PbIso: an R package and web app for calculating and plotting Pb isotope data

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Abstract

The package PbIso is a free and open R toolbox for commonly used calculations and plots of Pb-Pb isotope data and for generating Pb evolution models. In this paper, we review Pb isotope systematics and the calculations that are commonly used, such as model age, model source μ ($^{238}U/^{204}Pb$), time-integrated κ ($^{232}Th/^{238}U$), and initial Pb isotope ratios. These equations are implemented into R functions in the package PbIso. In addition, functions are provided for generating Pb evolution models, paleoisochrons, and isochrons. This allows users to apply calculations to their data in a straightforward way, while providing transparency and flexibility of the calculations used. We have implemented some basic features of the PbIso package into an online shiny R application (see https://shereearmistead.github.io/software/pbiso), which makes it easy for users without any R experience to use these calculations with their own data and to generate plots. We have provided a case study from the Superior Province in Canada, showing how different Pb evolution models can be generated in PbIso and compared to Pb isotope data.

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1 Introduction

Lead (Pb) isotopes are used in a range of science applications including, plate tectonics, studies of early Earth evolution and archaeometry. Pb isotopes have been used in geology since the early 1900's (Davis et al., 2003). The U-Th-Pb isotope system is based on the decay of two isotopes of uranium to two different isotopes of Pb and the decay of Th to a third isotope of Pb:

$^{238}U \rightarrow {}^{206}Pb$ half-life ~4468 million years

$^{235}U \rightarrow {}^{207}Pb$ half-life ~700 million years

$^{232}Th \rightarrow {}^{208}Pb$ half-life ~14000 million years

A fourth isotope of Pb, ^{204}Pb, which is of primordial origin and not produced by radioactive decay, is used to create isotope ratios ($^{206}Pb/^{204}Pb$, $^{207}Pb/^{204}Pb$ and $^{208}Pb/^{204}Pb$) which facilitate measurements using mass spectrometers. A major advantage of this combined U-Th-Pb isotope system is that three decay chains

should provide internally consistent results, a feature that is not available for other isotope systems. Decay constants for the three radioactive nuclides are very different, as are Th/U, U/Pb and Th/Pb ratios in many minerals and rocks, leading to many interesting uses for these isotope systems.

Two principal foci of endeavour based on the U-Th-Pb isotope system have been in: (1) geochronology, primarily using minerals with elevated U/Pb ratio, and (2) petrogenesis.

The first of these mostly uses minerals with elevated U/Pb or Th/Pb such as zircon, baddeleyite, titanite and monazite in which the radioactive decay of uranium or thorium produce large $^{206}Pb/^{204}Pb$, $^{207}Pb/^{204}Pb$ or $^{208}Pb/^{204}Pb$ ratios and is therefore generally referred to as the radiogenic U-Th-Pb system. Petrogenetic studies, in contrast, tend to concentrate on either whole rock samples or on minerals with fairly low to negligible U/Pb or Th/Pb and this version of the U-Th-Pb isotope system is thus typically referred to as the 'common Pb' system. The large difference in decay constant, and hence half-life, for ^{238}U and ^{235}U produces very different decay characteristics for old (Archean) rocks and minerals when compared with younger samples. Since ^{235}U decays much more rapidly than ^{238}U, the $^{207}Pb/^{204}Pb$ ratio increases much more rapidly than $^{206}Pb/^{204}Pb$ in early Earth history. At younger (Mesoproterozoic to Phanerozoic) times, there is little change in $^{207}Pb/^{204}Pb$ while $^{206}Pb/^{204}Pb$ continues to increase (Figure 1).

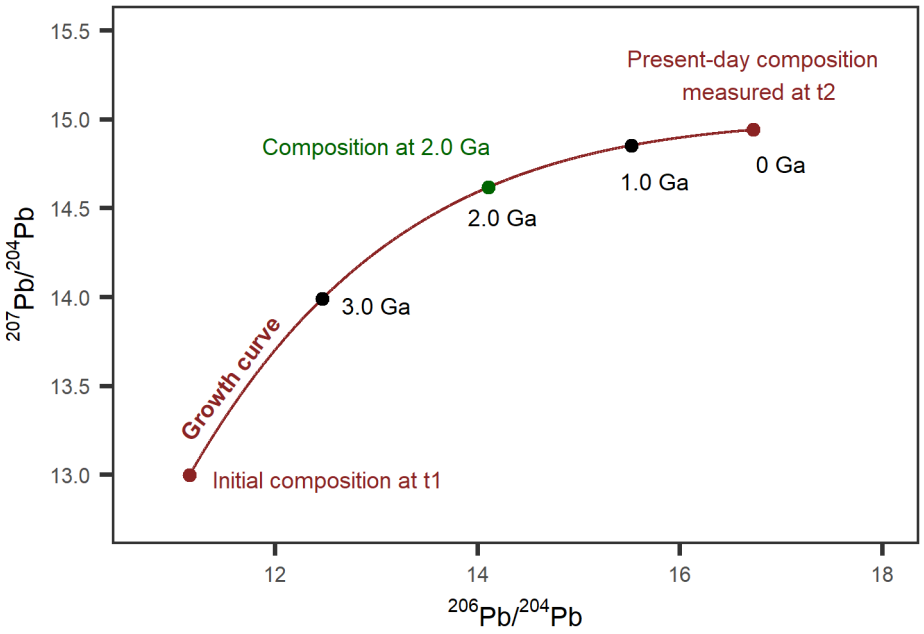


Figure 1: Single-stage growth curve. Evolution of the radiogenic isotopes ^{206}Pb and ^{207}Pb, relative to common ^{204}Pb, from t1 to the present-day. Reproduced from Halla (2018).

As with all isotope systems, complexity may be introduced by geological processes such as multiple dis-

turbance events or mixing of radiogenic products. Unlike some of the other petrogenetic isotope systems routinely used today (e.g. Lu-Hf and Sm-Nd) and in the past (Rb-Sr) which exclusively link to silicate petrogenetic processes, the U-Th-Pb isotope system provides insights for both silicate and sulphide processes. Although not frequently used, the Re-Os isotope system also provides information on sulphide petrogenetic processes but is not directly affected by silicate processes. U, Th and Pb concentrations are greater in crustal material than in most mantle lithologies, and therefore the Pb isotope system is sensitive to interaction (contamination or partial melting) of crust and introduction of this material to mantle-derived mafic lithologies.

The 'common Pb' isotope system was extensively used in the 1970's and 1980's, prior to development of ICPMS and ion microprobe capabilities for Lu-Hf investigations of zircon. It is often seen as a more difficult system to understand, in part because it uses graphs with radiogenic products on both axes, either ^{206}Pb/^{204}Pb vs ^{207}Pb/^{204}Pb for the uranogenic system or ^{206}Pb/^{204}Pb vs ^{208}Pb/^{204}Pb for the thorogenic system. As with other isotope decay systems, the isochron relationships for the U-Th-Pb system are described by relationships of the form:

$$\frac{^{206}Pb}{^{204}Pb}_{present} = \frac{^{206}Pb}{^{204}Pb}_{initial} + \frac{^{238}U}{^{204}Pb}(e^{\lambda_8 T_{initial}} - e^{\lambda_8 t}) \quad (1)$$

Where λ_8 is the decay constant for the radioactive isotope (^{238}U in this example), $T_{initial}$ is the age in years of the initial event and t is the age of a secondary event. For t=0 (present day) this latter term reduces to the value 1. The full set of equations for the three isotope systems are given in equations (2), (3) and (4). For simplicity, some ratios are often represented by Greek characters by convention. ^{238}U/^{204}Pb is represented by the letter μ, ^{232}Th/^{204}Pb by the letter ω and ^{232}Th/^{238}U by the letter κ.

