# UThwigl - 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 unvaluable 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 of open-system U-Th dating to the broad scientific community, here we provide an R package, named *UThwigl*, that implements the Diffusion-Adsorption-Decay model of Sambridge et al. (2012). 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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# Introduction

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

Closed-system U-Th dating has been successfully applied to a range of carbonates, from corals (Edwards, Gallup, and Cheng 2003) to speleothems (Richards and Dorale 2003). In corals and most speleothems, detrital correction is minimal; however, it can be significant when dating pedogenic carbonates, for instance (Ludwig and Paces 2002). In this case, detrital correction can be performed using the measured or assumed composition of the detrital fraction (e.g. K. Ludwig 2003). Alternatively, isochron techniques can be applied (Ludwig and Titterington 1994); the latter are beyond the scope of this article but IsoPlot is a commonly used software for isochron calculations and other geochronological applications (K. R. Ludwig 2003).

Closed-system conditions are seldom met in teeth and bones (although enamel can sometimes be quite impervious to isotope gain or loss). Thus, for teeth and bone, U-Th dating requires to take into account open system behaviour. The diffusion-adsorption-decay (DAD) model developed by Sambridge et al. (2012) was instrumental to implement successfully open-system U-Th dating. It allows for advective and diffusive transport of uranium and thorium isotopes, while include synchronous radioactive decay. The software implementation was written in Fortran and is available as a Java GUI (http://www.iearth.org.au/codes/iDaD/).

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

In this article, we propose a R package which offers functions to perform closed-system, `csUTh()`, and open-system, `osUTh()`, U-Th age calculations. The former implements formulations given in Ludwig (2003) while the latter applies the Diffusion-Adsorption-Decay (DAD) model of Sambridge et al. (2012). The motivation for providing an R package is to increase the transparency, reproducibility, and flexibility of the analytical workflow for computing U-Th ages. In particular, for open-system Currently it is difficult to include the Java GUI in a fully scripted data analysis so the method for computing the DAD model is not highly 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 reproducibiltiy of results. Reproducibility refers 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 (Medical Sciences 2015; Freedman, Cockburn, and Simcoe 2015; Institute 2013; Ioannidis 2005; Collaboration and others 2015; Camerer et al. 2018; Camerer et al. 2016). Consequently, the transparency, openness, and reproducibility of results and methods are receiving increased attention, and the norms of research in many fields are changing (Nosek et al. 2015; Miguel et al. 2014; Marwick 2016).

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, and others (Kattge, Díaz, and Wirth 2014; Ma 2018). However, the use of open source software such as R (Pebesma, Nüst, and Bivand 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 open-system 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 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 for each analysis to yield an age, ($^{234}$U/$^{238}$U), ($^{230}$Th/$^{238}$U) and ($^{232}$Th/$^{238}$U) activity ratios are measured (parentheses denote activity ratios throughout this article). The ($^{232}$Th/$^{238}$U) activity ratio is required for detrital correction (although it is needed to use `csUTh()` whether the detrital correction is performed or not).

*Open-system dating*

Data required for the DAD model are ($^{230}$Th/$^{238}$U) and ($^{234}$U/$^{238}$U) activity ratios collected along a transect perpendicular to the surface of the tooth or bone. Sampling for analysis can be done by micro-drilling or laser ablation.