ResAge Package Manual – Update Dec. 2015

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If you would use the F^{14}R or δ^{14}R metrics, please in addition cite: Soulet G, Skinner LC, Beaupré SR, Galy V, 2016. A note on reporting of reservoir ^{14}C disequilibria and age offsets. Radiocarbon, in press doi: 10.1017/RDC.2015.22

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Introduction

The Reservoir Age offset (ResAge) package is dedicated to proper calculation of reservoir age offsets, especially when dealing with pairs of ^{14}C and calendar ages (Soulet, in press). It consists of a set of ^{14}C calibration curves (IntCal09, IntCal13, and SHCal13), a template folder (/Templates), various examples (e.g. /InputData/example_rad2), this manual, and three scripts written in R (files *rad2.R*, *colyear.R*, and *radcal.R*). This package requires a recent version of the free open-source statistical software R (current version 3.1.2; R Development Core Team, 2014).

Before starting, install R on your computer. Unzip *ResAge.zip* to somewhere on your computer where you have write access (e.g., c:\ResAge\). Open R and change the working directory to where you have saved *ResAge*. To do so, click on the *File* (*Misc* for Mac) drop-down menu on the top-left (top-right for Mac) of the R screen, then click *Change Working Directory* and select the location of the (unzipped) *ResAge* folder.

Finally, depending on the data you would like to use for reservoir age offset calculation, load the appropriate script by typing *source('rad2.R')*, *source('colyear.R')* or, *source('radcal.R')* (press <enter> after every command). See the next section for an explanation of which script to choose.

Please cite *ResAge* (Soulet, 2015) in your publications, as well as the calibration curve(s) used to calculate your reservoir age offsets (Reimer et al., 2009, 2013 for IntCal09 and

IntCal13, respectively; Hogg et al., 2013 for SHCal13). Note that these scripts do not compute marine ΔR values, solely reservoir age offset compared to the atmosphere. Finally, note that *ResAge* is not designed to work with post-bomb samples (i.e., after AD 1950, or 0 cal. BP).

Choosing the appropriate script

Three scripts are available here for the reservoir age offset calculation. Each depends upon your data (see accompanying paper for further information):

1) If you have **pairs of radiocarbon ages** – namely reservoir-derived and atmospheric ^{14}C ages – you should **load script *rad2.R* by typing *source('rad2.R')*** (*rad2* stands for radiocarbon-radiocarbon). For example, this case arises when you have ^{14}C ages of a marine shell (reservoir-derived ^{14}C age) and a piece of wood (atmospheric ^{14}C age) embedded in the same sediment layer (e.g., Bondevik et al., 1999).

2) If you have **pairs of a reservoir-derived radiocarbon age and the corresponding perfectly known calendar age**, you should **load script *colyear.R* by typing *source('colyear.R')***. Typically, this case arises when working with reservoir-derived radiocarbon ages of shells obtained from a museum collection for which the exact calendar year is known (e.g. Siani et al., 2000).

3) If you have pairs of a reservoir-derived radiocarbon age and a corresponding weakly known calendar age – i.e., some uncertainty associated with the calendar age – you should **load script *radcal.R* by typing *source('radcal.R')*** (*radcal* stands for radiocarbon-calendar). For example, this case arises when working with reservoir-derived radiocarbon age and U/Th age obtained from corals or speleothems (e.g. Hall et al., 2010; Southon et al, 2012).

Running the scripts to calculate the reservoir age offsets

After choosing and loading the appropriate script for your data, you will now be able to run the script. However, before running the script, you need to enter your data following the appropriate template as a *.csv* file. Templates are available in folder called *Templates* (*ResAge\Templates*).

If your data file is called "MyData", create a *.csv* file using the appropriate template and save this file as *MyData.csv* in a folder called *MyData*. Save the folder *MyData* in the *InputData* folder.

(The file path should be *ResAge\InputData\MyData\Mydata.csv*). Do not change the headings of the columns of the templates.

Reservoir age offsets can be obtained by typing *rad2('MyData'), colyear('MyData')* or, *radcal('MyData')* [followed by <enter>], depending on your choice of script. Output files are stored in the *MyData* folder. As examples, check folders and associated files *example_rad2*, *example_colyear*, *example_radcal_Southon2012* stored in folder *InputData*. There are several additional options specific to each script (detailed below).

1) *rad2*

Data from *example_rad2* are from Bondevik et al. (1999). If you simply type *rad2()* or *rad2('example_rad2'),* reservoir age offsets corresponding to data file *example_rad2.csv* will be calculated and output file created in folder *example_rad2*.