The evolution of Pb isotope ratios through time for various conceptual Earth reservoirs is captured by a number of growth models. The simplest assumes a primordial Pb isotope composition equivalent to that of the Canyon Diablo meteorite (Blichert-Toft et al., 2010) and growth of the Pb isotope ratios to values representative of some modern environment. This model was first developed by Holmes and by Houtermans (Holmes (1946) and Houtermans (1946))and is generally referred to as either a single stage model or as the Holmes-Houterman model. It is known that this model does not provide a good representation of Pb isotope evolution for the Earth. More complex two-stage models have been developed, the most frequently used being that of Stacey and Kramers (1975). This model was based on the Pb isotope composition of a number of ore lead minerals and is more accurately described as representing well-mixed ore environments. It had a

first stage from the time of formation of the Earth (as represented by Canyon Diablo troilite) until 3.7 Ga, when the U/Pb and Th/Pb composition changed. Models such as that of Cumming and Richards (1975) and Tolstikhin et al. (2006), are more complex, with continually changing U/Pb ratios. Other models are defined for limited geographic regions (e.g. Thorpe (1999) for the Abitibi Belt of Canada) or so recently published that they have not yet been extensively used. Each of these two- or multistage models essentially describes a single evolution curve represented by a particular reservoir, although most are generally thought of as representing a version of 'average Earth'. In some cases, alternative curves with different U/Pb and Th/Pb composition may be calculated based on the age and composition of the second stage of the original model. Zartman and colleagues (Doe (1979), Zartman and Doe (1981), Zartman and Richardson (2005)) developed a model describing the evolution of several distinct reservoirs in the Earth, specifically lower crust, upper crust, mantle and orogene (a mix of material from the other three reservoirs). This model closely resembles that of Stacey and Kramers (1975) and Cumming and Richards (1975).

Original application of these various models was related to the study of U-Th-Pb in whole rock silicate systems as an additional tracer, supplementing Rb-Sr and Sm-Nd studies. It has, however, been recognised for some time that the various isotope systems may be decoupled from each other, either because of fluid-rock interaction processes (Eglington (2019), Johnson and DePaolo (1994)) or because the magmas involved tap material for each isotope system from multiple, distinct reservoirs (Stracke (2012), Vervoort et al. (1994)). The viability of the latter has become increasingly important with recent suggestions that distinct zones of concentration of sulphide minerals may occur in the crust and mantle lithosphere which may be tapped by younger mantle melts (Holwell et al. (2022)) and the recognition that there may be distinct spatial variations in Pb isotope composition of different ore deposits and crustal domains (Be'eri-Shlevin et al. (2010), Carr et al. (1995), Champion and Huston (2016), Eglington (2018a), Gulson (1986), Halla (2018), Huston et al. (2016), Luais and Hawkesworth (2002), Warren and Thorpe (1994)).

Since $^{206}Pb/^{204}Pb$ or $^{207}Pb/^{204}Pb$ ratios are different at different times, as is the case for epsilon values of Nd or Hf isotopes, it does not help to plot these values on maps. A more distinctive parameter is the model source $^{238}U/^{204}Pb$ (μ) which is a function of model starting composition, model age and event age (mineralisation or crust-forming episode) and the isotope composition of the material produced. The $^{238}U/^{204}Pb$ ratio needed to derive an initial composition for one or more samples may be calculated by rearranging the uranogenic isochron equations and solving iteratively if the age of the samples is known (Albarède et al. (2012), Andersen (1998), Champion and Huston (2016), Eglington (2018a), Gale and Mussett (1973), Halla (2018), Harmer et al. (1995)). The model source μ ($^{238}U/^{204}Pb$) derived in this way may be thought of as the composition of the source region from which rocks or minerals are produced. Calculation of this parameter is quite routine

for aficionados of Pb isotopes but is not routinely understood by most geologists, even though its use is again becoming more common in the ore deposit research community. A variety of software have been produced over time for use with isotope data. Some are primarily intended for calculating isochrons, regression ages and initial compositions (Andersen (1998), Eglington (2018b), Vermeesch (2018), Ludwig (2001)). Some have explicit capabilities for model source μ calculations and the form that these occur in has varied through time as a function of the preferred software development language or environment at the time. Ludwig (2001) and Andersen (1998) provided ways to perform the calculations in Excel spreadsheets, Eglington (2018b) using a stand-alone graphical user package and Gaab et al. (2006) using the Octave environment. Here, we provide a standalone R package and R code to perform the calculations since R is becoming increasingly popular for scientific investigations.

More comprehensive introductions to Pb isotope plots and their interpretation have been provided elsewhere and are not repeated here (Faure (1977), Gale and Mussett (1973), Halla (2018)).

1.1 Introduction to `PbIso`

In recent years, several tools have been developed and adapted for various isotopic and geochemical datasets, including, `IsoplotR` (Vermeesch, 2018) (an R implementation of the Excel Isoplot plugin (Ludwig, 2001)), `provenance` (Vermeesch et al., 2016), and `detzrcr` (Andersen et al., 2018) in R, and `pyrolite` (Williams et al., 2020) in Python. Some of these packages have a linked graphic user interface (GUI), which makes them accessible to users of various programming experience. The power of these tools is the ability to apply them to large datasets, and integrate them with other powerful statistical and visualisation packages, which is becoming increasingly important as many disciplines within Earth Sciences involve big data analytics.

Typically Pb isotope calculations and Pb evolution models are performed in makeshift spreadsheets with little transparency of how they are actually calculated. The methods for calculating these different values also vary among publications, often with poor documentation, making reproducibility difficult. Our aim is to provide a review of Pb isotope systematics and how these are incorporated into various Pb isotope calculations. We document the different calculations used for Pb isotope data and Pb evolution models and how they have been implemented into the `PbIso` R package. The `PbIso` functions allow for simplicity in only requiring minimal Pb isotope measurements as inputs, while also allowing users the flexibility of setting optional input values, or defining their own Pb evolution models.

`PbIso` is intended for users interested in modelling the evolution of various systems from Pb isotopes, such as calculating model age, model source μ, and initial isotope ratios. These calculations are particularly

applicable to a wide range of ore deposit studies (e.g. Huston et al. (2010)), and plate tectonic studies (e.g. Blichert-Toft et al. (2016)). `PbIso` also allows rapid modelling of user-defined Pb evolution curves, which is important for understanding Earth evolution as well as the evolution of many ore-forming regions around the world. For individual samples, we recommend using the functions in `IsoplotR` (Vermeesch, 2018), which allows details such as factoring in uncertainties, performing regressions and sample statistics to be calculated.

1.2 Pb isotope systematics

The decay of ^{238}U to ^{206}Pb; ^{235}U to ^{207}Pb and ^{232}Th to ^{208}Pb and the non-radiogenic ^{204}Pb can be used to understand the history of certain crustal and mantle processes of a mineral or rock. The abundance of the radiogenic isotopes increases with time (Figure 2), so samples with significantly different ages cannot easily be compared using the ^{206}Pb/^{204}Pb, ^{207}Pb/^{204}Pb, and ^{208}Pb/^{204}Pb ratios. To allow easy comparison of samples across broad time periods, the model source μ (^{238}U/^{204}Pb) and κ (^{232}Th/^{238}U) values can be used, calculated using an independently constrained age for each sample. These also allow us to compare samples/deposits of varying ages to modelled reservoirs such as upper crust, mantle and lower crust (Zartman and Doe, 1981); Bulk Silicate Earth (Maltese and Mezger, 2020); or region specific models (e.g. Abitibi-Wawa in Superior Province (Thorpe, 1999)).

