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‘RCarb’: Dose Rate Modelling of Carbonate-Rich Samples - an Implementation of *Carb* in R -

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Abstract

Geochemical conditions (e.g., pH-value, temperature, availability of CO₂) in carbonate-rich sedimentary environments lead to cementation processes, i.e., air or water in the pore space are substituted by mineral phases. Consequently, in such environments the conventional formalism of estimating the environmental dose rate from U, Th and K concentrations (pores are filling by air or water) cannot be overall correct. In 2008, Nathan & Mauz (2008) presented a model to account for dose-rate changes occurring when carbonate minerals replace air and water in the pore space between mineral grains. The underlying MATLAB® code (*Carb*) was later published by Mauz & Hoffmann (2014). Here we present an implementation of this tool using the statistical programming environment R. Our implementation does not alter the underlying model and its assumption but comes with an updated code basis published as R package under GPL-3 licence conditions.

Keywords: Luminescence dating; Dose rate; R

1. Motivation

Over the last decades the luminescence dating community has developed various software tools (cf. Kreutzer et al., 2017) to facilitate automatised analytical workflows and processing of data from samples originating from sedimentary environments that underwent post-depositional changes with consequences for the dose-rate estimation. Some of these tools are likely to be used only occasionally, but nevertheless

carefully collected and archived for the moment when they are needed. In contrast to good Bordeaux wine, sadly, software does not mature with age: Software that had worked perfectly in the past eventually renders itself unusable when needed. It was such an event that revealed the need for the creation of ‘RCarb’ (Kreutzer et al., 2019).

At the IRAMAT-CRP2A in Bordeaux, we processed carbonate-rich sediment samples using routine luminescence dating techniques (e.g., optically stimulated luminescence, Huntley et al., 1985), for which the ages were not in stratigraphic order. We hypothesised that this was caused by the replacement of pore water by carbonate minerals, which promotes dose-rate changes through time. To test this hypothesis, the work by Nathan & Mauz (2008) and Mauz & Hoffmann (2014) and the published MATLAB® software *Carb* seemed to offer a convenient starting point without the need to run a full simulation in *DosiVox* (Martin et al., 2015), which would be further complicated by the assumed post-depositional dose-rate alterations. Problems with running the code in an updated version of MATLAB® motivated us to translate it into R (R Core Team, 2019) and deploy it to the trapped-charge dating community as R package; henceforth named ‘RCarb’. The implementation of ‘RCarb’ aimed at:

- Providing a version of *Carb* based on open-source software and published under GPL-3,
- updating and refitting the code basis to extend its availability to the community by another 5 to 10 years,
- supplementing *Carb* with an updated documentation of the code for developers as well as for end-users to facilitate the usage of the software,
- enabling future, community driven, developments by using the open-source repositories such as GitHub (<https://github.com>).

In the following, we outline the main implementation aspects of ‘RCarb’ and provide **R** code snippets (typed in monospace letters). *Carb* was designed to model dose rate through time for quartz grains $> 100\mu\text{m}$. Typically, these grains are etched in concentrated HF and, thereby, the external α -dose contribution is removed (Fleming, 1966, 1970) and does not need be considered for the modelling. However, not in all cases an etching of the grains is feasible or desired (e.g., a limited amount of material). To be able to consider the full radiation field for special sample cases, we additionally discuss the impact of α -radiation on the dose-rate modelling, simulated for grain diameters of $4\mu\text{m}$ and $250\mu\text{m}$.

2. Implementation

The original MATLAB[®] program (Mauz & Hoffmann, 2014, their supplement) consists of 51 individual files in a single folder. These files represent the code necessary to run the model and to provide a graphical user interface (GUI). The files further comprise reference and example data, tests scripts and cached graphical and numerical output. MATLAB[®] and **R** are both numerical computation environments which mainly evaluate code during runtime. With some knowledge of the syntax differences, MATLAB[®] code can be translated easily into **R**. However, translating non-**R** code into a full **R** package requires substantial effort to meet the basic requirements of the Comprehensive R Archive Network (CRAN, <https://cran.r-project.org>) which is the central **R** package repository. In the following, we detail the implementation of *Carb* in ‘RCarb’ to provide a better understanding of the package structure and to highlight similarities and differences between the two programs.

