into two segments, pre-Rn and after-Rn. Users can enter any value between 0 and 1 for the 'Rn_loss' parameter in the CSV template. For example, a value of 0 means no Rn loss, and a value of 0.25 means 25 % Rn loss. The degree of Rn loss can be estimated from ^{210}Pb/^{226}Ra activity ratios, in case the samples have been measured by gamma-ray spectrometry (De Corte et al., 2006). We tested the influence of Rn loss on the total dose rates, using sediments from the Rodderberg crater basin, Germany (Zhang et al., 2024b). With a 25 % Rn loss, the dose rates will be 4–5 % lower compared to the dose rate without Rn loss (Fig. 2A).

2.2. Alpha efficiency

Alpha irradiation is less efficient in generating trapped charges (luminescence or ESR signals) than beta and gamma irradiation, per unit of energy deposited. The k-value is defined to describe the alpha efficiency (Zimmerman, 1971), which is equal to the ratio of the beta or gamma dose to the alpha dose that generates the same amount of luminescence. However, by losing the same amount of energy (e.g., 0.1 MeV), an alpha particle with a higher energy (e.g., 4.0 MeV) is more effective than an alpha particle with a lower energy (e.g., 3.0 MeV) in generating luminescence signals. As a result, the k-value will decrease when the alpha particle has a lower energy (Zimmerman, 1971, 1972). The alpha efficiency values were measured using artificial alpha sources, such as ^{210}Po (Zimmerman, 1971, 1972), ^{242}Cm (Aitken and Bowman, 1975), ^{238}Pu (Tribolo et al., 2001), ^{244}Cm (Zhang and Wang, 2020) and ^{241}Am (Mauz et al., 2006; Lai et al., 2008; Biswas et al., 2013; Kreutzer et al., 2014, 2018; Schmidt et al., 2018), which have different alpha energies. In the pioneering work of Zimmerman (1971), the author assumed that all alpha particles emitted by a ^{210}Po source arriving at the sample were mono-energetic at around 3.7 MeV. Hence, the k-value measured by Zimmerman was termed $k_{3.7}$. While the k-value is dependent on the alpha particle's energy, it is found that the luminescence signal produced per unit length of alpha track is nearly independent of the energy (Zimmerman, 1971, 1972; Aitken and Bowman, 1975; Aitken, 1985). Thus, the a-value system was proposed to describe alpha efficiency in terms of generated luminescence per unit track length (Aitken and Bowman, 1975; Aitken, 1985). From the definition of the a-value, it is equal to $k_{3.7}$ for quartz, and $r \times k_{3.7}$ for other minerals, where r represents the ratio of alpha particle stopping powers between a certain mineral and quartz (Aitken, 1985). According to our calculation, r is 0.98, 1.02 and 1.04 for K-feldspar, calcite and dolomite, respectively (Table S4). Therefore, we can still approximate the a-value as $k_{3.7}$ for these minerals.

In natural environments, the alpha particles received by a fine grain (from U and Th decay chains) have a wide energy spectrum. The average efficiency of these alpha particles in generating luminescence is lower than that of a 3.7 MeV alpha particle (Zimmerman, 1971; Aitken, 1985). Consequently, the effective k-value (k_{eff}) in nature is typically smaller than the $k_{3.7}$ or the a-value. When calculating the natural alpha dose rate, a correction factor should be applied to the a-value or $k_{3.7}$ to obtain the k_{eff}. The correction factors are slightly different between different minerals (Zimmerman, 1971; Aitken, 1985). For quartz, a correction factor of 0.83 was deduced assuming equal U and Th activities (Zimmerman, 1971; Aitken, 1985). It is worth noting that this correction factor is based on TL signals, and such correction factors for OSL and ESR signals have not been reported yet. The correction factors before and after Rn in the decay chain of ^{238}U are also slightly different (Zimmerman, 1971). We have not accounted for the influence of Rn loss on the correction factors, and have applied a constant correction factor of 0.83 in our scripts. If needed, users can change the correction factor in the functional R scripts **calc_dr_alpha_fine.R** and **calc_dr_alpha_coarse.R**, by the parameter of 'a2k' in the code.

Using the a-value to calculate alpha dose rates without converting it to the k_{eff}, the alpha dose rates will be overestimated by ∼20 %. Taking the sediments from the Rodderberg crater basin as an example, alpha dose rates contribute approximately 22 % and 11 % to the total dose rates of fine-grained feldspar and quartz, respectively (Zhang et al., 2024b). Thus, 20 % overestimation in the alpha dose rates will result in 4.4 % and 2.2 % overestimation in the total dose rates for fined-grained feldspar and quartz, respectively (Fig. 2B). In cases where the alpha dose rate makes a major contribution, such as in carbonate rocks, the correction factor from a-value to k_{eff} will be crucial.

