

Package ‘RCarb’

December 9, 2018

Type Package

Title Dose Rate Modelling of Carbonate-Rich Samples

Version 0.1.2

Date 2018-12-02

Author Sebastian Kreutzer [aut, trl, cre, dtc]
(<https://orcid.org/0000-0002-0734-2199>),
Roger P. Nathan [aut, cph],
Barbara Mauz [aut, cph] (<https://orcid.org/0000-0003-1504-333X>)

Maintainer Sebastian Kreutzer sebastian.kreutzer@u-bordeaux-montaigne.fr

Description Translation of the 'MATLAB' program 'Carb' (Nathan and Mauz 2008 <[DOI:10.1016/j.radmeas.2007.12.012](https://doi.org/10.1016/j.radmeas.2007.12.012)>; Mauz and Hoffmann 2014) for dose rate modelling for carbonate-rich samples in the context of trapped charged dating (e.g., luminescence dating) applications.

Depends R (>= 3.3.0), utils

Imports interp (>= 1.0), matrixStats (>= 0.50.0)

Suggests testthat (>= 2.0), R.rsp (>= 0.42.0)

License GPL-3

Encoding UTF-8

LazyData true

VignetteBuilder R.rsp

RoxygenNote 6.1.1

NeedsCompilation no

Repository CRAN

Date/Publication 2018-12-09 15:10:12 UTC

R topics documented:

| | |
|---------------------|---|
| RCarb-package | 2 |
| Example_Data | 2 |
| model_DoseRate | 3 |
| Reference_Data | 6 |
| write_InputTemplate | 7 |

| | |
|---------------|--|
| RCarb-package | <i>RCarb - Dose Rate Modelling of Carbonate-Rich Samples</i> |
|---------------|--|

Description

The package provides a dose rate modelling for carbonate-rich samples in the context of trapped charged dating (e.g., luminescence dating) applications.

Package: RCarb
Type: Package
Version: 0.1.2
Date: 2018-12-02
License: GPL-3

References

This package bases on a 'MATLAB' programme with name 'Carb', details can be found the following references:

Mauz, B., Hoffmann, D., 2014. What to do when carbonate replaced water: Carb, the model for estimating the dose rate of carbonate-rich samples. *Ancient TL* 32, 24–32. http://ancienttl.org/ATL_32-2_2014/ATL_32-2_Mauz_p24-32.pdf

Nathan, R.P., Mauz, B., 2008. On the dose-rate estimate of carbonate-rich sediments for trapped charge dating. *Radiation Measurements* 43, 14–25. doi: [10.1016/j.radmeas.2007.12.012](https://doi.org/10.1016/j.radmeas.2007.12.012)

Further reading

Nathan, R.P., 2010. Numerical modelling of environmental dose rate and its application to trapped-charge dating. DPhil thesis, St Hugh's College, Oxford. <https://ora.ox.ac.uk/objects/ora:6421>

| | |
|--------------|---------------------|
| Example_Data | <i>Example data</i> |
|--------------|---------------------|

Description

Example data as shipped with *Carb* by Mauz & Hoffmann (2014). In contrast to the original data, NA values have been replaced by 0 and columns and rows have been transposed. Samples are now organised in rows and parameters in columns.

The data can be used to test 'RCarb' and play with the secondary carbonatisation process. Sample HD107 was renamed to LV107 for the sake of consistency with Fig. 4 in Mauz & Hoffmann (2014).

Format

Example_Data: `data.frame` (28 x 29)

Each column has two attributes:

- UNIT: the unit, so far applicable, e.g. "ppm"
- DESCRIPTION: the column description

Version

0.1.0

Author(s)

Mauz & Hoffmann (2014), with minor modifications by Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS-Université Bordeaux Montaigne (France)

References

Mauz, B., Hoffmann, D., 2014. What to do when carbonate replaced water: Carb, the model for estimating the dose rate of carbonate-rich samples. *Ancient TL* 32, 24-32.

Examples

```
## show first elements of the example data
data(Example_Data, envir = environment())
head(Example_Data)

##show only column U238
Example_Data$U238
```

model_DoseRate

Model dose rate evolution in carbonate-rich samples

Description

This function models the dose rate evolution in carbonate enrich environments. For the calculation internal functions are called.