2.1. Central premise and code structure

‘RCarb’ was designed with the intention to keep the original code recognisable, notwithstanding more efficient or elegant solutions would exist in **R**. The names of variables as well as large parts of the code structure remained almost identical to that presented in Nathan & Mauz (2008); Mauz & Hoffmann (2014). Basic MATLAB[®] functions were replaced by **R** equivalents and, consequently, a new syntax had to be adopted. Comments were added where they appeared to be necessary for the understanding of the code. Likewise, the code structure (Fig. 1) was modified and broken down into separate functions. Three of these functions are for internal use only and not accessible by the user (see below).

2.2. Reference and example data

In a first step, the file structure was reorganised to meet the CRAN **R** package requirements. Reference data, which are (1) water/carbonate correction factors for β and γ -radiation after Nathan & Mauz (2008), (2) β -dose attenuation factors after Mejdahl (1979), (3) and example data taken from Mauz & Hoffmann (2014), were imported into **R** and integrated as package (example) data. In the **R** terminal they are now ac-

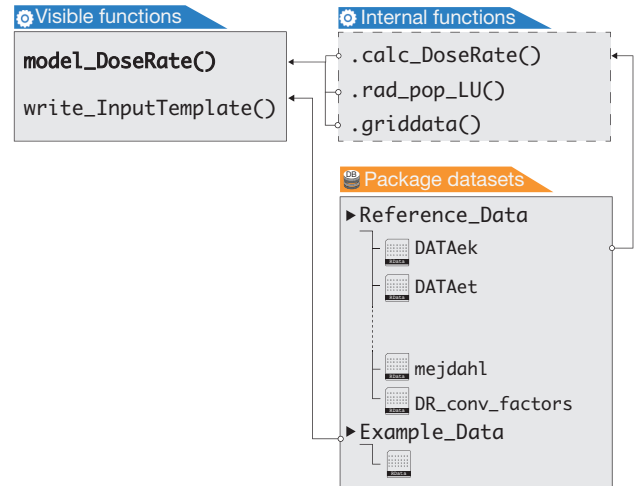


Figure 1: The threefold structure of the R package ‘RCarb’. In its current state, the package has only two visible functions. Additional internal functions (e.g., `.calc_DoseRate()`) are not meant for user interaction. These functions are not displayed to the user and they show no documentation (but are supplied with comments in the code). Package datasets are (1) reference data needed for the calculation, e.g., `mejdahl`, which refers to the β -dose attenuation dataset published by Mejdahl (1979) and (2) example datasets from *Carb*. For further details see main text.

cessible via, e.g., `data(Example_Data)`. Additionally, appropriate documentation was added for the reference as well as the example data. The reference data are used extensively by the internal functions, while the example data serve as test dataset to the user.

2.3. The modelling core

The second step consisted of a line by line translation of the MATLAB[®] code and removal of unused code lines. *Carb* is started in MATLAB[®] by executing `carb_2007a.m` which then internally calls the files `daterlu1.m` and `rad_pop_LU.m`. Other files, e.g., those preceding with the word ‘test’, are not needed to run the program and have been removed. In ‘RCarb’, the internal workhorse function is called `.calc_DoseRate()` and it is based on the file `daterlu1.m` from *Carb*. The function `rad_pop_LU()` is the **R** equivalent of `rad_pop_LU.m` and `.griddata()`, and provides a match to the MATLAB[®] function `griddata` for the interpolation of irregular gridded data. Actually, an equivalent does not exist in base **R** so that we had to implement the package ‘interp’ (Gebhardt et al., 2019). All three functions are not exported, i.e. they do not appear in the help page index and are not directly visible to the user.¹ The new

¹Such internal functions in **R** packages mainly serve the package developers and do not usually provide a documented interface. Although such functions can still be called, e.g., `RCarb:::calc_DoseRate()`, they should not be employed by the user without having a profound reason (and knowledge). Besides, CRAN itself does not allow calling such “non-exported” functions from inside other packages.

entry point for the user is the function `model_DoseRate()`. This function has a full documentation and provides terminal and graphical output very similar to *Carb* (see Sec. 3 for examples).