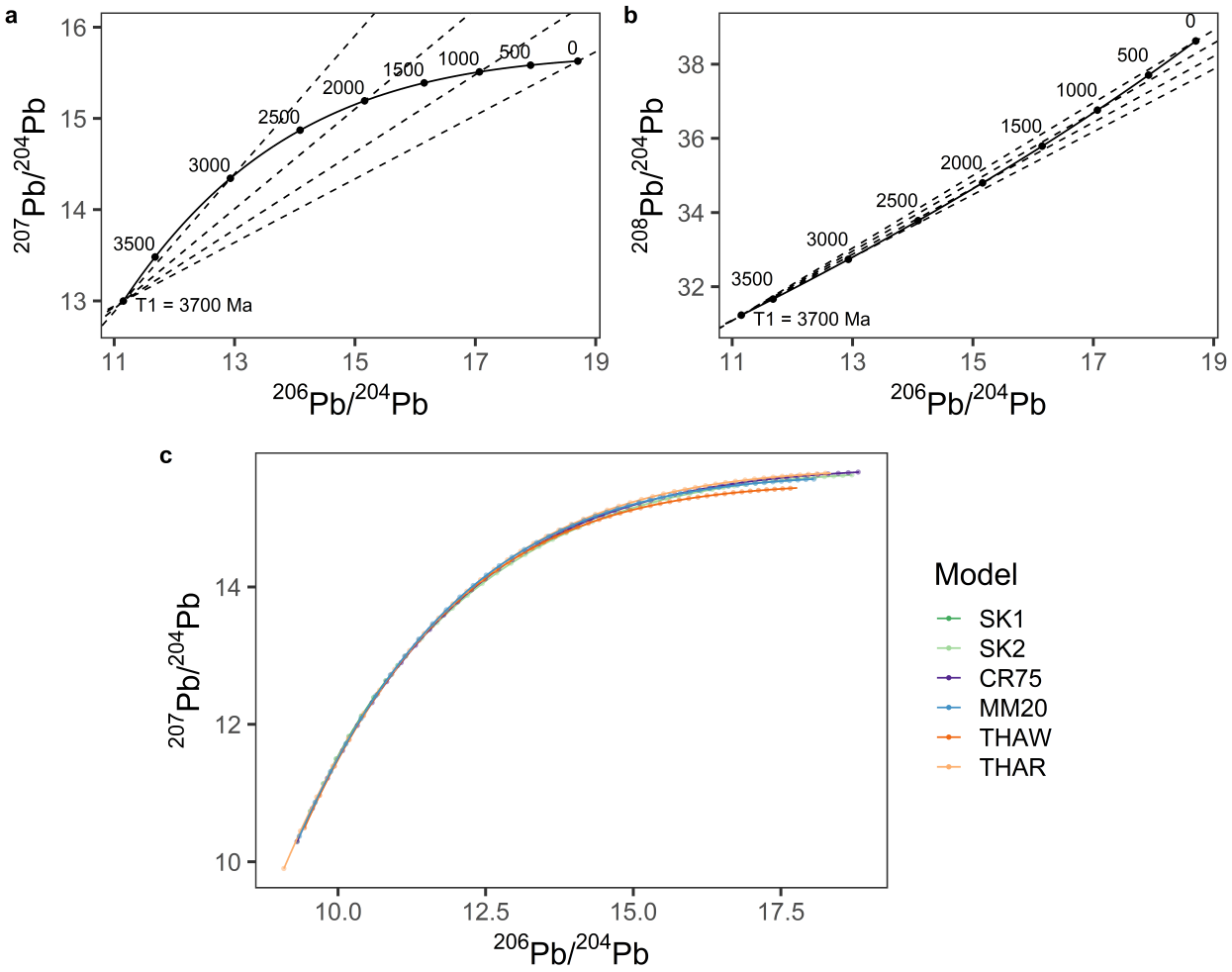


Figure 2: Pb isotopic evolution through time, a) evolution of $^{206}Pb/^{204}Pb$ and $^{207}Pb/^{204}Pb$; b) evolution of $^{206}Pb/^{204}Pb$ and $^{208}Pb/^{204}Pb$; both using the 2nd stage model parameters from Stacey and Kramers (1975). Paleoisochrons for 3000 Ma, 2000 Ma, 1000 Ma and the isochron for 0 Ma are shown as dashed lines in both plots. c) Pb evolution curves using models packaged within `PbIso`, see Table 3 for model parameters and references. Points are shown along each curve at 100 Ma intervals. See section 4 for how to generate the model curves and section 5.2.1 for the paleoisochron/isochron lines shown in (a) and (b).

2 Using `PbIso` in R

`PbIso` includes functions for calculating initial Pb isotope ratios, model age, model source μ ($^{238}U/^{204}Pb$) and time-integrated κ ($^{232}Th/^{238}U$), as well as plotting parameters such as model curves, paleoisochron lines and y-intercepts, and isochrons. Using the package within R allows flexibility in applying the functions to the user's own datasets and the ability to use the wide array of plotting and statistical tools available in R.

We have also implemented some of the basic features of `PbIso` into an online Shiny R application (see https://shereearmistead.github.io/software/pbiso), which requires no knowledge of R, making it accessible

for users. The app allows input of user data including sample name/ID, age, $^{206}Pb/^{204}Pb$, $^{207}Pb/^{204}Pb$, and $^{208}Pb/^{204}Pb$ ratios. Users can then export the processed data as a .xlsx file, which will include the calculated columns for initial Pb isotope ratios, model age, model source μ ($^{238}U/^{204}Pb$) and time-integrated κ ($^{232}Th/^{238}U$), as well as a sheet containing the model parameters. Four basic plots are automatically generated in the Shiny application based on the user data, and can be downloaded as .pdf figures.

The functions in `PbIso` take one or more of the basic input parameters t (time (Ma)), x ($^{206}Pb/^{204}Pb$), y ($^{207}Pb/^{204}Pb$) and z ($^{208}Pb/^{204}Pb$) to perform the calculations. For advanced usage, the functions can also optionally take the values for different model parameters (summarised in Table 1). The calculations and functions used in `PbIso` assume a starting composition and model following Stacey and Kramers (1975) 2nd stage model, although this can easily be changed if an alternative model (e.g. Stacey and Kramers (1975) single stage; Maltese and Mezger (2020) Bulk Silicate Earth or others) is preferred.

Table 1: Default model parameters used in `PbIso` functions. These can be changed if an alternative model is preferred.

Parameter	Description	Default value	Reference
T1	Model start time (Ma)	3700	Stacey and Kramers (1975)
X1	$^{206}Pb/^{204}Pb$ model starting composition	11.152	Stacey and Kramers (1975)
Y1	$^{207}Pb/^{204}Pb$ model starting composition	12.998	Stacey and Kramers (1975)
Z1	$^{208}Pb/^{204}Pb$ model starting composition	31.23	Stacey and Kramers (1975)
Mu1	$^{238}U/^{204}Pb$ model (μ_1)	9.74	Stacey and Kramers (1975)
Ka1	$^{232}Th/^{238}U$ model (κ_1)	3.78	Stacey and Kramers (1975)
W1	$^{232}Th/^{204}Pb$ model (ω_1)	36.84	Stacey and Kramers (1975)
L5	^{235}U decay constant (λ_5)	$9.8485 * 10^{-10}$	Jaffey et al. (1971)
L8	^{238}U decay constant (λ_8)	$1.55125 * 10^{-10}$	Jaffey et al. (1971)
L2	^{232}Th decay constant (λ_2)	$0.49475 * 10^{-10}$	Le Roux and Glendenin (1963)
U8U5	Present-day $^{238}U/^{235}U$ ratio	137.88	Stacey and Kramers (1975)
E1	ϵ_1 rate factor for change in μ over time	0	see Cumming and Richards (1975)
E2	ϵ_2 rate factor for change in κ over time	0	see Cumming and Richards (1975)

2.1 Installation

The package can be downloaded from https://github.com/ShereeArmistead/PbIso or can be installed within R by running the following:

```
install.packages(devtools)
devtools::install_github("shereearmistead/PbIso")
library(PbIso)
```

Note: the first two lines only need to be run once to install the package on a user's computer. The third line needs to be run every time a user wants to use PbIso in a new R session.

2.2 Running functions

All of the functions in `PbIso` are designed for ease of use, while also allowing flexibility in changing model parameters. The required inputs are outlined in subsequent sections of this manuscript, but we have included a brief overview of the different ways these functions can be used below, using the `Calc64()` function as an example, which only requires one input (age). The formatted code in the following sections includes the input line of code (e.g. Calc64(2700) in the example below), and the output value given by R (e.g. 13.63662 in the example below), indicated by the line beginning with [1].

The most basic usage is to simply include the one required input parameter, in this case age:

```
Calc64(2700)
```

```
[1] 13.63662
```

2.3 Customising model parameters

As stated previously, the default starting parameters are based on Stacey and Kramers (1975) 2nd stage model, however, these can be manually overridden by specifying them in the function. For further information about how to generate a table with values for a customised Pb evolution model, see section 4. The optional parameters, in this case, T1, X1, Mu1, can be specified as:

```
Calc64(2700, T1 = 4000, X1 = 9.5, Mu1 = 7)
```

```
[1] 11.87765
```

Not all of the optional parameters need to be defined. For example, accepting the defaults for T1 and X1, but modifying Mu1 to 8:

```
Calc64(2700, Mu1 = 8)
```

```
[1] 13.19276
```

Table 2 summarises the `PbIso` functions and their required and optional input parameters. See Table 1 for the descriptions and default values for these model parameters. Note that the decay constants are included as optional arguments in `PbIso` functions for maximum flexibility, however, we advise against modifying these unless there are good constraints on alternative values.