Usage

```
model_DoseRate(data, length_step = 1L, max_time = 500L, n.MC = 100,
  method_control = list(), txtProgressBar = TRUE, verbose = TRUE,
  plot = TRUE, ...)
```

Arguments

| | |
|----------------|---|
| data | data.frame (required) : input data following the structure given in the example data set <code>data(Example_Data)</code> . The input <code>data.frame</code> should have at least one row (i.e. values for one sample). For multiple rows the function is automatically re-called. |
| length_step | numeric (with default): step length used for the calculation |
| max_time | numeric (with default): maximum temporal search range |
| n.MC | numeric (with default): number of Monte Carlo runs used for the error calculation |
| method_control | <i>(optional)</i> : additional arguments that can be provided to the control the the modelling. See details for further information. |
| txtProgressBar | logical (with default): enables/disables the <code>txtProgressBar</code> for the MC runs |
| verbose | logical (with default): enables/disables verbose mode |
| plot | logical (with default): enables/disables plot output |
| ... | further arguments passed to the underlying plot functions, see also details for further information. Supported standard arguments are <code>mfrow</code> , <code>xlim</code> , <code>xlab</code> . |

Details

This function is the starting point for the dose rate modelling for carbonat enrich environments. It provides basically the same functionality as the original version of 'Carb', i.e. you should be also aware of the limitations of this modelling approach. In particular: The model assumes a linear carbonate mass increase due to post-depositional processes. Please read the references cited blow.

Uncertainty estimation

For estimating the uncertainties, Monte-Carlo (MC) simulation runs are used. For very small values (close to 0) this can, however, lead to edge effects (similar in 'Carb') since values below 0 are set to 0.

Value

The function returns numerical and graphical output

[NUMERICAL OUTPUT]

- A `data.frame` which is the combination of the input and values calculated by this function.

[GRAPHICAL OUTPUT]

Upper plot: Dose rate evolution over time backwards. The solid black line is the calculation output, the grey shaded area indicates the 2-sigma error margins. The dashed blue line is an indicator

of the quality of the error estimations based on Monte Carlo (MC) runs. The closer it follows the black line, the more reliable are the given error margins.

Lower plot: Totally absorbed dose over time. The plot is an representation of the 'new' age based on the carbonat modelling.

Function version

0.1.0

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, Université Bordeaux Montaigne (France); based on 'MATLAB' code given in file Carb_2007a.m of *Carb*

References

Mauz, B., Hoffmann, D., 2014. What to do when carbonate replaced water: Carb, the model for estimating the dose rate of carbonate-rich samples. *Ancient TL* 32, 24–32. http://ancienttl.org/ATL_32-2_2014/ATL_32-2_Mauz_p24-32.pdf

Nathan, R.P., Mauz, B., 2008. On the dose-rate estimate of carbonate-rich sediments for trapped charge dating. *Radiation Measurements* 43, 14–25. doi: [10.1016/j.radmeas.2007.12.012](https://doi.org/10.1016/j.radmeas.2007.12.012)

Further reading

Nathan, R.P., 2010. Numerical modelling of environmental dose rate and its application to trapped-charge dating. DPhil thesis, St Hugh's College, Oxford. <https://ora.ox.ac.uk/objects/ora:6421>

Examples

```
##load example data
data("Example_Data", envir = environment())

##run the function for one sample from
##the dataset
model_DoseRate(
  data = Example_Data[14,],
  n.MC = 2,
  txtProgressBar = FALSE
)
```

Reference_Data *Reference data*

Description

Correction factors for beta and gamma radiation used for internal calculations. These values are used instead of the correction factors given in Aitken (1985) for the carbonate model.

Format

Reference_Data: [list](#)

| NAME | TYPE | DIM | DESCRIPTION |
|-----------|------------|--------|--|
| DATAek | matrix | 4 x 4 | correction factors for electrons for water and carbonate to sediment mass ratio for K |
| DATAet | matrix | 4 x 4 | correction factors for electrons for water and carbonate to sediment mass ratio for Th |
| DATAet230 | matrix | 4 x 4 | correction factors for electrons for water and carbonate to sediment mass ratio for Th-230 |
| DATAeu | matrix | 4 x 4 | correction factors for electrons for water and carbonate to sediment mass ratio for U |
| DATAeu234 | matrix | 4 x 4 | correction factors for electrons for water and carbonate to sediment mass ratio for U-234 |
| DATAeu238 | matrix | 4 x 4 | correction factors for electrons for water and carbonate to sediment mass ratio for U-238 |
| DATApk | matrix | 4 x 4 | correction factors for photons for water and carbonate to sediment mass ratio for K |
| DATApt | matrix | 4 x 4 | correction factors for photons for water and carbonate to sediment mass ratio for T |
| DATApt230 | matrix | 4 x 4 | correction factors for photons for water and carbonate to sediment mass ratio for Th-230 |
| DATApu | matrix | 4 x 4 | correction factors for photons for water and carbonate to sediment mass ratio for U |
| DATApu234 | matrix | 4 x 4 | correction factors for photons for water and carbonate to sediment mass ratio for U-234 |
| DATApu238 | matrix | 4 x 4 | correction factors for photons for water and carbonate to sediment mass ratio for U-238 |
| mejdahl | data.frame | 36 x 4 | beta-dose attenuation values for quartz grains according to Mejdahl (1979) |

Details

The reference values are used internally to account for: (1) grain size depend beta-attenuation factors (Mejdahl, 1979) and (2) to correct nuclide dependent beta and gamma radiation for water/carbonate proportions. The latter values are given as matrix and precise values are interpolated during the modelling process.