2.4. Graphical user interface and miscellaneous

In a third step, the MATLAB® code providing the GUI was removed. This code only works in MATLAB® and cannot be translated easily into R. As a consequence, 'RCarb' is light-weighted, uses base R syntax and does not depend heavily on other R packages. The reduced overhead may simplify and encourage the code inspection by others. However, to improve the usability, in particular for users not familiar with R, we provide a new (separate) GUI to 'RCarb' through the R 'RLumShiny' package (Burow et al., 2016, 2019) (cf. Fig. 3, see below).

In the last step, code example and reference data were compiled as R package and submitted to CRAN. Although 'RCarb' does not depend on other packages of the 'RLum' family (e.g., 'RLumShiny'), it is hosted and developed through the same version control hosting service GitHub (<https://github.com/R-Lum/RCarb>). Thereby, 'RCarb' benefits from established development workflows and testing routines ensuring robust and smooth execution on the three major platforms (Windows®, Linux™, macOS®) as detailed by Kreutzer et al. (2017).

2.5. Enhancements and code modifications

Besides code structure alterations required by the translation from MATLAB® to R, two additional modifications slightly changed the calculation output in comparison to *Carb*. The first difference concerns a bug: In case values for ^{238}U and $^{234}\text{U}/^{238}\text{U}$ activity ratios were provided, erroneously the same water correction factor (for the concept of those factors cf. Zimmerman, 1971) applied to correct the β -dose rate was also used for the γ -dose rate. 'RCarb' now applies the correct factors, i.e. the β -dose correction factors to the β -dose rate and the γ -correction factors to the γ -dose rate.

The second modification relates to the dose-rate conversion factors. The latest version of *Carb* uses dose-rate conversion factors downloaded from the ENSDF database as of January 16, 2002 (Roger Nathan, personal communication, July 24, 2019; archived database versions available at <http://www.nndc.bnl.gov/ensarchivals/>). These factors are slightly different to published values used by the trapped-charge dating community (e.g., Adamiec & Aitken, 1998). Considering the overall uncertainties of the dose-rate modelling for carbonate-rich samples, the differences are, however, negligible. Nevertheless, to provide a consistent and up-to-date approach, 'RCarb' supports, on top of the dataset from *Carb*, now named 'Carb2007', the selection of dose-rate conversion factors published by Adamiec & Aitken (1998), Guérin et al. (2011), and Liritzis et al. (2013). These datasets are part of the package reference data (cf., `Reference_Data`, Fig. 1). The default set-

ting is 'Carb2007' to yield modelling results consistent with the original *Carb*. To see the implemented datasets type `RCarb::Reference_Data$DR_conv_factors` in your R terminal.

3. Running examples

Before outlining two examples for how to run 'RCarb' in the R terminal, we wish to remind the reader that these software examples can provide only a first impression. The manuscript remains static, while 'RCarb' may evolve. Consequently, our examples are kept short and we point the reader to the always up-to-date HTML-document shipped alongside the package (a so called 'vignette') via CRAN.

3.1. Example 1 - example dataset

Users who are not familiar with R should first look at the example section in the package manual. It provides a good start (type `?model_DoseRate` in the R terminal) and 'RCarb' includes the example data of *Carb*. The code lines in listing 1 first load the package itself before loading the example data into the working environment. Subsequently, line 6 (listing 1) calls row 14 from the table with the example data (without modifying the function arguments). This example is similar to the one shown in Mauz & Hoffmann (2014) (their Fig. 4).

Listing 1: Running 'RCarb' using the package example dataset.

```
1 ##load example data and example data
2 library(RCarb)
3 data("Example_Data", envir = environment())
4
5 ##model dose rate for sample LV107
6 model_DoseRate(data = Example_Data[14,])
```

The terminal and graphical output (Fig. 2) is very similar to the one provided by *Carb*. Our example output (listing 2) shows that the conventional age calculation, i.e. without considering the pore filling by carbonate, overestimates the age by ca 15 %.