2.3. Comparison with DRAC

The dose rates of quartz and feldspar calculated from our R scripts are compared with those calculated by the DRAC software (Durcan et al., 2015). Dose rates were calculated with no Rn loss, as DRAC cannot directly account for Rn loss in its calculation. In the input CSV template of DRAC, we entered the k_{eff} values rather than the a-values. The k_{eff} values were calculated by multiplying a correction factor of 0.83 with the a-values, which are 0.04 ± 0.01 for quartz and 0.09 ± 0.02 for feldspar, respectively. The dose rate results from our R scripts are identical to those from DRAC (Table S5; Fig. 2C).

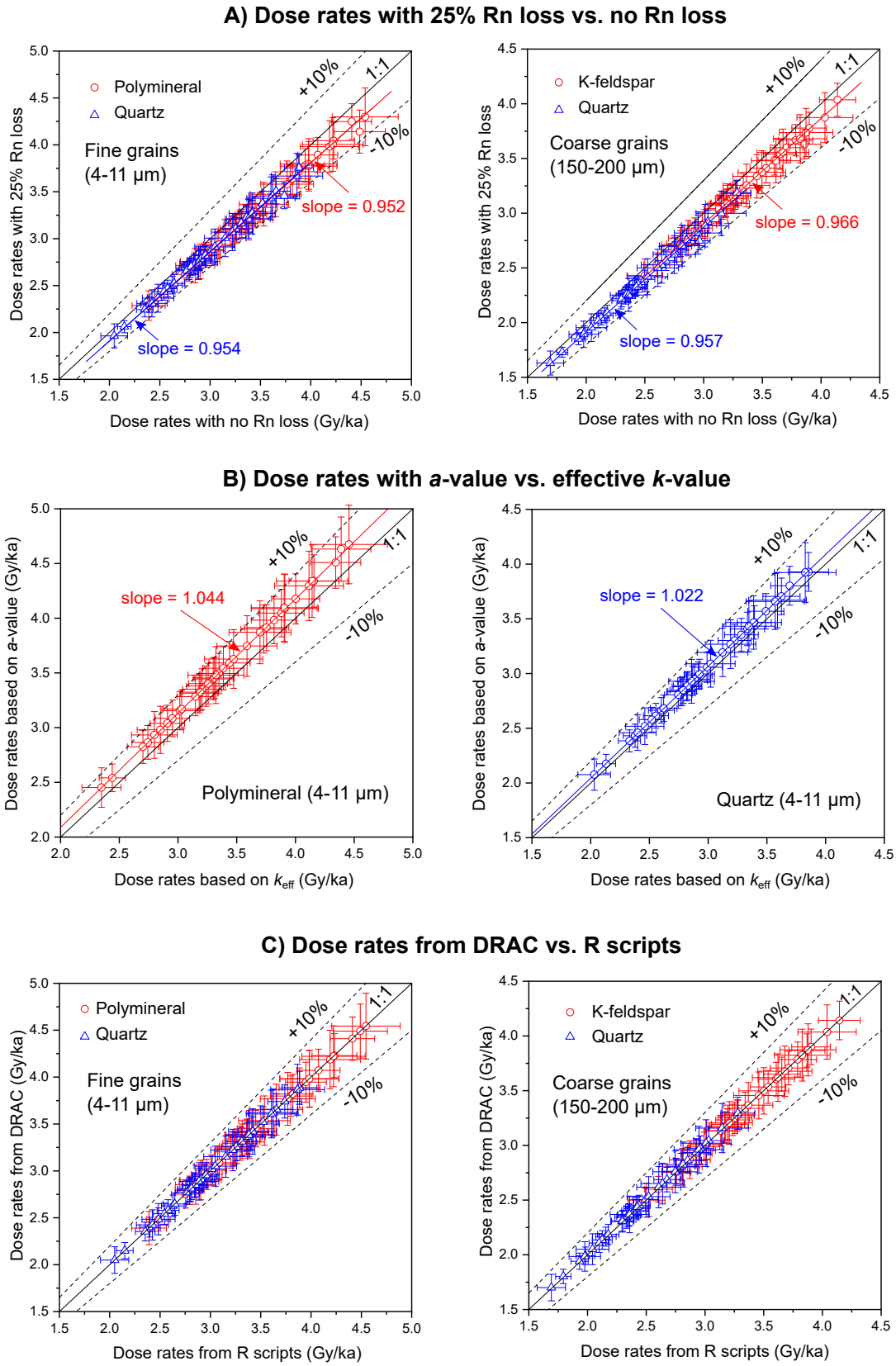

Figure 2: A) Comparison between dose rates calculated with 25 % Rn loss and no Rn loss, for fine grains and coarse grains. B) Comparison between dose rates calculated with the *a*-value and the effective *k*-value (k_{eff}) for fine-grained polymineral material and quartz. C) Comparison between dose rates calculated by DRAC and our R scripts for fine grains and coarse grains. For the coarse grains, the HF etched thickness is set as 10 μm for quartz and 0 μm for K-feldspar. The samples are loess and lacustrine sediments from the Rodderberg crater basin, Germany (Zhang et al., 2024b).

3. R scripts for carbonates

The existing MATLAB™ code 'Carb' (Mauz and Hoffmann, 2014) and its translation to R ('RCarb'; Kreutzer et al., 2019) were developed for dose rate calculation of quartz grains inside carbonate rich sediments, to account for the dose rate change with time resulting from the replacement of air and water in the pore space by carbonates. We have prepared two R scripts for dose rate estimation of carbonate minerals in carbonate rocks (e.g., speleothem, limestone, dolostone), using the assumption of an infinite homogeneous medium. These two scripts are **doserate_carbonate_keff.R** and **doserate_carbonate_sa.R**, in the folder named 'doserate_homogeneous_carbonate' under the doserate_rProject. If users apply the effective k-value for the alpha dose rate calculation, the script of **doserate_carbonate_keff.R** should be used in combination with the **Template_carbonate_keff.csv** file. In the template CSV file, users need to enter