

UThwgl - an R package for closed- and open-system uranium-thorium dating

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Abstract

For several decades, uranium-thorium (U-Th) dating has allowed geochronologists to precisely date geological materials, providing invaluable geochronological constraints on Quaternary processes. Open-system dating of bones and teeth has also provided ages of human and faunal remains of archaeological significance.

To facilitate access to closed- and open-system U-Th dating to the broad scientific community, here we provide an R package, named *UThwgl*. Description of input and output parameters is given, as well as a guide for running the model. The package can be used three different ways: (i) as a web application, (ii) through a web browser with an internet connection, or (iii) in R (most efficiently with RStudio). Examples of application of the model are also provided, showing that it yields ages within error of previously published values.

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1 Introduction

2 Uranium-thorium (U-Th) dating has revolutionised Quaternary science and
3 archaeology. Dating uses the decay of ^{238}U into ^{230}Th , with ^{234}U and a few
4 short-lived nuclides as intermediary products. It is based on the principle that
5 the age of formation of a material can be dated as it incorporates U and no or
6 little Th at the time of formation, so all the ^{230}Th in the sample comes from
7 decay of ^{238}U . If detrital Th is incorporated into the sample, a correction must
8 be included to account for the fraction of ^{230}Th which is detrital and not derived
9 from ^{238}U decay. Another requirement is that there is no gain or loss of ^{230}Th ,
10 ^{234}U or ^{238}U after formation of the material (*closed system*).

11 Closed-system U-Th dating can be used to date materials as young as a
12 few years up to samples over 600,000 years old (Edwards et al., 2003). It has
13 been successfully applied to a range of marine and lacustrine carbonates. For
14 instance, dating of corals (coralline aragonite) has had a pivotal role in re-
15 constructing past sea levels (Lambeck and Chappell, 2001). Closed-system U-
16 Th dating has also been applied to speleothems (cave carbonates) which are
17 commonly used as continental palaeo-climate archives (Richards and Dorale,
18 2003). In corals and most speleothems, detrital correction is minimal; however,
19 it can be significant when dating pedogenic carbonates, for instance (Ludwig
20 and Paces, 2002). In this case, detrital correction can be performed using the
21 measured or assumed composition of the detrital fraction (e.g. Ludwig, 2003a).
22 Alternatively, isochron techniques can be applied (Ludwig and Titterton,
23 1994); the latter are beyond the scope of this article but IsoPlot is a commonly
24 used software for isochron calculations and other geochronological applications
25 (Ludwig, 2003b), now also available as a R package (Vermeesch, 2018).

26 Closed-system conditions are seldom met in shells, teeth and bones (although
27 enamel can sometimes be quite impervious to isotope gain or loss). Thus, U-Th
28 dating requires to take into account open system behaviour. The diffusion-
29 adsorption model of Pike and Hedges (2002) and the Diffusion-Adsorption-
30 Decay (DAD) model of Sambridge et al. (2012) were instrumental to imple-
31 ment successfully open-system U-Th dating. They allow for advective and dif-
32 fusive transport of uranium and thorium isotopes, while including synchronous
33 radioactive decay. Software implementation for the DAD model was written
34 in Fortran and is available as a Java GUI ([http://www.earth.org.au/codes/](http://www.earth.org.au/codes/iDaD/)
35 [iDaD/](http://www.earth.org.au/codes/iDaD/)).

36 Open-system U-Th dating of teeth and bones, while challenging, has provided
37 quantitative ages for human and faunal remains (Eggins et al., 2005; Grün et al.,
38 2014; Hoffmann et al., 2018; Pike and Hedges, 2002; Sambridge et al., 2012).
39 Thus, this approach has significantly improved our understanding of human
40 evolution (e.g. Dirks et al., 2017; Hoffmann et al., 2018; Sutikna et al., 2016).

41 In this article, we present a R package, *UThwgl*, which offers functions to
42 perform closed-system, `csUTh()`, and open-system, `osUTh()`, U-Th age calcu-
43 lations. The former implements formulations given in Ludwig (2003a) while
44 the latter applies the DAD model of Sambridge et al. (2012). The R package
45 *IsoPlotR* provides a more extensive tool for closed-system U-Th dating (Ver-

meesch, 2018), and *UThwigl* only includes closed-system U-Th age calculations for the sake of offering both closed- and open-system calculations.