Listing 2: Typical 'RCarb' terminal output.

```
[model_DoseRate()]

Sample ID:          LV107
Equivalent dose:    53 ± 2 Gy
Diameter:           215 µm
MC runs error estim.: 100
-----
Age (conv.):        149.73 ± 10.667 ka
Age (new):          130.642 ± 7.754 ka

Dose rate (conv.):  0.354 ± 0.018 Gy/ka
Dose rate (onset):  0.499 ± 0.027 Gy/ka
Dose rate (final):  0.361 ± 0.017 Gy/ka
-----
```

3.2. Example 2 - own dataset

Using own data requires the replacement of the input data (in listing 1: `data = Example_Data[14,]`) by an own `data.frame`. Because this particular user interaction likely increases the chance to crash the function and then becoming a frustrating experience, we aimed at minimising the probability of such events. In the next example (listing 3), after loading ‘RCarb’, the function `write_InputTemplate()` first generates a template CSV-file (if the argument `file` is left blank, a template `data.frame` is returned to the **R** terminal). The CSV-file can be filled easily with every spreadsheet software (e.g., *Excel*®) and re-imported into **R** (code lines 9–12). In the final call of `model_DoseRate()`, `data = Example_Data[14,]` it is replaced by `data = own_data`. The subsequent calculation does not require user interaction but may take a while.

Listing 3: Working with own data.

```
1 ##load package
2 library(RCarb)
3
4 ##write template CSV
5 write_InputTemplate(
6     file = 'YOUR_PATH/MyData.csv')
7
8 ##import after filled with external program
9 own_data <- read.table(
10     file = 'YOUR_PATH/MyData.csv',
11     header = TRUE,
12     sep = ',')
13
14 ##run model
15 model_DoseRate(data = own_data)
```

3.3. Remarks

If the input table has more than one row, `model_DoseRate()` automatically iterates over all rows, i.e. multiple samples. Entries leading the function to fail are skipped and removed from the output. The uncertainties are estimated using a resampling approach similar to *Carb*. By default, the function uses 100 Monte Carlo (MC) runs (argument `n.MC`). More MC runs likely increase the quality of the error estimate but also the computation time.

4. Limitations and further considerations

Carb (and so ‘RCarb’) does not model the dose-rate effect of α -radiation. Instead, *Carb* was written to model post-depositional dose-rate alteration by which the sediment is subject to gradual infilling of carbonate in the pore space. Within the range of sedimentary deposits suitable for luminescence dating, those containing sand-sized components are most likely to be affected by this process. As a consequence, *Carb* was designed for sand-sized quartz grains and these are usually treated with HF (cf. Porat et al., 2015; Duval et al., 2018, for recent discussions) in order to remove the

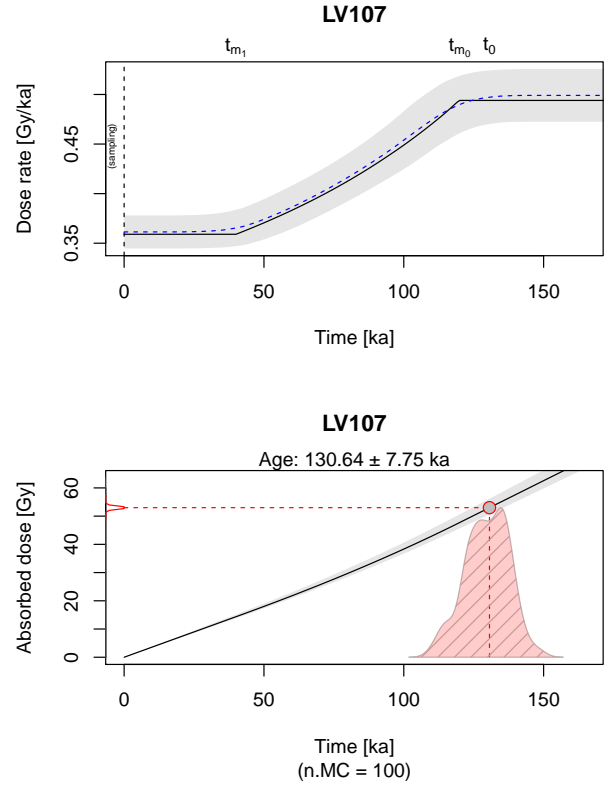


Figure 2: Graphical output of ‘RCarb’ for a sample from the example dataset (here: HD107, which corresponds to the sample LV107 shown in Mauz & Hoffmann 2014, their Fig. 4).