Rather than setting the optional parameters manually for every calculation, a predefined model can be used. We have incorporated several commonly used models (see Table 3), for example the Stacey and Kramers (1975) 1st stage model:

```
Calc64(2700, model = SK1)
```

```
[1] 12.98544
```

Or the Maltese and Mezger (2020) Bulk Silicate Earth Model:

```
Calc64(2700, model = MM20)
```

```
[1] 13.57078
```

Alternatively, users may define starting parameters for their own Pb evolution models, which is particularly useful if this is needed for multiple calculations, and to generate model curves (see section 4). To define your own model, use the `list()` function in R to define the starting parameters:

Table 2: Summary of 'PbIso' functions and their input parameters

Function	Description	Required inputs	Optional inputs
`Calc64()`	Calculates $^{206}Pb/^{204}Pb$ at a given time, for a given model	t	T1, X1, Mu1, L8, model
`Calc74()`	Calculates $^{207}Pb/^{204}Pb$ at a given time, for a given model	t	T1, Y1, Mu1, U8U5, L5, model
`Calc84()`	Calculates $^{208}Pb/^{204}Pb$ at a given time, for a given model	t	T1, Z1, W1, L2, model
`CalcModAge()`	Calculates the model age	x, y	T1, X1, Y1, U8U5, L5, L8, model
`CalcMu()`	Calculates the model source μ_1	t, x, y	T1, X1, Y1, U8U5, L5, L8, model
`CalcKa()`	Calculates the time-integrated κ_1	t, z, x	T1, X1, Z1, L2, L8, model
`Calc64in()`	Calculates the initial $^{206}Pb/^{204}Pb$ ratio	t, x, y	T1, X1, Y1, U8U5, L5, L8, model
`Calc74in()`	Calculates the initial $^{207}Pb/^{204}Pb$ ratio	t, x, y	T1, X1, Y1, U8U5, L5, L8, model
`Calc84in()`	Calculates the initial $^{208}Pb/^{204}Pb$ ratio	t, x, y, z	T1, X1, Y1, Z1, U8U5, L5, L8, L2, model
`modelcurve()`	Generates a dataframe for a Pb evolution model	t	T1, X1, Y1, Z1, Mu1, W1, U8U5, L5, L8, L2, E1, E2, model
`isochron76slope()`	Paleoisochron slope on a $^{206}Pb/^{204}Pb$ vs $^{207}Pb/^{204}Pb$ plot	t	T1, X1, Y1, Mu1, U8U5, L5, L8, model
`isochron76yint()`	Paleoisochron y-intercept on a $^{206}Pb/^{204}Pb$ vs $^{207}Pb/^{204}Pb$ plot	t	T1, X1, Y1, Mu1, U8U5, L5, L8, model
`isochron86slope()`	Paleoisochron slope on a $^{206}Pb/^{204}Pb$ vs $^{208}Pb/^{204}Pb$ plot	t	T1, X1, Z1, Mu1, W1, L8, L2, model
`isochron86yint()`	Paleoisochron y-intercept on a $^{206}Pb/^{204}Pb$ vs $^{208}Pb/^{204}Pb$ plot	t	T1, X1, Z1, Mu1, W1, L8, L2, model
`mslope()`	Isochron for a given time	t	U8U5, L5, L8
`LeastRad()`	Filters a dataset for the least radiogenic value	df, group, value	

```
my_model <- list(T1 = 4000, X1 = 10.5, Y1 = 11.5, Z1 = 30, Mu1 = 10, W1 = 33)
Calc64(2700, model = my_model)
```

```
[1] 13.89664
```

Note, that for `Calc64()`, only age, T1, X1 and Mu1 are required (not Y1, Z1 or W1), however to make the user-defined model applicable to other `PbIso` functions, it is best to include parameters required for all functions of interest.

Models that we have included as options in `PbIso` are given in Table 3.

Table 3: Predefined models that can be used in the `PbIso` functions. [1] Stacey and Kramers (1975); [2] Cumming and Richards (1975); [3] Maltese and Mezger (2020); [4] Thorpe (1999); [5] Thorpe et al. (1992)

Model	R name	T1	X1	Y1	Z1	Mu1	W1	E1	E2
Single stage model [1]	SK1	4570	9.307	10.294	29.487	7.2	33.2	0	0
2nd stage model [1]	SK2	3700	11.152	12.998	31.230	9.7	36.8	0	0
Variable μ model [2]	CR75	4509	9.307	10.294	29.476	10.8	41.2	$5*10^{-11}$	$3.7*10^{-11}$
Bulk Silicate Earth [3]	MM20	4500	9.345	10.370	29.510	8.6	35.0	0	0
Abitibi-Wawa [4]	THAW	4490	9.431	10.495	29.681	8.3	33.9	0	0
Archean Sulphide [5]	THAR	4560	9.082	9.900	29.343	9.0	34.0	0	0

3 A review of Pb isotopes and how to perform calculations with `PbIso`

3.1 The evolution of radiogenic Pb isotopes with time

The following equations describe the evolution of Pb isotopes with time:

$$\left(\frac{^{206}Pb}{^{204}Pb}\right)_t = \left(\frac{^{206}Pb}{^{204}Pb}\right)_{T_1} + \mu_1(e^{\lambda_8 T_1} - e^{\lambda_8 t}) \quad (2)$$

$$\left(\frac{^{207}Pb}{^{204}Pb}\right)_t = \left(\frac{^{207}Pb}{^{204}Pb}\right)_{T_1} + \frac{\mu_1}{137.88}(e^{\lambda_5 T_1} - e^{\lambda_5 t}) \quad (3)$$

$$\left(\frac{^{208}Pb}{^{204}Pb}\right)_t = \left(\frac{^{208}Pb}{^{204}Pb}\right)_{T_1} + \omega_1(e^{\lambda_2 T_1} - e^{\lambda_2 t}) \quad (4)$$

Note that ω (^{232}Th/^{204}Pb) in equation (4) can also be expressed as $\mu \cdot \kappa$, which is equivalent to ^{238}U/^{204}Pb $\cdot$ ^{232}Th/^{238}U.

The above equations are implemented in `PbIso` by the functions `Calc64()`, `Calc74()` and `Calc84()`, respectively. These functions can be used in a number of ways. For simply calculating the value of each isotope ratio on the Stacey and Kramers (1975) average ore lead curve at a given time, only the age is required.

For example, the ^{206}Pb/^{204}Pb, ^{207}Pb/^{204}Pb and ^{208}Pb/^{204}Pb ratios on the Stacey and Kramers (1975) curve at a given time, say 2700 Ma, is given by:

```
Calc64(2700)
```

```
[1] 13.637
```

```
Calc74(2700)
```

```
[1] 14.69
```

```
Calc84(2700)
```

```
[1] 33.366
```

See Table 2 for the optional parameters for each of these functions to allow a different Pb evolution model to be used.

3.2 Model age

Pb-Pb model ages are calculated by assuming a starting composition (typically Stacey and Kramers (1975) 2nd stage values), and calculating the time needed to reach the present-day measured values. To visualise

this, in Figure 3a, the line connecting the model starting composition (X1, Y1 at T1) and the sample (red circle) intersects the Stacey and Kramers (1975) curve at the model age for this sample. This is numerically given by the following equation:

$$\frac{\frac{^{207}Pb}{^{204}Pb}_{t_{sample}} - \frac{^{207}Pb}{^{204}Pb}_{T_1}}{\frac{^{206}Pb}{^{204}Pb}_{t_{sample}} - \frac{^{206}Pb}{^{204}Pb}_{T_1}} = \frac{1}{137.88} \cdot \frac{e^{\lambda_5 T_1} - e^{\lambda_5 t_{sample}}}{e^{\lambda_8 T_1} - e^{\lambda_8 t_{sample}}} \quad (5)$$

It is not possible to solve this equation directly for the model age (t_{sample}), so a Newton-Raphson iterative calculation is implemented using the `uniroot()` function in the `stats` package in R. This is implemented in `PbIso` using the `CalcModAge()` function. Only the $^{206}Pb/^{204}Pb$ (x) and $^{207}Pb/^{204}Pb$ (y) ratios are needed to solve for the model age.