Providing an R package aims at increasing the transparency, reproducibility, and flexibility of the analytical workflow for computing U-Th ages. For instance, with open-system dating, it is difficult to include the Java GUI in a fully scripted data analysis so the method for computing the DAD model is not fully transparent. This can obscure steps where key decisions are made that are important for others to see to verify the reliability of the analysis. Enabling a scripted workflow for computational analysis of geoscience data is important for improving the reproducibility of results. Reproducibility refers to the ability to recreate the results or retest the hypotheses leading to a scientific claim, either by rerunning the same code used by the original authors, or by writing new code. High rates of irreproducibility of research results have been estimated in several fields and disciplines (Camerer et al., 2018; Camerer et al., 2016; Freedman et al., 2015; Institute, 2013; Ioannidis, 2005; Open Science Collaboration, 2015). Consequently, the transparency, openness, and reproducibility of results and methods are receiving increased attention, and the norms of research in many fields are changing (Marwick, 2016; Miguel et al., 2014; Nosek et al., 2015).

There is strong interest in open, transparent, and reusable research in the geoscience community (Gil et al., 2016) and substantial progress toward open data has been made in the geosciences with the widespread use of data services of NASA, USGS, NOAA and community-built data portals such as OneGeology, EarthChem, RRUFF, PANGAEA, PaleoBioDB, SISAL and others (Comas-Bru et al., 2020; Kattge et al., 2014; Ma, 2018). However, the use of open source software such as R (Pebesma et al., 2012), and sharing of scripted data analysis workflows with research publications is not yet widespread (Hutton et al., 2016). With this R package our goal is to make scripted and reproducible data analysis easy for uranium-thorium dating. This will improve the transparency of geochronology research, and provide a more credible and robust foundation for scientific advancement (Hutton et al., 2016).

To enable re-use of our materials and improve reproducibility and transparency, all the results and visualisations in this paper can be reproduced using the RMarkdown vignette document included with the *UThwigl* package. We have archived these files at <http://doi.org/10.17605/OSF.IO/D5P7S> to ensure long-term accessibility. Our code is released under the MIT licence, our data as CC-0, and our figures as CC-BY, to enable maximum re-use (for more details, see Marwick, 2016).

Methods

Closed-system U-Th dating is based on the premise that the dated material takes up U during formation, but no Th (and thus no ^{230}Th). This is because U-Th dating focuses on materials that precipitate from solution (e.g. carbonates) and Th has a very low solubility in most cases. In this case, the age of material formation (e.g., precipitation of coralline aragonite) is quantified. Carbonates

are particularly amenable to U-Th dating because, in most cases, they take up U during formation but very little Th.

U-Th dating is undertaken by measuring the $^{234}\text{U}/^{238}\text{U}$ and $^{230}\text{Th}/^{238}\text{U}$ of the material. In this case, the measured $[\frac{^{230}\text{Th}}{^{238}\text{U}}]$ activity ratio in the sample is written as follows (brackets denote activity ratios):

$$[\frac{^{230}\text{Th}}{^{238}\text{U}}] = 1 - e^{-\lambda_{230}t} + (\frac{\delta^{234}\text{U}_m}{1000}) \cdot (\frac{\lambda_{230}}{\lambda_{230} - \lambda_{234}}) \cdot (1 - e^{-(\lambda_{230} - \lambda_{234})t})$$

where λ_{230} and λ_{234} are ^{230}Th and ^{234}U decay constants, respectively (in yr^{-1}), t is the age of the material (i.e. the time elapsed since onset of ^{230}Th in-growth; in yr), and $\delta^{234}\text{U}_m = ([\frac{^{234}\text{U}}{^{238}\text{U}}] - 1) \cdot 1000$, with the measured $[\frac{^{234}\text{U}}{^{238}\text{U}}]$ activity ratio in the material.