The *upper plot* reads from right to left and displays the dose-rate evolution over time with t_0 the burial time, t_{m0} the inset of the cementation and t_{m1} the completion of the cementation. The grey shaded error indicates the error margins determined by MC runs. The dashed blue line provides a quality measure for the number of the MC runs. If the dashed blue line closely matches the solid line, the number of MC runs have been sufficient. Please note that the match will be never perfect.

The *lower plot* shows the absorbed dose over time indicating the resulting age (red lines). Dashed lines and grey shaded area indicate error margins. The superlinear evolution of the absorbed dose is a consequence of the modelling and no display error.

α -radiation affected outer rim of the grains. However, what can we do with a sample that has not been etched?

The travel range of (natural) α -particles in silicate-rich sediments is a few micrometres so that only those grains situated in close vicinity to the emitter receive an external α -dose. If the pore space between the grain and emitter, typically occupied by air or water, is gradually filled with carbonate instead of air or water, the α -dose changes over time. Therefore, we provide additional information on the α -correction factors needed to estimate the environmental dose rate and calculate the luminescence age. In the appendix (Tables A1–A4) we list α -correction factors following the style

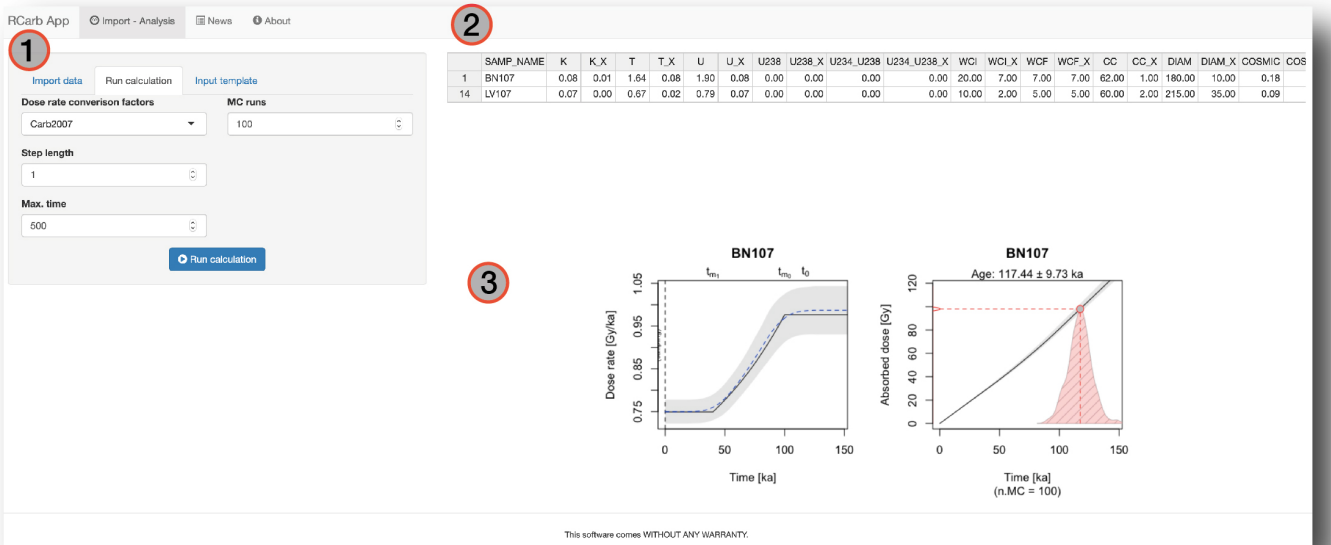


Figure 3: Screenshot of the Shiny app ‘RCarb App’ providing a graphical user interface to the package ‘RCarb’. (1) Data import and calculation menu, (2) central data table with input and output data and (3) graphical output similar to Fig. 2.

of Table 1 in [Mauz & Hoffmann \(2014\)](#) for different water- and carbonate-mass fractions for a grain size of 250 μm (Tables A1–A2) and 4 μm (Tables A3–A4). Values for the U-series and the Th-series are quoted for each grain size, and the lower rows of each table list the corresponding 2σ uncertainties.