To apply `CalcModAge()` to a hypothetical sample with $^{206}Pb/^{204}Pb = 13.5$ and $^{207}Pb/^{204}Pb = 14.5$:

```
CalcModAge(13.5, 14.5)
```

```
[1] 2510
```

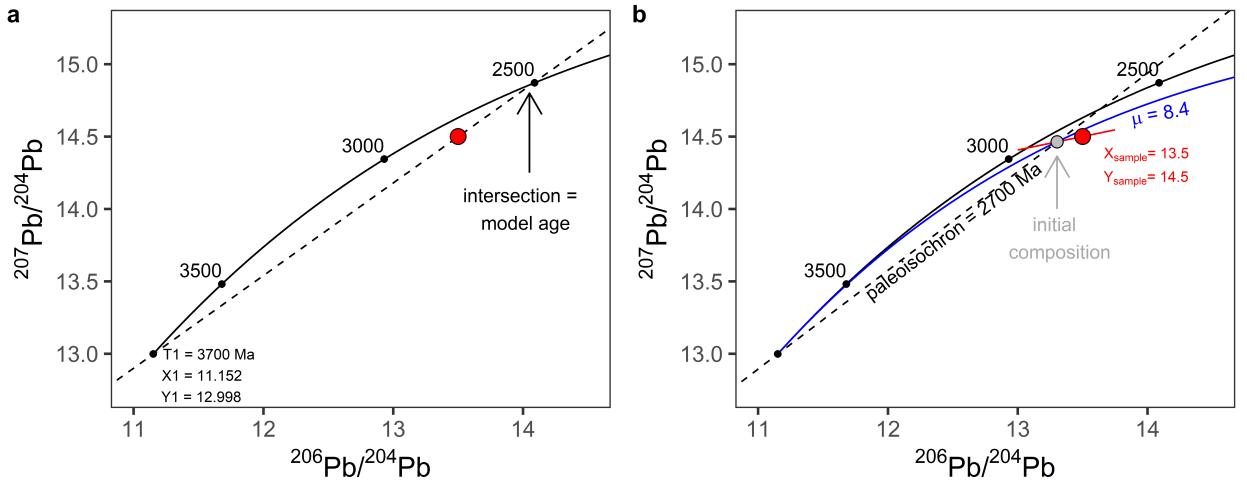


Figure 3: Hypothetical sample (red circle) plotted on a standard Stacey and Kramers (1975) 2nd stage model curve (black line), showing a) that a line connected between a model starting composition and the sample composition, will project onto the Stacey and Kramers (1975) model curve at the corresponding model age, and b) additional values that can be calculated if the actual sample age (in this case 2700 Ma) is known. Grey circle represents the calculated initial ratios, the blue curve represents the corresponding model source μ value for this sample, and the dashed line is the sample age (2700 Ma) paleoisochron.

3.3 Model source μ ($^{238}U/^{204}Pb$)

All calculations from here onwards require that the sample age is known. Preferably an independently obtained age, such as a zircon U–Pb age is used. When comparing Pb isotope signatures across different time periods, it is often more useful to compare the model source μ ($^{238}U/^{204}Pb$) rather than the Pb isotope ratios, as μ does not vary with time in a closed system.

Rocks or minerals that formed within the same reservoir will have Pb isotopic compositions that cluster along an isochron line on a $^{206}Pb/^{204}Pb$ vs $^{207}Pb^{204}Pb$ plot (red line in Figure 3b). The least radiogenic samples will fall near the lower left end of this isochron, while more radiogenic samples will fall near the upper right end. One way to calculate a rock's age is to regress multiple sample analyses. The slope of this line is directly related to its mineralisation age. A more robust way of doing this though is to use the known age of a sample, whereby the slope (m) for a sample with a known age (t_{sample}) is defined by:

$$m_{sample} = \frac{e^{\lambda_5 t_{sample}} - 1}{137.88(e^{\lambda_8 t_{sample}} - 1)} \tag{6}$$

This is implemented in `PbIso` by the function `mslope()`, which takes the argument t and additional optional arguments (see documentation). Substituting equation (6) into the following equation gives us the model source μ ($^{238}U/^{204}Pb$) (Harmer et al. (1995), Eglington (2018a)):

$$\mu = \frac{m_{sample}(X_1 - X_{sample}) + Y_{sample} - Y_1}{\frac{e^{\lambda_5 T_1} - e^{\lambda_5 t_{sample}}}{137.88} - m_{sample}(e^{\lambda_8 T_1} - e^{\lambda_8 t_{sample}})} \tag{7}$$

This is implemented in `PbIso` by the function `CalcMu()`, using the sample age (t) in Ma, $^{206}Pb/^{204}Pb$ (x) and $^{207}Pb/^{204}Pb$ (y) ratios. Optional arguments T1, X1, Y1, U8U5, L5 and L8 can also be applied in the format `CalcMu(t, x, y, T1, X1, Y1, U8U5, L5, L8)`. For example, if we have a sample with a known deposit age (independently obtained using a robust method such as U-Pb zircon crystallisation) of t = 2700 Ma; $^{206}Pb/^{204}Pb$ = 13.5, and $^{207}Pb/^{204}Pb$ = 14.5, and accepting the default Stacey and Kramers (1975) model values, we can calculate the model source μ by:

```
CalcMu(2700, 13.5, 14.5)
```

```
[1] 8.43
```

These calculations can be visualised in Figure 3b. The intersection of the isochron (m_{sample}; red line in Figure 3b), the paleoisochron associated with the sample age (2700 Ma in this case), and the model source μ curve of 8.43 (blue curve in Figure 3b), mark the initial Pb isotope composition of the sample. For samples with very low U concentrations, such as galena, the initial compositions will be approximately the same as the measured values. See section 3.5 for calculating initial Pb isotope ratios, and section 5.2 for generating the model curves and paleoisochron and isochron lines shown in Figure 3b.

3.4 Time-integrated κ (^{232}Th/^{238}U)

Somewhat similar to using the model source μ (^{238}U/^{204}Pb) for a sample, we can use the time-integrated κ (^{232}Th/^{238}U) to look at thorogenic Pb isotopic trends for samples or regions over different time scales.

The time-integrated κ (^{232}Th/^{238}U) is given by:

$$\kappa = \frac{Z_{sample} - Z_1}{X_{sample} - X_1} \times \frac{e^{\lambda_8 T_1} - e^{\lambda_8 t_{sample}}}{e^{\lambda_2 T_1} - e^{\lambda_2 t_{sample}}} \tag{8}$$

This is implemented in `PbIso` as the `CalcKa()` function, using the sample age (t), ^{208}Pb/^{204}Pb (z) and ^{206}Pb/^{204}Pb (x). Again, let's assume a sample with ^{206}Pb/^{204}Pb = 13.5; t = 2700 Ma and now with ^{208}Pb/^{204}Pb = 33:

```
CalcKa(2700, 33, 13.5)
```

```
[1] 3.32
```

This calculation can be visualised in Figure 4, where the red circle is the sample, the blue curve is evolution of the sample κ, and the grey circle is the initial Pb isotope ratio.

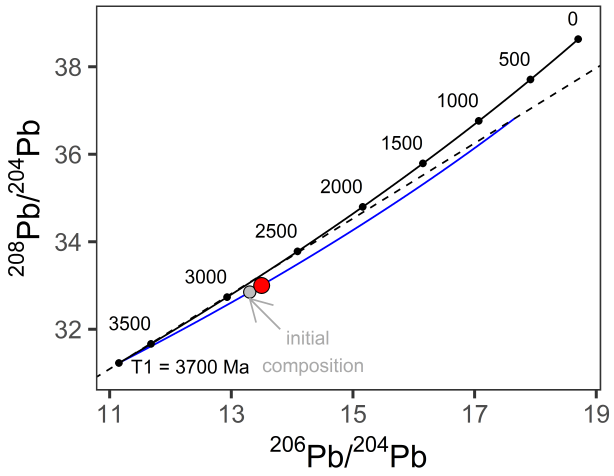


Figure 4: Plot of $^{208}Pb/^{204}Pb$ vs $^{206}Pb/^{204}Pb$ with the same hypothetical sample as previous plots, with the 2700 Ma paleoisochron (dashed line), corresponding kappa curve (blue) and initial isotope composition (grey circle)

3.5 Initial Pb isotope ratios

Often we are interested in the initial Pb isotope composition of a sample at the time of formation, particularly for more radiogenic samples.