This approach assumes that (i) all the ^{230}Th measured is produced by decay of ^{238}U and (ii) the system is closed at $t=0$, i.e. there is no loss or gain of any nuclides after the time of formation. In corals, the second assumption can be tested using the mineralogy of the sample: corals precipitate as aragonite. Open system behaviour exemplified as diagenetic alteration generally involves the replacement of aragonite by calcite. Thus, prior to ^{230}Th dating, coral mineralogy should be quantified. Samples exhibiting calcite are deemed unsuitable for dating. The initial $[\frac{^{234}\text{U}}{^{238}\text{U}}]$ activity ratio, calculated along the age, should also be similar to the seawater value [1.145; Henderson (2002)], which has not changed significantly over the past 800,000 yr. In speleothems, the closed system assumption can be tested by looking for any age inversions. In pedogenic carbonates, there is no straightforward way to test this assumption. The first assumption (^{230}Th measured is only produced by decay of ^{238}U) is tested for any sample type using ^{232}Th as an index of detrital Th. Any significant amount of ^{232}Th in the sample implies a detrital contribution of Th to the sample, and thus that a fraction of the ^{230}Th measured does not result from decay of ^{238}U , but from detrital input of Th. The $[\frac{^{230}\text{Th}}{^{232}\text{Th}}]$ or $[\frac{^{232}\text{Th}}{^{238}\text{U}}]$ activity ratios are used as indices of the quantity of detrital Th present in the sample. Arbitrary values are set to define whether the presence of detrital Th is significant; $[\frac{^{230}\text{Th}}{^{232}\text{Th}}]$ ratios greater than 20 or $[\frac{^{232}\text{Th}}{^{238}\text{U}}]$ ratios less than 0.01 are usually recommended. If significant detrital Th is present, correction is necessary (in fact, even if the contribution of detrital Th is minimal, correction should still be applied). Ideally, one would measure the $[\frac{^{230}\text{Th}}{^{238}\text{U}}]$, $[\frac{^{234}\text{U}}{^{238}\text{U}}]$ and $[\frac{^{230}\text{Th}}{^{232}\text{Th}}]$ activity ratios of the detrital component; however it is rarely possible to isolate this fraction, let alone measure its U-series isotope composition. Often, correction is undertaken assuming a $[\frac{^{230}\text{Th}}{^{232}\text{Th}}]$ of 0.8 ± 0.4 for the detrital component, which is the average value for the continental crust. Alternatively, detrital correction can be undertaken by measuring several samples assumed to have the same ^{230}Th age, but variable amounts of detrital Th. In this case, it is possible to define an isochron or derive a single age for the same of isochronous samples.

Open-system U-Th dating operates on the principles that little U (and Th) are incorporated at the time of the material formation (shell, tooth or bone),

and it is only after death and burial of the material in soil or sediments, that U (and Th to a lesser extent) are taken up and diffuse into the material. When dating teeth, enamel is often preferred over dentine, as the former is denser and thus less prone to complex nuclide movement. For samples exhibiting open system behaviour, the analytical strategy generally involves measuring ^{238}U , ^{234}U , ^{230}Th and ^{232}Th in several aliquots along a transect perpendicular to the surface of the sample (Figure @ref(fig:femurpic)). Then, U concentrations and $[\frac{^{230}\text{Th}}{^{238}\text{U}}]$, $[\frac{^{234}\text{U}}{^{238}\text{U}}]$ activity ratios can be modelled to derive a single open-system age. Aliquots can be collected by micro-drilling or using laser ablation.

Several open-system models have been developed (Pike and Pettitt, 2003). The Diffusion-Adsorption model (Pike and Pettitt, 2003) was later modified to a Diffusion-Adsorption-Decay model (Sambridge et al., 2012), and is the most commonly employed to U-Th date archaeological materials such as teeth and bones. Profiling of uranium concentrations across the sample is used to determine whether the sample has experienced loss of uranium (inverted “U” shaped profile) or shows an irregular pattern of uranium concentration variation. If the sample presents either of these profiles, it is rejected for dating. Ideally, the uranium concentration profile shows a “U” shape (illustrating uranium diffusion) or homogenous concentrations (indicating that equilibrium in uranium diffusion has been achieved). Once these tests have been performed, closed-system U-Th ages for each analysis can then be computed. If they show an inverted “U” shaped profile, this is diagnostic of recent uranium uptake, and the sample is rejected. Otherwise, the profile of U-series isotope data can then be used to derive a single open-system age.

Analytically, two types of measurements are possible: bulk or in-situ. For bulk analysis, a fraction of the samples is dissolved and the solution processed through ion exchange chromatography to separate U and Th (e.g. Luo et al., 1997). Each element is then analysed separately for their isotope ratios by mass spectrometry. For in-situ analysis, laser ablation is commonly used (Eggins et al., 2005). In this case, a laser with a spot size ranging from a few μm to several hundreds of μm produces an aerosol which is carried using a gas (helium or preferably a mixture of helium and nitrogen; Eggins et al. (1998)). While laser ablation offers a better spatial resolution and is less time consuming than bulk analysis, the precision of the data is inferior because of the much smaller amount of material sampled.