These new α -correction factors were determined by simulations with the software *GEANT4* ([Agostinelli et al., 2003](#)) with a setup similar to [Martin et al. \(2014\)](#). Our sediment composition used for the simulation followed [Nathan & Mauz \(2008\)](#) who relied on [Garrels & Mackenzie \(1971\)](#). Thus, the sediment was dominated by quartz with a significant contribution of feldspar represented by the following chemical composition: SiO_2 (66 %), Al_2O_3 (18 %), Fe_2O_3 (6 %) and KAlSi_3O_8 (10 %)². The initial density (without water and carbonate) was set to 1.8 g cm^{-3} . CaCO_3 was used to simulate carbonate.

The obtained values seem to show a similar trend for both silt and sand (simulated grain diameters: 4 μm and 250 μm) but are characterised by increasing uncertainty with decreasing grain size owing to the very low probability for an α -particle to hit the (simulated) grain. Additional simulations would improve the precision of the quoted values. Unfortunately, this would require access to a large computer cluster over several months. Such resources were not available for this article and, besides, more precise factors do not necessarily improve the overall accuracy of the dose-rate modelling.

Additionally, we performed simulations (data not shown) for the case of detrital carbonate, i.e. the carbonate is part of the sediment components (i.e., no cementation). The re-

sulting α -correction factors, averaged for U- and Th-series, estimate at 1.36–1.37 for reasonable water contents inferior or equal to 20 %. Such values are close to the values reported by [Martin et al. \(2014\)](#) for a clay sediment matrix. We did not include those correction factors into ‘RCarb’ since it would require extensive modification of the code basis, unjustified by the significant uncertainties of the correction factors (cf. Tables A1–A4). Instead, if needed, the listed factors can be used to roughly estimate the impact of the pore filling process on the luminescence ages in particular environments.

5. Graphical user interface (GUI)

We provide a simple GUI via the R ‘RLumShiny’ (cf. [Burow et al., 2016](#)). To run the GUI the user needs to install the two packages ‘RCarb’ and ‘RLumShiny’. Alternatively, an installation of ‘RLumShiny’ will force ‘RCarb’ to install, but not *vice versa*. The GUI can be started in the R terminal via (listing 4):

Listing 4: Starting the Shiny app ‘RCarb’.

```
##load package
library(RLumShiny)

##start app
app_RLum(app = 'RCarb')
```

In case a valued colleague runs a local *Shiny* server (<https://shiny.rstudio.com/>) in your institution, the ‘RCarb App’ can be started like every other web-based application. We do not provide the ‘RCarb App’ via the *Shiny* hosting service (<http://www.shinyapps.io>), since

²We tested different feldspar phases but found no significant differences.

the few free calculation hours would be quickly exhausted by a few users and the commercial service is rather costly.

‘RCarb App’ (Fig. 3) is split into three sub-windows: (1) The import and settings panel, (2) the modifiable spreadsheet and (3) a graphical output similar to the one presented in Fig. 2. Clicking on the table rows (Fig. 3-2) switches the graphical output, i.e. (3) shows the figures corresponding to the selection in (2). The central table supports various standard user interactions such as copy & paste, deletion and insertion of rows. Please note that the modelling feature set of ‘RCarb’ determines the functionality of “RCarb App”.

6. Conclusion and outlook

We presented a new **R** package called ‘RCarb’. This package is a translation of the MATLAB[®] software *Carb* introduced by Nathan & Mauz (2008) and Mauz & Hoffmann (2014). While the package is new, it does not enhance or substantially modify the features set by *Carb*. However, with ‘RCarb’, we provide a refitted open-source and open-access solution to the community. The code is maintained via the platform GitHub and we invite interested readers to contribute to further developments. A graphical user interface to ‘RCarb’ is available through the **R** package ‘RLumShiny’.