the k_{eff} values for each individual sample, as alpha efficiency values may vary significantly between different calcite and dolomite samples (e.g., Debenham and Aitken, 1984; Zhang et al., 2025). The alpha dose rate contributes more than 50 % to the total dose rate for carbonate samples in an infinite homogeneous medium (Fig. 3). Therefore, we recommend measuring the alpha efficiency for each individual sample as part of routine procedures in dating carbonates.

In addition to the k-value and a-value systems, the S_α-value system (Guérin and Valladas, 1980) has also been used in calculating the alpha dose rate. With the S_α-value, the effective alpha dose rate can be obtained directly from the alpha flux. If users apply the S_α-value system, the **doserate_carbonate_sa.R** script should be used in combination with the file **Template_carbonate_sa.csv**. S_α-values need to be entered for each sample. The alpha fluxes of 1 µg g^{-1} (ppm) U or Th in calcite and dolomite are slightly different. In the 'mineral' column of the CSV template, either 'calcite' or 'dolomite' should be entered. The ranges (in mg cm^{-2}) of alpha particles with different energies for calcite (ρ = 2.71 g cm^{-3}) and dolomite (ρ = 2.85 g cm^{-3}) were obtained from the software 'The Stopping and Range of Ions in Matter' (SRIM version 2013; Ziegler and Biersack, 1985). With these alpha ranges, the alpha fluxes of 1 µg g^{-1} U or Th in calcite and dolomite were calculated based on the energy spectrum of emitted alpha particles in their decay chains using an MS Excel™ sheet (provided by Norbert Mercier, see Supplementary Materials). For calcite, the alpha fluxes of 1 µg g^{-1} U and 1 µg g^{-1} Th are 18,468 and 5,166 cm^{-2} a^{-1}. For dolomite, the corresponding values are 18,013 and 5,047 cm^{-2} a^{-1}, respectively. Previous studies have reported alpha ranges for quartz, feldspar and calcite (e.g., Brennan and Lyons, 1989; Valladas, 1988). We have updated these alpha range data with the SRIM 2013 software. Though the ranges of alpha particles are slightly different between different minerals, the alpha fluxes from 1 µg g^{-1} U or Th differ by less than 3 % between quartz, K-feldspar, calcite and dolomite (see Table S6).