Uranium and thorium isotope ratios are analysed by multi-collector inductively-coupled plasma mass spectrometry (e.g. Luo et al. (1997); although bulk analysis can also be performed by thermal ionisation mass spectrometry). A plasma ionises U and Th atoms, their isotopes are separated through a magnetic field and each are collected in a different collector (Faraday cups or ion counters). If using laser ablation, it is best to have two ion counters so ^{230}Th and ^{234}U can be collected simultaneously.

Closed-system dating

Pending closed-system behaviour can be assessed, it is possible to derive an age for each U-Th analysis. The closed-system function `csUTh()` requires that



Figure 1: (ref:femurpicap)

(#fig:femurpic)

for each analysis to yield an age, $[\frac{^{234}\text{U}}{^{238}\text{U}}]$, $[\frac{^{230}\text{Th}}{^{238}\text{U}}]$ are measured, as well as $[\frac{^{232}\text{Th}}{^{238}\text{U}}]$ or $[\frac{^{230}\text{Th}}{^{232}\text{Th}}]$. The $[\frac{^{232}\text{Th}}{^{238}\text{U}}]$ activity ratio is required for detrital correction (note it is needed to use `csUTh()` whether the detrital correction is performed or not). If $[\frac{^{230}\text{Th}}{^{232}\text{Th}}]$ is provided instead, $[\frac{^{232}\text{Th}}{^{238}\text{U}}]$ is calculated with `csUTh()`.

Open-system dating

Data required for the DAD model are $[\frac{^{230}\text{Th}}{^{238}\text{U}}]$ and $[\frac{^{234}\text{U}}{^{238}\text{U}}]$ activity ratios collected along a transect perpendicular to the surface of the tooth or bone.

The x-y coordinates of each analysis, and of the inner and outer surfaces of the sample are also needed as input data. `osUTh()` uses these coordinates to calculate normalised positions, where the outer surface of the sample is given a reference coordinate of 1, the inner surface -1, and analyses take values in between (Figure @ref(fig:femurpic)).

(ref:femurpicap) Modern human femur (132A/LB/27D/03) from Liang Bua, Flores, Indonesia. Two analysis transects can be seen. For a given transect, the x and y coordinates of the outer and inner surfaces, and of the analyses, are used by `osUTh()` to calculate normalised positions where the outer surface is given 1 as reference coordinate, the inner surface -1, and normalised positions of the analyses take values in between. Modified from Sutikna et al. (2016).

Working with the package

We provide three methods for using this package to suit different levels of familiarity with the R programming language. The simplest way to use the pack-

age is our web applications, online at <https://anthony-dosseto.shinyapps.io/csUTh/> and <https://anthony-dosseto.shinyapps.io/osUTh/> (Figure @ref(fig:shinyfig)). Using the web application requires no familiarity with R. To use the web application we upload a CSV file, then click through a series of tabs to inspect the data, adjust the model parameters, run the model, and inspect the output. The interface is mouse-driven and requires no programming. In the web application we upload the data file on the *Load the data* tab, set parameters from the *Set model parameters* tab, run the model by clicking the button *Run Simulation* on the same tab, and observe the results on the *Visualise the model* and *Inspect the model* tabs. We can change the parameters and re-run the model by clicking the button *Run Simulation*. Once done, close the window.

(ref:shinyfigcap) Screenshots of the web application for open-system U-Th dating. A: Upload a CSV file of the data to model, B: Inspect a table of the uploaded data. C: Set the model parameters and run the model. D: Inspect visualisations of the model's output. E: Inspect and download the numeric output from the model.

The second way to use the package is with Binder, a browser-based instance of R and RStudio that includes our package ready to work with (Figure @ref(fig:binderfig)). Binder is a server technology that turns computational material, such as an R package, into interactive computational environments in the cloud. Using Binder requires a novice level of familiarity with R, for example to use the code in this paper and adapt it to work with a different CSV file. Because Binder provides a complete R environment, custom R code can be written during a Binder instance to further explore the model's output in the browser. These two methods, the web application and Binder, do not require any software to be downloaded and installed on the user's computer, all computation occurs in the browser. The web application and Binder are suitable for getting a quick start on working with the package, but they require a connection to the internet, and they have limited memory and compute time available per instance.