Finally, we wish to remind the reader about limits and assumptions underpinning the *Carb* model. They are detailed in Nathan & Mauz (2008) and Mauz & Hoffmann (2014).

‘RCarb’ is available

- as **R** package via CRAN: <https://CRAN.R-project.org/package=RCarb>,
- as development version under <https://github.com/R-Lum/RCarb>,
- and we host a package webpage at <https://r-lum.github.io/RCarb/>.

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Reviewer

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Appendix

A1: α -radiation correction factors - 250 μm

Table A1: U-series correction factor x for α -radiation for water and carbonate to sediment mass ratios (m_s : sediment mass; m_c : carbonate mass; m_w : water mass). Values in *italic* do not exist in nature. The lower table quotes corresponding 2σ uncertainties.

U-series — α -radiation — 250 μm				
m_w/m_s	m_c/m_s			
	0.00	0.04	0.20	1.00
0	-	0.99	1.03	1.02
0.04	1.36	1.18	1.08	1.03
0.20	1.38	1.31	1.19	1.07
1.00	1.37	1.36	1.32	1.19
<i>corresponding 2σ uncertainty</i>				
0	-	38.2 %	5.8 %	2.5 %
0.04	29.6 %	15.7 %	4.8 %	2.1 %
0.20	8.7 %	4.4 %	3.0 %	2.2 %
1.00	3.0 %	2.2 %	2.0 %	2.1 %

Table A2: Th-series correction factor x for α -radiation for water and carbonate to sediment mass ratios (m_s : sediment mass; m_c : carbonate mass; m_w : water mass). Values in *italic* do not exist in nature. The lower table quotes corresponding 2σ uncertainties.

Th-series — α -radiation — 250 μm				
m_w/m_s	m_c/m_s			
	0.00	0.04	0.20	1.00
0	-	0.96	1.01	1.01
0.04	1.38	1.17	1.07	1.03
0.20	1.36	1.29	1.18	1.07
1.00	1.36	1.34	1.30	1.19
<i>corresponding 2σ uncertainty</i>				
0	-	36.0 %	8.9 %	2.5 %
0.04	18.0 %	18.5 %	4.6 %	3.9 %
0.20	6.3 %	5.4 %	4.1 %	3.2 %
1.00	3.5 %	3.8 %	4.5 %	3.4 %

A2: α -radiation correction factors - 4 μm

Table A3: U-series correction factor x for α -radiation for water and carbonate to sediment mass ratios (m_s : sediment mass; m_c : carbonate mass; m_w : water mass). Values in *italic* do not exist in nature. The lower table quotes corresponding 2σ uncertainties.

U-series — α -radiation — 4 μm				
m_w/m_s	m_c/m_s			
	0.00	0.04	0.20	1.00
0	-	1.38	0.99	1.03
0.04	1.62	1.00	1.36	1.06
0.20	1.43	1.42	1.12	1.04
1.00	1.42	1.41	1.37	1.20
<i>corresponding 2σ uncertainty</i>				
0	-	240.0 %	68.8 %	27.8 %
0.04	256.6 %	183.2 %	45.9 %	22.0 %
0.20	69.1 %	48.5 %	37.6 %	23.9 %
1.00	37.6 %	21.9 %	20.0 %	19.3 %

Table A4: Th-series correction factor x for α -radiation for water and carbonate to sediment mass ratios (m_s : sediment mass; m_c : carbonate mass; m_w : water mass). Values in *italic* do not exist in nature. The lower table quotes corresponding 2σ uncertainties.

Th-series — α -radiation — 4 μm				
m_w/m_s	m_c/m_s			
	0.00	0.04	0.20	1.00
0	-	0.88	1.08	1.06
0.04	1.41	0.97	1.04	1.05
0.20	1.43	1.33	1.19	1.07
1.00	1.36	1.36	1.34	1.21
<i>corresponding 2σ uncertainty</i>				
0	-	313.9 %	56.5 %	20.5 %
0.04	212.5 %	149.8 %	49.8 %	22.1 %
0.20	62.7 %	40.6 %	30.6 %	18.7 %
1.00	27.6 %	17.2 %	18.5 %	17.1 %