The S_α-value is almost independent of the energy of alpha particles. However, when alpha particle energies fall below 2 MeV, the luminescence generated per unit track length decreases significantly (Zimmerman, 1971, 1972; Aitken and Bowman, 1975; Aitken, 1985). The S_α-values we provide in **Template_carbonate_sa.csv** were measured with an ^{241}Am source at Archéosciences Bordeaux, CNRS-Université Bordeaux Montaigne (Zhang et al., 2024a, 2025). These values are slightly different from the S_α-values in nature, as the energy spectrum of the alpha particles emitted by the Bordeaux ^{241}Am source arriving at the aliquots differs from that of the U and Th decay chains in nature (Kreutzer et al., 2018). Correction factors of 0.92 for U and 0.96 for Th have been simulated for the measured S_α-values, respectively (personal communication with Norbert Mercier by email on 29 March 2023). Thus, inside the **doserate_carbonate_sa.R** script, these two correction factors have been multiplied with the S_α-values when calculating alpha dose rates. These correction factors likely differ for different alpha sources used for measuring the S_α-values.

These two R scripts for carbonate dose rate calculation are based on the secular equilibrium state of ^{238}U. When dating the crystallization event of carbonates (e.g., speleothem growth, shell formation), U-series disequilibrium should be considered. Variation of dose rate through time since carbonate crystallization can be modelled by the **doserate_simulation.R** script in the folder 'correction_for_238U_disequilibrium'. Results are saved as **doserate_simulated_238U_disequilibrium.csv**. The simulation is based on the U concentration and the initial ^{234}U/^{238}U activity ratio. The activities of ^{238}U, ^{234}U and ^{230}Th (Bq kg^{-1}) are calculated from their decay constants (Fig. 4A). The dose rates from three segments of the ^{238}U decay chain (^{238}U to ^{234}U, ^{234}U to ^{230}Th, ^{230}Th to ^{206}Pb) are calculated separately and summed up to obtain the dose rate of the full decay chain (Fig. 4B). Adding the constant dose rates from the ^{232}Th decay chain, ^{40}K and cosmic ray, the totally accumulated dose (D_e) with time can be simulated (Fig. 4C). The script **doserate_simulation_for_age_err.R** is used to deduce the age error by the Monte Carlo method. The **age_iteration.R** is another R script to deduce the crystallization age, by an iteration method modified from Ikeya and Ohmura (1983). More details about the modelling can be found in Zhang et al. (2024a).

4. Access to the code and supplementary materials

The R scripts are freely available on GitHub at `https://github.com/JunjieZhang113/R-scripts-dose-rate-calculator`, and on Zenodo at `https://doi.org/10.5281/zenodo.15856401`.

Together with the R scripts, supplementary materials are uploaded. These supplementary files include MS Excel™ tables showing the fitting of grain size related parameters, the raw data of stopping powers and ranges of alpha particles in different minerals from the SRIM2013 software, and

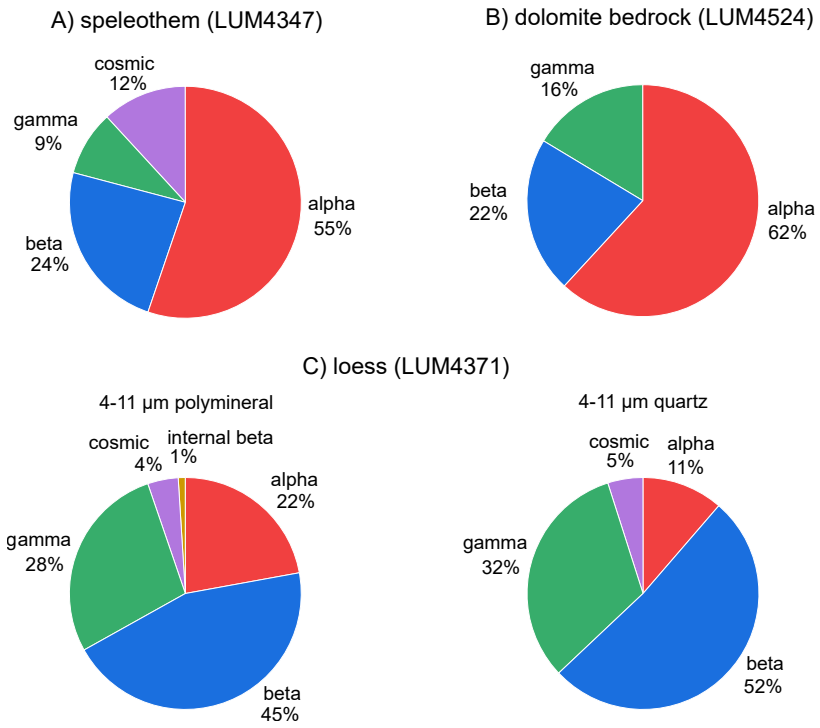

Figure 3: Pie charts showing dose rate compositions of two carbonate samples and one loess sample. A) The speleothem sample is from the Bleßberg cave, Germany (Zhang et al., 2024a). B) The dolomite bedrock sample is from the central Apennines, Italy (Zhang et al., 2025). C) The loess sample is from the Rodderberg crater basin, Germany (Zhang et al., 2024b). Note that for the carbonate samples, alpha dose rates contribute more than half to the total dose rates.