$$\left(\frac{^{206}Pb}{^{204}Pb}\right)_{initial} = \left(\frac{^{206}Pb}{^{204}Pb}\right)_{T_1} + \mu_{sample}(e^{\lambda_8 T_1} - e^{\lambda_8 t_{sample}}) \quad (9)$$

$$\left(\frac{^{207}Pb}{^{204}Pb}\right)_{initial} = \left(\frac{^{207}Pb}{^{204}Pb}\right)_{T_1} + \frac{\mu_{sample}}{137.88}(e^{\lambda_5 T_1} - e^{\lambda_5 t_{sample}}) \quad (10)$$

$$\left(\frac{^{208}Pb}{^{204}Pb}\right)_{initial} = \left(\frac{^{208}Pb}{^{204}Pb}\right)_{T_1} + \omega_{sample}(e^{\lambda_2 T_1} - e^{\lambda_2 t_{sample}}) \quad (11)$$

The above equations are identical to the Pb isotope equations in section 3.1, so we could use those same functions, but substitute the sample μ (or ω) in. However, this would require two steps: 1) calculate the model source μ (or ω) using the `CalcMu()` (or `CalcMu()`·`CalcKa()` for ω), which requires t_{sample}, X_{sample}, Y_{sample} (and Z_{sample} for equation (11)) as input parameters, and 2) use that calculated μ (or ω) value to input into equations `Calc64()`, `Calc74()` and `Calc84()`. To eliminate the need to do this in two steps, we have added the functions `Calc64in()`, `Calc74in()` and `Calc84in()` to calculate the initial Pb isotope ratios directly. Note: the X_{sample}, Y_{sample} and Z_{sample} are compulsory arguments because these are required

to calculate μ and/or κ. The initial Pb isotope ratios can be calculated using our hypothetical sample as follows:

```
Calc64in(2700, 13.5, 14.5)
```

```
[1] 13.304
```

```
Calc74in(2700, 13.5, 14.5)
```

```
[1] 14.464
```

```
Calc84in(2700, 13.5, 14.5, 33)
```

```
[1] 32.852
```

4 Pb evolution models

Pb evolution models can be generated using the `modelcurve()` function in `PbIso`. This function takes the arguments for time (t) – usually given as a time interval e.g. 0:3700 – as well as optional arguments for model starting parameters, μ_1, ω_1 values and decay constants (see Table 2). Additionally, parameters ϵ_1 and ϵ_2 can be specified to allow a variable μ with time (see Cumming and Richards (1975) for further information). These two ϵ parameters are rate factors that account for accelerated or decelerated Pb isotope evolution, and therefore the changes in μ of a Pb source over time. The `modelcurve()` function will generate a dataframe with columns t, x, y, z. These correspond to time, $^{206}Pb/^{204}Pb$, $^{207}Pb/^{204}Pb$ and $^{208}Pb/^{204}Pb$, respectively. The values x, y and z are calculated following equations (2), (3) and (4) in section 3.1, with the added parameters ϵ_1 and ϵ_2 to allow a variable μ through time. The model curves shown in Figure 2c and Figure 5 are generated using the `modelcurve()` function, and we have detailed the steps to do this below.

To generate a simple (Stacey and Kramers, 1975) 2nd stage Pb evolution model, only the time (t) is needed in the function `modelcurve()`. The 'SKcurve' dataframe will have 3701 rows of data, each corresponding to a 1 Ma time interval (Table 4).

```
SKcurve <- modelcurve(0:3700)
```

Table 4: First ten rows of the 'SKcurve' dataframe produced using the `modelcurve()` function.

t	x	y	z
0	18.703	15.629	38.631
1	18.702	15.629	38.629
2	18.700	15.629	38.627
3	18.699	15.629	38.625
4	18.697	15.629	38.623
5	18.696	15.629	38.621
6	18.694	15.628	38.620
7	18.693	15.628	38.618
8	18.691	15.628	38.616
9	18.690	15.628	38.614

The `modelcurve()` function can be used to produce model curves with different model parameters. For example the 'modelex1' curve in Figure 5, which corresponds to a model μ of 8 is generated by the following:

```
modelex1 <- modelcurve(0:3700, Mu1 = 8)
```

Using the same parameters as above, but using a variable μ with time (specified by parameters ϵ_1 and ϵ_2)

```
modelex2 <- modelcurve(0:3700, Mu1 = 8, E1 = 0.05 * 10^-9, E2 = 0.037 * 10^-9)
```

The `modelcurve()` function can be used to produce model curves over different time ranges with optional arguments. For example, in the code below, 'modelex3' is a hypothetical model using a custom model 'my_model'. These three example curves are shown in Figure 5.

```
my_model <- list(T1 = 4000, X1 = 10.5, Y1 = 11.5, Z1 = 30, Mu1 = 10, W1 = 33)
modelex3 <- modelcurve(0:3500, model = my_model)
```

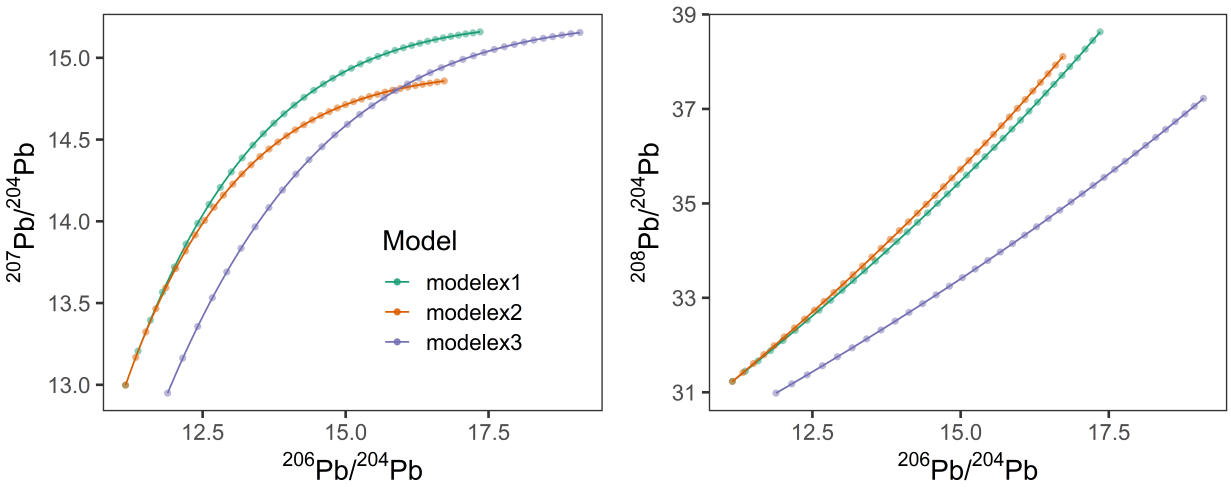


Figure 5: Model curves generated using the `modelcurve()` function for three hypothetical models. Points on curves are shown for every 100 Ma.

5 Other `PbIso` functions

5.1 Least radiogenic calculation

Usually in Pb isotope studies of ore deposits, multiple samples will be obtained from an individual deposit, which produce analyses with a range of Pb isotope values. When doing large regional-scale studies, often only the least radiogenic sample from each deposit will be used.

In `PbIso` we have implemented the function `LeastRad()` which filters a dataset (e.g. df), based on the lowest analysis of an isotope ratio (e.g. $^{207}Pb/^{204}Pb$ or $^{206}Pb/^{204}Pb$) from each group (e.g. ore deposit), in the format: `LeastRad(df, group, value)`.

For example, to filter a sample dataset 'df', based on the lowest $^{207}Pb/^{204}Pb$ analysis from each deposit we would use:

```
LeastRad(df, DepositName, Pb74)
```

Note that this function can only be applied to a dataframe in R, not to individual measurements. More information on using `PbIso` with dataframes is included in the sections below.

5.2 Plotting parameters

In addition to plotting sample data, there are also several plotting features such as paleoisochron and isochron lines.