(ref:binderfigcap) Screenshot of Binder running R and RStudio in a web browser window.

The third method is to download and install the package locally to the user's computer, and work with it in the user's local installation of R and RStudio. This method requires some familiarity with R, but gives the most flexibility when working with the model because we are not limited by the memory and compute time of the cloud services. Our recommendation is to use Binder or a local installation of UThwgl because then the user can save an R script file that includes the name of the input file, the specific parameters used to generate the model output, and any downstream processing and visualisation. This script file and the CSV file can then be archived in a data repository to ensure long-term accessibility for other researchers. In the following sections we demonstrate the use of UThwgl with a local installation of R and RStudio.

A UThwgl::osUTh : compute open-system uranium-thorium ages using the diffusion-adsorption-decay (DAD) model

Load the data Inspect the data Set model parameters

Visualise the model Inspect the model

Before uploading, check that your CSV file contains columns with these names:

- **U234_U238**: $^{234}\text{U}/^{238}\text{U}$ activity ratios
- **U234_U238_2SE**: the 2 sigma errors of the activity ratios
- **Th230_U238**: $^{230}\text{Th}/^{238}\text{U}$ activity ratios
- **Th230_U238_2SE**: the 2 sigma errors of the activity ratios
- **U_ppm**: uranium concentrations (in ppm)
- **U_ppm_2SE**: the 2 sigma errors of the uranium concentrations
- **x**: x coordinates (in mm) of the analyses, and the outer and inner surfaces of the sample
- **y**: y coordinates (in mm) of the analyses, and the outer and inner surfaces of the sample
- **Comments**: two rows must show 'outer surface' and 'inner surface' (with the corresponding x and y coordinates)

Choose CSV file

Browse... Hobbitt_Mh2T_for_UAD.csv

Upload complete

Go to inspect the data

C UThwgl::osUTh : compute open-system uranium-thorium ages using the diffusion-adsorption-decay (DAD) model

Load the data Inspect the data Set model parameters

Visualise the model Inspect the model

Number of iterations: Age min (yr):

100 1000

Value of squared sum: Age max (yr):

0.01 20000

Uranium concentration at the sample surface (ppm): Min U diffusion coefficient:

25 0.0000000000001

Min [234U/238U] at the surface: Max U diffusion coefficient:

1.265 0.00000000001

Max [234U/238U] at the surface:

1.275

Run simulation and visualise the output

E UThwgl::osUTh : compute open-system uranium-thorium ages using the diffusion-adsorption-decay (DAD) model

Load the data Inspect the data Set model parameters

Visualise the model Inspect the model

Age	Age	Age	U234_U238_0	U234_U238_0	U234_U238_0
(ka)	(ka)	(ka)		+1SD	-1SD
6.78	1.37	1.18	1.27	0.01	0.00

diff	T_final	K_final	T_sol
238.71	6778.23	0.00	6989.85
863.99	6778.23	0.00	7615.14
-1326.73	6778.23	0.00	5424.41
1160.64	6778.23	0.00	7911.79
-151.03	6778.23	0.00	6600.12
-237.46	6778.23	0.00	6513.69
-946.60	6778.23	0.00	5904.55
-1114.49	6778.23	0.00	5636.65
2864.52	6778.23	0.00	8815.66

B UThwgl::osUTh : compute open-system uranium-thorium ages using the diffusion-adsorption-decay (DAD) model

Load the data Inspect the data Set model parameters

Visualise the model Inspect the model

Here is the raw data from the CSV file

Show 10 entries Search:

	U234_U238	U234_U238_2SE	Th230_U238	Th230_U238_2SE	U_ppm	U_ppm_2SE
1						
2						
3	1.2696216	0.00421	0.0733	0.00236	12.3	0.615
4	1.2729341	0.00424	0.0732	0.00239	12.7	0.635
5	1.2654235	0.00372	0.076	0.00177	12.5	0.625
6	1.2673451	0.00454	0.077	0.00193	14.2	0.71
7	1.2691554	0.00291	0.0721	0.00188	19.8	0.99
8	1.2655151	0.00284	0.0769	0.00167	16	0.9
9	1.269979	0.00255	0.0816	0.00169	20	1
10	1.2760185	0.00231	0.0766	0.00136	27.2	1.36