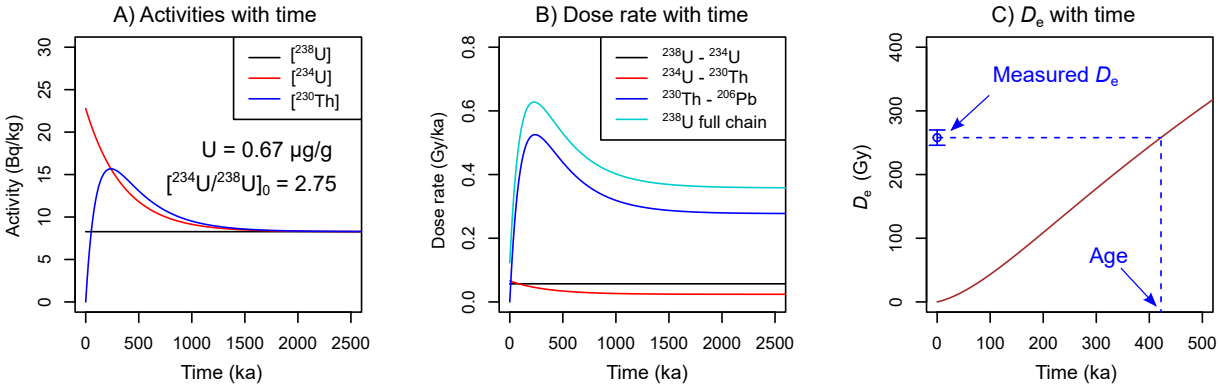

Figure 4: Example for simulating the dose rate change with time since the carbonate crystallization. The sample here is a speleothem (LUM4347) from the Bleßberg cave, Germany (Zhang et al., 2024a).

the summary of alpha fluxes. DRAC dose rate results of the sediment samples from the Rodderberg crater basin are also attached for comparison with dose rate results from the R scripts.

Data availability. All data generated in this study are included in this article, its Supplementary Materials and archived on GitHub and Zenodo.

Conflict of interest. The authors declare that they have no conflict of interest that could have biased their scientific work.

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Review. This article was reviewed by Sebastian Kreutzer.

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portunities to measure S_α-values of calcite and dolomite samples at Archéosciences Bodeaux, CNRS-Université Bordeaux Montaigne (France) and the Justus-Liebig University of Giessen (Germany), as well as the discussion about S_α-value evaluation. Norbert Mercier prepared the MS Excel™ table to calculate the alpha flux from alpha ranges, and simulated the correction factors for the measured S_α-values to account for the energy spectrum difference between the ^{241}Am alpha source in Bordeaux and the natural environment. We are grateful to Sebastian Kreutzer whose constructive comments have greatly helped us to improve the manuscript and the R code.

Disclaimer by the reviewer. In 2024, I participated in an extensive scientific discussion via email with the authors and the group in Bordeaux regarding the calculation of the alpha efficiency. Consequently, I was included in the acknowledgements regardless of the provided review. Additionally, during the review process, I recommended incorporating two additional references to this manuscript, where I am the first author (simulation of the ^{241}Am energy spectrum, RCarb; Kreutzer et al., 2018, 2019). I deem both references relevant to the given context. However, due to my personal bias, it was the authors' prerogative to include them (or not).

Reviewer comment. In my experience with research software development, I have observed over the years that not every newly developed tool is automatically appreciated. Users may be overwhelmed by the abundance of possibilities, leading to confusion about the advantages and disadvantages, and sometimes "yet another tool" mindset. Here, I would like to take the opportunity to highlight three aspects I consider relevant from a research software perspective, underscoring the significance of such contributions. First, through the development of their solution, the authors spent considerable time double-checking existing solutions, thereby verifying and documenting their calculations; a vital aspect of reproducible science. Second, for carbonate and radon loss, they added new code that can be easily used by others, avoiding the need to reinvent the wheel. Lastly, any open-source software alternative is always highly welcome, as it provides users with a choice and allows them to pick their preferred solution.

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