Several options are available:

- If you want to calibrate each atmospheric ^{14}C age, use option: *calibrate=TRUE* (default value is *calibrate=FALSE*). In that case you need to select the atmospheric calibration curve you want to use by entering *cc=1* (for IntCal13, default value), *cc=2* (for SHCal13), *cc=3* (for IntCal09). Ranges of the calibrated distribution are calculated at 95% confidence (*prob=0.95*, default value). It is recommended to keep prob=0.95 to have a good estimate of your calibrated ranges. Nevertheless, you can change the confidence interval by typing *prob=0.70* for example to calculate ranges at 70% confidence.
- If you want to export the calibrated probability density functions of each sample, use option: *export.cal.pdf=TRUE* (default value is *export.cal.pdf=FALSE*).

As an example, typing:

rad2('example_rad2', calibrate=TRUE, cc=3, prob=0.95, export.cal.pdf=TRUE)

calculates the reservoir age offset of *example_rad2* data file, calibrates associated atmospheric radiocarbon ages using Intcal09, provides the calibrated ranges at 95% and exports calibrated pdfs as .csv files. All output files are stored in the folder *example_rad2*. Note that the calibration function is the most basic one detailed in Clam v2.2 and the ranges are calculated according to the hpd function from Clam v2.2 (for more information see Blaauw, 2010).

2) colyear

Data from *example_colyear* are from Siani et al. (2000). If you simply type *colyear()* or *colyear('example_colyear')*, by default reservoir age offsets corresponding to data file *example_colyear.csv* will be calculated using IntCal13 and output file created in folder *example_colyear*. You can change the atmospheric calibration curve by using the option: *cc=1* (for IntCal13, default value), *cc=2* (for SHCal13), *cc=3* (for IntCal09).

For example, typing:

colyear('example_colyear', cc=1)

calculates the reservoir age offset of *example_colyear* data file by using the IntCal13 calibration curve.

3) radcal

Data from *example_radcal_Southon2012* are from Southon et al. (2012). If you simply type *radcal()* or *radcal('example_radcal_Southon2012')*, by default the function “uncalibrates” the calendar ages using IntCal13 and then computes the corresponding reservoir age offset pdfs following approach described in accompanying paper and reports ranges at 95% confidence. All reservoir age offset probability density functions are exported as a .csv file. Output files are stored in the folder *example_radcal_Southon2012*.

Several options are available:

- If you want to compute the reservoir age offset pdf mixture type: *mixture.pdf=TRUE* (default is *mixture.pdf=FALSE*). This may be useful for a rough estimate of the long-term changes in the speleothem dead carbon fraction (see Case study section in Soulet, 2015). Ranges of the reservoir age offset and uncalibrated distributions are given by default at 95% (*prob=0.95*, default value).
- If you want to export and get the ^{14}C ranges of all the uncalibrated probability density functions type *export.uncal.pdf=TRUE* (default value is *export.uncal.pdf=FALSE*).

- You may change the atmospheric calibration curve by typing *cc=1* (IntCal13), *cc=2* (SHCal13), or *cc=3* (IntCal09).

As an example, typing:

radcal('example_radcal_Southon2012', cc=1, export.uncal.pdf=TRUE, prob=0.95, mixture.pdf=TRUE)

computes the uncalibrated and the reservoir age offset pdfs of *example_radcal_Southon2012* data file by using the IntCal13 calibration curve, reports resulting ranges at 95% and exports both the uncalibrated and reservoir age offset pdfs. The mixture pdf is also exported and ranges reported. All outputs are stored in *example_radcal_Southon2012* folder.

Data presented in accompanying paper Soulet (2015) can be obtained by typing:
radcal('example_radcal_Southon2012', mixture.pdf=TRUE) for Southon et al. (2012) data
radcal('Hoffmann2010', mixture.pdf=TRUE) for Hoffmann et al. (2010) data
radcal('Beck2001', mixture.pdf=TRUE) for Beck et al. (2001) data

Summary of useful options

Option	Script	Default value	Description
name	all scripts	example_...	name of your data folder and file
cc	all scripts	1	calibration curve (1, 2 or 3)
calibrate	rad2.R	FALSE	calibrates atmospheric ^{14}C ages
export.cal.pdf	rad2.R	FALSE	exports the calibrated pdfs
mixture.pdf	radcal.R	FALSE	calculates the mixture of all reservoir age offset pdfs
export.uncal.pdf	radcal.R	FALSE	exports the uncalibrated pdfs
prob	rad2.R and radcal.R	0.95	confidence interval (between 0 and 1)
storedat	rad2.R and radcal.R	FALSE	stores all data within R
threshold	rad2.R and radcal.R	1e-6	below which value should probabilities be excluded from calculations
f.14R	all scripts	FALSE	returns the $F^{14}R$ metric
delta.14R	all scripts	FALSE	returns the $\delta^{14}R$ metric
dcp	all scripts	FALSE	returns the dcp metric

About ResAge

The *ResAge* package is an open-source program; you are free to use, copy, distribute and modify it, but please read this manual and accompanying paper before using the scripts.

 Please cite Soulet (2015) if you modify or use this program, applied settings and calibration curves.

Updates

All scripts include the functions to computes the $F^{14}R$, $\delta^{14}R$, and dcp metrics – Oct. 2015

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