Showing 1 to 10 of 22 entries Previous 1 2 3 Next

Go to set the model parameters

D UThwgl::osUTh : compute open-system uranium-thorium ages using the diffusion-adsorption-decay (DAD) model

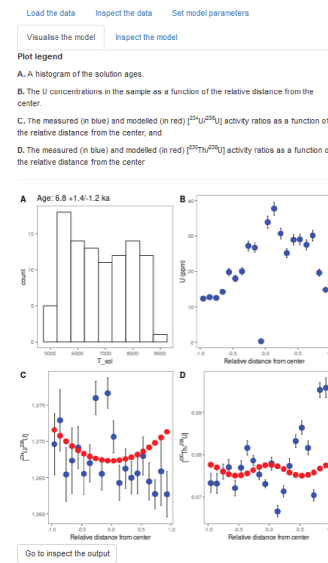


Figure 2: (ref:shinyfigcap)

(#fig:shinyfig)

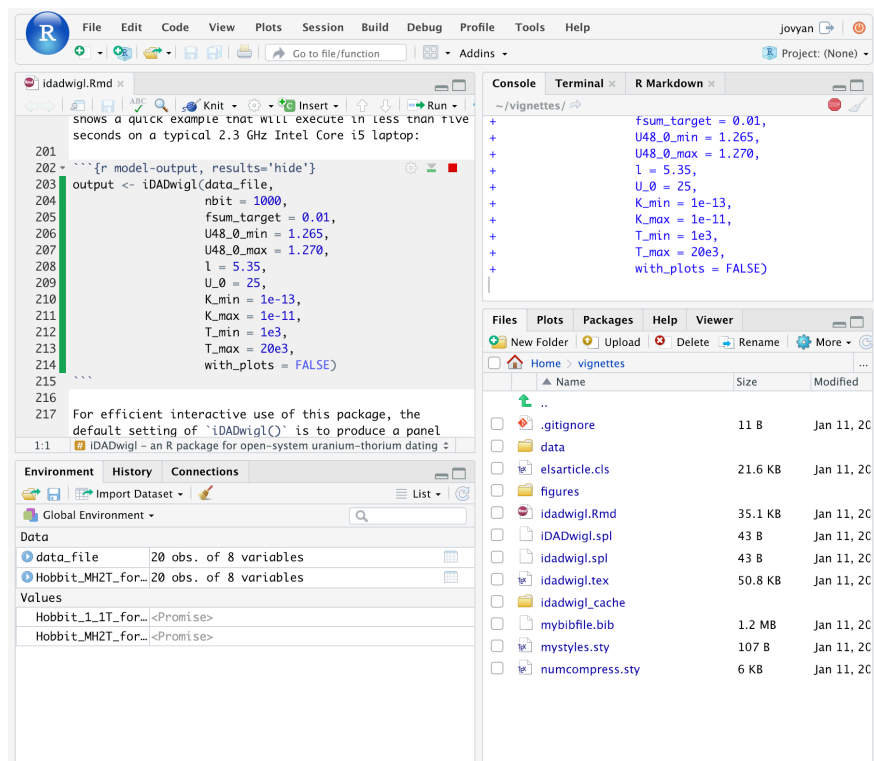


Figure 3: (ref:binderfigcap)

(#fig:binderfig)

239 Installing and attaching the package

240 First the user will need to download and install R, and we also recommend
241 downloading and installing RStudio. To run the model, start `RStudio` and
242 install the package from GitHub. There are many ways to do this, one simple
243 method is shown in the line below. This only needs to be done once per
244 computer.

```
if(!require("remotes")) install.packages("remotes")  
remotes::install_github("tonydoss/UThwigl")
```

245 For routine data analysis, R scripts need to contain the following line to
246 attach the package to the current working environment. This line needs to be
247 run at the start of each analysis:

```
# attach the package  
library(UThwigl)
```

248 Closed-system U-Th dating

249 *Input data format*

250 Our package provides the function `csUTh()` for closed-system U-Th dating.
251 Data for this function needs to be in a data frame (a form of table in R) with
252 the following column names:

- 253 • `Sample_ID`
- 254 • `U234_U238`
- 255 • `U234_U238_2SE`
- 256 • `Th230_U238`
- 257 • `Th230_U238_2SE`

258 and

- 259 • `Th232_U238`
- 260 • `Th232_U238_2SE`

261 or

- 262 • `Th230_Th232`
- 263 • `Th230_Th232_2SE`

264 To help with preparing data for input into our function, we have included
265 an example of an input file, taken from Pan et al. (2018). Before reading in the
266 data file, the user needs to set the working directory to the folder containing
267 the data file. This can be done in RStudio using the menu item ‘Session’ >
268 ‘Set Working Directory’ > ‘To Source File Location.’ Alternatively, the working
269 directory can be defined interactively at the R prompt in the Console panel
270 using `setwd()`. However, we do not recommend including `setwd()` in script
271 files because it is bad for reproducibility, since the path to one user’s working
272 directory will not exist on another user’s computer.