Different values quoted for U-238 and U-234 accounts for different activity ratios. For further details on the origin of these data we refer to Nathan & Mauz (2008) and Nathan (2010).

Nuclear data origin according to Nathan & Mauz (2008)

The gamma primary energy spectra of uranium, thorium and potassium are drawn from Evaluated Nuclear Structure Data File (ENSDF) database at <http://www.nndc.bnl.gov> (2002-01-16) and the beta primary energy spectra was derived from ENSDF end-point energies using a Fermi beta decay model (Evans, 1955) modified by Behrens & Szybisz (1976). For the simulations of the collisional mass stopping powers for quartz the software ESTAR (Berger et al., 2000) was used. The mass energy-absorption coefficients for quartz were tabulated by Hubbell & Seltzer (2004).

For further details and references please read Nathan & Mauz (2008)

Version

0.1.0

References

Mejdahl, V., 1979. Thermoluminescence dating: beta-dose attenuation in quartz grains. *Archaeometry* 21, 61-72. http://ancientt1.org/ATL_32-2_2014/ATL_32-2_Mauz_p24-32.pdf

Nathan, R.P., Mauz, B., 2008. On the dose-rate estimate of carbonate-rich sediments for trapped charge dating. *Radiation Measurements* 43, 14-25. doi: [10.1016/j.radmeas.2007.12.012](https://doi.org/10.1016/j.radmeas.2007.12.012)

Nathan, R.P., 2010. Numerical modelling of environmental dose rate and its application to trapped-charge dating. DPhil thesis, St Hugh's College, Oxford. <https://ora.ox.ac.uk/objects/ora:6421>

Further reading

Aitken, M.J., 1985. Thermoluminescence dating. Academic Press.

Berger, M.J., Coursey, J.S., Zucker, M.A., 2000. ESTAR, PSTAR, and ASTAR: Computer Programs for Calculating Stopping-Power and Range Tables for Electrons, Protons, and Helium Ions (version 1.2.2). <http://physics.nist.gov/Star> (2005-08-09). National Institute of Standards and Technology, Gaithersburg, MD.

Behrens, H., Szybisz, L., 1976. Shapes of beta spectra. *Physics Data* 6-1, Zentralstelle fuer Atomkernenergie-Dokumentation (ZAED), Germany.

Evans, R.D., 1955. *The Atomic Nucleus*. McGraw-Hill, NY.

Hubbell, J.H., Seltzer, S.M., 2004. Tables of X-Ray Mass Attenuation Coefficients and Mass Energy-Absorption Coefficients (version 1.4). <http://physics.nist.gov/xaamdi> (2005-08-09). National Institute of Standards and Technology, Gaithersburg, MD.

Examples

```
data(Reference_Data, envir = environment())
str(Reference_Data)
Reference_Data$DATAek
```

write_InputTemplate *Write table input template*

Description

This function creates a template table that can be used as input for the function [model_DoseRate](#)

Usage

```
write_InputTemplate(file = NULL, ...)
```

Arguments

file [character](#) (optional): output path, if NULL nothing is written, but a template [data.frame](#) is returned.

... additional arguments that can be passed to function [write.table](#) if file != NULL. Supported arguments are: sep, dec, fileEncoding‘

Function version

0.1.0

Author(s)

Sebastian Kreutzer, IRAMAT-CRP2A, UMR 5060, CNRS - Université Bordeaux Montaigne (France)

See Also[Example_Data](#), [write.table](#)**Examples**

```
##create template without file creation
write_InputTemplate()

## Not run:
##Example with file output
##To run: uncomment and modify path
#write_InputTemplate(file = "[YOUR PATH]")

## End(Not run)
```


Index

- *Topic **datasets**
 - Example_Data, 2
 - Reference_Data, 6
- *Topic **dplot**
 - model_DoseRate, 3
- *Topic **manip**
 - model_DoseRate, 3
- *Topic **package**
 - RCarb-package, 2

- character, 8

- data.frame, 3, 4, 8

- Example_Data, 2, 8

- list, 6
- logical, 4

- model_DoseRate, 3, 7

- numeric, 4

- RCarb (RCarb-package), 2
- RCarb-package, 2
- Reference_Data, 6

- write.table, 8
- write_InputTemplate, 7