5.2.1 Paleoisochrons

To generate paleoisochron lines for a given time (t), the slope and y-intercept are needed. To calculate the slope of a paleoisochron line on a $^{206}Pb/^{204}Pb$ vs. $^{207}Pb/^{204}Pb$ plot, the function `isochron76slope()` is used, which takes the argument t as well as optional arguments (see documentation). The associated y-intercept for that paleoisochron is given by the function `isochron76yint()`. These can then be used to plot the paleoisochron line along with a model curve. Similarly, to calculate the paleoisochron slope and y-intercept on a $^{206}Pb/^{204}Pb$ vs. $^{208}Pb/^{204}Pb$ plot, the functions `isochron86slope()` and `isochron86yint()` can be used. Paleoisochron lines (and isochron line for t = 0) in Figure 2 are plotted using the below functions for t = 3000 Ma, t = 2000 Ma, t = 1000 Ma and t = 0 Ma. These values can then be used to plot paleoisochron lines, or the function can be called directly, for example by using `abline(a = isochron76yint(2700), b = isochron76slope(2700))` in base R plotting, or `geom_abline(slope = isochron76slope(2700), intercept = isochron76yint(2700))` in ggplot2 (this command is used to produce the black dashed line in 3b). For a $^{206}Pb/^{204}Pb$ vs. $^{208}Pb/^{204}Pb$ plot, the ggplot2 command would be `geom_abline(slope = isochron86slope(2700), intercept = isochron86yint(2700))` (black dashed line in 4). To use this function to generate the slope and y-intercept of a paleoisochron at time 2700 Ma:

```
isochron76slope(2700)
```

```
[1] 0.681
```

```
isochron76yint(2700)
```

```
[1] 5.4
```

```
isochron86slope(2700)
```

```
[1] 0.86
```

```
isochron86yint(2700)
```

```
[1] 21.6
```

6 Applying PbIso functions to a dataset, case study: Superior Province, Canada

We have shown above that the PbIso package allows for straightforward calculations of various Pb isotope parameters such as model age, model source μ ($^{238}U/^{204}Pb$), time-integrated κ ($^{232}Th/^{238}U$) and initial Pb isotope ratios. However, usually we will want to apply these calculations to an entire dataset rather than to just one sample. Using the standard base R function `mapply()` we can apply the PbIso functions to a dataframe. PbIso is packaged with a sample dataset, which is a subset of sulphide Pb isotope analyses from the Superior Province in Canada obtained from the DepIso database (see: https://sil.usask.ca/databases.php and Eglington (2018a)). We briefly document below how to apply functions to this dataset, using the 'SampleData.csv'.

Import the SampleData.csv file:

```
df <- read.csv("SampleData.csv")
```

The dataframe that we have imported as 'df', before any calculations have been applied, is shown in Table 5.

Table 5: First ten rows of sample data input with sample information and measured Pb isotope ratios

DepositName	age	DepClan	Pb64	Pb74	Pb84
Bachelor Lake	2697	Lode Au	13.492	14.544	33.219
Bachelor Lake	2697	Lode Au	13.607	14.547	33.252
Birchtree Mine	1880	Ni-PGE-Cr	17.318	15.463	37.435
Birchtree Mine	1880	Ni-PGE-Cr	17.320	15.480	36.723
Birchtree Mine	1880	Ni-PGE-Cr	17.320	15.480	36.723
Bousquet	2698	VMS	13.335	14.473	33.200

DepositName	age	DepClan	Pb64	Pb74	Pb84
Bousquet	2698	VMS	13.273	14.448	33.117
Chibougamau	2726	VMS	13.262	14.441	33.186
Chibougamau	2726	VMS	13.279	14.422	33.172
Chibougamau	2726	VMS	13.444	14.477	33.306

We can now apply the `PbIso` functions to the dataframe in the same way we do to individual analyses. Each of the new calculations below will be added as separate columns to the 'df' dataframe.

```
df$Mu     <- CalcMu(df$age, df$Pb64, df$Pb74)
df$Ka     <- CalcKa(df$age, df$Pb84, df$Pb64)
df$Pb64in <- Calc64(df$age, df$Pb64, df$Pb74)
df$Pb74in <- Calc74in(df$age, df$Pb64, df$Pb74)
df$Pb84in <- Calc84in(df$age, df$Pb64, df$Pb74, df$Pb84)
```

Like applying the functions to individual analyses, we can specify optional arguments (e.g. T1, X1, Y1) or specify a predefined or user-defined model (see section 2.2 for defining your own model 'my_model'):

```
df$Mu2 <- CalcMu(df$age, df$Pb64, df$Pb74, T1 = 4570)
df$Mu3 <- CalcMu(df$age, df$Pb64, df$Pb74, model = SK1)
df$Mu4 <- CalcMu(df$age, df$Pb64, df$Pb74, model = my_model)
```

The model age function is slightly more complex, so we need to use the base R function `mapply()`. Instead of using 'model' to add a predefined or user-defined model, we need to use 'MoreArgs'.

```
df$ModAge  <- mapply(CalcModAge, df$Pb64, df$Pb74)
df$ModAge2 <- mapply(CalcModAge, df$Pb64, df$Pb74, T1 = 4570)
df$ModAge3 <- mapply(CalcModAge, df$Pb64, df$Pb74, MoreArgs = SK1)
df$ModAge4 <- mapply(CalcModAge, df$Pb64, df$Pb74, MoreArgs = my_model)
```

The resulting 'df' dataframe with calculations applied (we have removed the extra columns demonstrating the optional arguments and models) is shown in Table 6:

Table 6: First ten rows of dataframe after the `PbIso` functions have been applied

DepositName	age	DepClan	Pb64	Pb74	Pb84	Mu	Ka	Pb64in	Pb74in	Pb84in	ModAge
Bachelor Lake	2697	Lode Au	13.49	14.54	33.22	8.8	3.7	13.64	14.53	33.14	2608
Bachelor Lake	2697	Lode Au	13.61	14.55	33.25	8.6	3.6	13.64	14.50	33.05	2467
Birchtree Mine	1880	Ni-PGE-Cr	17.32	15.46	37.44	9.7	4.2	15.41	15.24	35.49	721
Birchtree Mine	1880	Ni-PGE-Cr	17.32	15.48	36.72	9.8	3.8	15.41	15.26	35.04	753
Birchtree Mine	1880	Ni-PGE-Cr	17.32	15.48	36.72	9.8	3.8	15.41	15.26	35.04	753
Bousquet	2698	VMS	13.34	14.47	33.20	8.5	4.0	13.64	14.47	33.18	2676
Bousquet	2698	VMS	13.27	14.45	33.12	8.3	3.9	13.64	14.45	33.13	2711
Chibougamau	2726	VMS	13.26	14.44	33.19	8.4	4.1	13.58	14.44	33.17	2712
Chibougamau	2726	VMS	13.28	14.42	33.17	8.2	4.0	13.58	14.41	33.10	2648
Chibougamau	2726	VMS	13.44	14.48	33.31	8.4	4.0	13.58	14.44	33.13	2537

The dataframe is now ready to use for plotting various parameters against each other or for performing a wide range of statistical analyses that is possible with other R functions and packages.

Users may wish to only use the least radiogenic sample from each deposit, which can be performed using the `LeastRad()` function, either as the first step in this workflow (immediately after importing the dataset) or the last (after running the various calculations above).

In either case:

```
dfLR <- LeastRad(df, DepositName, Pb74)
```

This produces a dataframe (dfLR) that contains only the sample with the lowest $^{207}Pb/^{204}Pb$ value from each deposit (DepositName).

6.1 Pb evolution models for Superior Province

Often Pb isotope models are developed to help understand the evolution of Pb isotopes in particular regions. Two models are commonly referred to when dealing with Superior Province data, the Abitibi-Wawa model (Thorpe (1999)) and an Archean model based on sulphide data from the Pilbara Craton in Australia and

other Archean terranes (Thorpe et al. (1992)). We refer to these below as the 'Abitibi Model' and 'Archean Model', respectively.

```
AbitibiModel <- modelcurve(4000:0, model = THAW, Mu1 = 8)
ArcheanModel <- modelcurve(4000:0, model = THAR, Mu1 = 9)
```

With `PbIso`, it's very straightforward to generate multi-stage models. In the hypothetical example below, let's assume we want to model an extraction event from the Stacey and Kramers (1975) 2nd stage model curve at 3200 Ma, with a new μ value of 5. First, the starting parameters need to be obtained. To do this, we can just filter the 'SK2model' dataframe for our starting time, t=3200 Ma, as follows:

```
SK2model <- modelcurve(3700:0)
new_start_params <- filter(SK2model, t == 3200)
new_start_params
```

```
     t           x           y           z
1 3200 12.44246395 14.04849329 32.31097509
```

The `new_start_params` values are now the starting composition for our 'NewSuperior' model below, using our desired μ value of 5. We can then use the `modelcurve()` function to generate the dataframe for this model and plot it on Figure 6.

```
new_Superior_model <- list(T1 = 3200, X1 = 12.442, Y1 = 14.048, Z1 = 32.311, Mu1=5)
new_Superior_curve <- modelcurve(3200:0, model = new_Superior_model)
```

The above steps can be repeated indefinitely to generate additional model 'stages' using the PbIso functions, although caution should be applied to whether this is geological reasonable. By plotting the Pb isotope data along with the model curves, we can begin to interrogate different Pb evolution models for what might be realistic for the source of Pb in sulphides from the Superior Province. Note that the 'NewSuperior' model is very much a hypothetical example to demonstrate how this can be done in the `PbIso` package, and is not being suggested here as a suitable model for Pb isotope evolution in the Superior Province.