273 Inspecting the included data sets will be helpful for understanding how to pre-
274 pare new data for use with this package. After attaching the package, we can
275 access the built-in datasets with the `data()` function, like this:

```
# access the data included in the UThwigl package
data("Pan2018")
```

276 This will make the built-in data available in the R environment to inspect
277 and explore how to use the `csUTh()` function. To download the built-in data
278 to the user’s computer as a CSV file, so it can be inspected and modified
279 in a spreadsheet program (e.g. as a template for the user’s own data), use
280 `write.csv()`:

```
# download the data included in the package
write.csv(Pan2018, "Pan2018.csv")
```

The code chunk below shows how to read the CSV file created above into the R environment. We assume that the user's working directory contains a directory called `data` and the CSV file is in this `data` directory, and so the data can be imported as follows:

```
# read in one of the example CSV files included in the package
input_data_cs <- read.csv('data/Pan2018.csv')
```

To use new data with this package, the user needs to import a CSV or Excel file with the U-Th data into the R environment. This can be done using a generic function such as `read.csv` or `read_excel` from the `readxl` package (Wickham and Bryan, 2018).

Table @ref(tab:pan) shows the data contained in the `Pan2018.csv` file included in the package.

Sample_ID	U234_U238	U234_U238_2SE	Th230_U238	Th230_U238_2SE	Th232_U238	Th232_U238_2SE
YP002A	1.150	0.005	0.794	0.007	0.010	0.00005
YP002B	1.120	0.004	0.788	0.006	0.004	0.00002
YP003-1_1	1.125	0.004	0.752	0.010	0.000	0.00001
YP003-1_2	1.113	0.007	0.761	0.011	0.000	0.00000
YP003-1_3	1.122	0.005	0.748	0.008	0.001	0.00001
YP003-1_4	1.122	0.005	0.726	0.007	0.001	0.00001
YP003-1_5	1.119	0.006	0.757	0.006	0.002	0.00001
YP002-1_1	1.129	0.006	0.722	0.008	0.001	0.00001
YP002-1_2	1.137	0.005	0.767	0.008	0.001	0.00001
YP002-1_3	1.118	0.008	0.739	0.009	0.002	0.00002
YP002-1_4	1.114	0.006	0.749	0.008	0.003	0.00003
YP002-1_5	1.105	0.007	0.764	0.011	0.003	0.00004

Table 1: Data contained in the example CSV file `Pan2018.csv` included in the package

The columns `Sample_ID`, `U234_U238`, `U234_U238_2SE`, `Th230_U238`, `Th230_U238_2SE` and either `Th232_U238` and `Th232_U238_2SE`, or `Th230_Th232` and `Th230_Th232_2SE` must be present in the input data frame with these exact names for the model to function. The `csUTh()` function will check if the input data frame has these columns, and will stop with an error message if it does not find these columns. The `names()` function can be used to update column names of a data frame to

297 ensure they match the names that the model function requires. Alternatively
 298 the user can edit the column names in a spreadsheet program such as Microsoft
 299 Excel. The order of the columns in the data frame is not important.

300 Columns U234_U238 and U234_U238_2SE are the $[\frac{^{234}\text{U}}{^{238}\text{U}}]$ activity ratios and
 301 their 2σ errors. Columns Th230_U238 and Th230_U238_2SE are the $[\frac{^{230}\text{Th}}{^{238}\text{U}}]$
 302 activity ratios and their 2σ errors. Columns Th232_U238 and Th232_U238_2SE
 303 are the $[\frac{^{232}\text{Th}}{^{238}\text{U}}]$ activity ratios and their 2σ errors. Columns Th230_Th232 and
 304 Th230_Th232_2SE are the $[\frac{^{230}\text{Th}}{^{232}\text{Th}}]$ activity ratios and their 2σ errors.

305 If Th230_Th232 and Th230_Th232_2SE are provided instead of Th232_U238
 306 and Th232_U238_2SE, columns Th232_U238 and Th232_U238_2SE are calculated
 307 by `csUTh()`.

308 *Details of the input parameters of closed-system analysis*

309 `sample_name` is the name of the sample to calculate closed-system ages
 310 for. The function will partially match by sample prefix. For example in Ta-
 311 ble @ref(tab:pan) one sample is indicated by the Sample ID ‘YP003.’ If the
 312 user inputs ‘YP003’ for the `sample_name`, then this will match rows where the
 313 Sample ID is ‘YP003-1,’ ‘YP003-2,’ ‘YP003-3,’ and so on.

314 `nbitchoice` is the number of iterations in the model (it is recommended
 315 to have at least 10,000). `detcorrectionchoice` is a parameter for choosing
 316 whether or not to apply a detrital correction to the calculation.

317 `R28det` (0.8) and `R28det_err` (0.4) are the values for the $[\frac{^{232}\text{Th}}{^{238}\text{U}}]$ activity
 318 ratio of the detritus and its standard error (default values in parentheses). Sim-
 319 ilarly, `R08det` (1) and `R08det_err` (0.05) are the values for the $[\frac{^{230}\text{Th}}{^{238}\text{U}}]$ activity
 320 ratio of the detritus and its standard error, and `R48det` (1) and `R48det_err`
 321 (0.02) are the corresponding values for $[\frac{^{234}\text{U}}{^{238}\text{U}}]$ activity ratio of the detritus.

322 *How to run the model*

323 Assuming that the package is attached with `library(UThwigl)`, and the
 324 data have been imported to the working environment as noted above into a
 325 data frame named `input_data_cs`, the user can then run `csUTh()`, specifying
 326 the input data frame and the input parameters as described above. The code
 327 block below shows a typical example that will execute in less than a minute on
 328 a typical 2.3 GHz Intel Core i5 laptop:

```
# Solve for sample YP003
output_cs <-
  csUTh(
    input_data_cs,
    sample_name = 'YP003',
    nbitchoice = 10000,
    detcorrectionchoice = TRUE,
    R28det = 0.8,
    R28det_err = 0.4,
```

```

R08det = 1,
R08det_err = 0.05,
R48det = 1,
R48det_err = 0.02,
keepfiltereddata = FALSE,
print_age = TRUE,
with_plots = TRUE,
save_plots = FALSE,
save_output = FALSE
)

```

For efficient interactive use of this package, the default setting of `csUTh()` is to produce a panel plot as seen in Figure @ref(fig:csuthvizfig). The setting `with_plots = FALSE` prevents plots from being generated which is more useful when the function is part of a longer sequence of code. The function runs faster when not producing plots, which is helpful when replicating many runs. The setting `save_output = TRUE` will save a csv file to the current working directory so the output data can be used in other contexts. The csv file that is created when `save_output = TRUE` will be given a name that includes a date and time stamp so that the output of each time the function is run can be saved to a unique file.

When run on the R console, the function will print a confirmation that the input data frame has the required columns. If `print_age` is set to `TRUE`, it will also print the resulting mean age value of several analyses on a single sample, with an error reported as 2 Standard Deviation, for example:

```

All required columns are present in the input data
[1] "Mean age: 117.1 +/- 3.7 ka"

```

`print_age` should be set to `FALSE` if ages computed are not for analyses of the same sample, since this mean age would be meaningless.

Inspecting and visualizing the models' output

The function returns a data frame with the age, error and summary output for each measurement, as shown in Table @ref(tab:panoutput). This includes calculated ages (with or without detrital correction, depending how `detcorrectionchoice` was set), initial $[\frac{^{234}\text{U}}{^{238}\text{U}}]$ activity ratios, along with their uncertainties, calculated as the 2.1 and 97.9 percentiles of the population of solutions determined with the Monte Carlo simulation.

The plots produced by the `csUTh()` function are stored as list objects in the output of the function. We can show the plots by accessing the list like this:

(ref:csuthvizfigcap) Example of the visualisations produced by the `csUTh()` function, using the demonstration run described above, and five in-situ analyses by laser ablation of coral sample YP003. A: closed-system ages and B: initial $[\frac{^{234}\text{U}}{^{238}\text{U}}]$ activity ratios for each sample analysis.