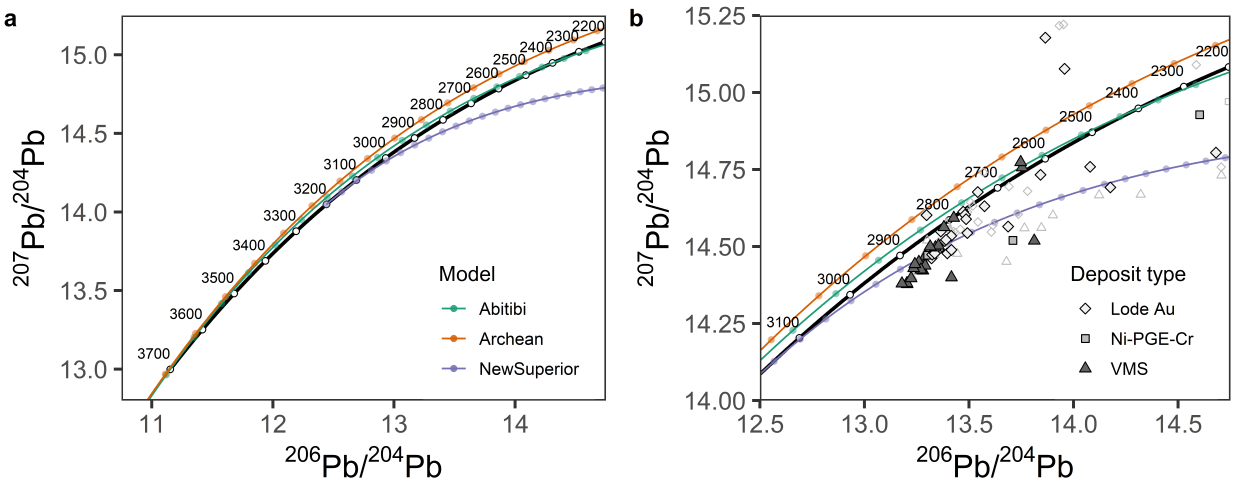
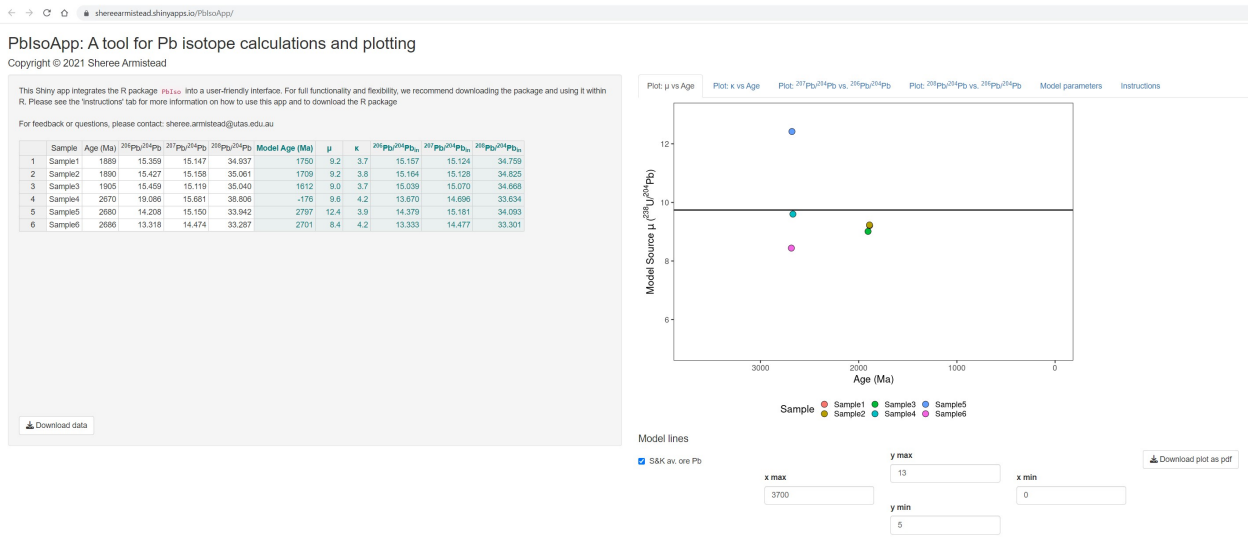


Figure 6: a) Stacey and Kramers (1975) model curve (black line) with three Pb evolution model curves, including two published models (Thorpe (1999) and Thorpe et al. (1992)), and a hypothetical NewSuperior model; and b) the same model curves as (a) but showing the extent of Superior Province Pb isotope data from selected ore deposits. Filled symbols are the least radiogenic value from each deposit and the unfilled symbols include all data from deposits. Circles along model curves are shown at 100 Ma intervals.

7 Shiny application

Using the above functions within R allows for flexibility in applying them to different datasets and using models that are appropriate for specific regions of interest. For a quick and easy to use approach, and to demonstrate some of the capabilities of `PbIso`, we have deployed the `PbIso` package into a Shiny application (see: https://shereearmistead.github.io/software/pbiso). The app allows users to add their own data by simply copying and pasting data into an excel-like spreadsheet. The app will then automatically generate the values for model age, model source μ ($^{238}U/^{204}Pb$), time-integrated κ ($^{232}Th/^{238}U$) and the three initial Pb isotope ratios. The app also plots these data onto a series of standard plots. These include; 1) model source μ ($^{238}U/^{204}Pb$) vs. age; 2) time-integrated κ ($^{232}Th/^{238}U$) vs. age; 3) $^{206}Pb/^{204}Pb$ vs. $^{207}Pb/^{204}Pb$; and 4) $^{206}Pb/^{204}Pb$ vs. $^{208}Pb/^{204}Pb$. The app also allows users to modify the model parameters such as T1, X1, Y1 and decay constants, or select from one of the included models.



	Sample	Age (Ma)	206Pb/204Pb	207Pb/204Pb	208Pb/204Pb	Model Age (Ma)	μ	κ	206Pb/204Pb$_m$	207Pb/204Pb$_m$	208Pb/204Pb$_m$
1	Sample1	1889	15.359	15.147	34.937	1750	9.2	3.7	15.157	15.124	34.759
2	Sample2	1890	15.427	15.158	35.061	1709	9.2	3.8	15.164	15.128	34.825
3	Sample3	1905	15.459	15.119	35.040	1612	9.0	3.7	15.039	15.070	34.668
4	Sample4	2670	19.086	15.681	38.806	-176	9.6	4.2	13.670	14.696	33.634
5	Sample5	2680	14.208	15.150	33.942	2797	12.4	3.9	14.379	15.181	34.093
6	Sample6	2686	13.318	14.474	33.287	2701	8.4	4.2	13.333	14.477	33.301

Figure 7: Screenshot of the PbIso shiny application. Left side is where the user can copy and paste data, and values are subsequently calculated. The right side has a series of tabs that include four commonly used Pb isotope plots and a tab for modifying the model parameters

The spreadsheet with newly calculated values can be exported as a .xlsx file by clicking the 'Download data' button. The downloaded spreadsheet contains two tabs, the 'DataOutput' tab contains the input data with the new calculations as shown on the left hand side of the Shiny App screen. The second tab in the .xlsx spreadsheet is the 'ModelParameters' tab and contains all of the values from the 'Model parameters' tab in the Shiny App that were used to generate the calculated values. The four plots can be downloaded separately as .pdf files by clicking the 'Download plot as pdf' button in the lower right corner. If the input sample data is 12 samples or less, these will be differentiated by colour and the sample ID included in a legend below the plots. For more than 12 samples, differentiating by colour becomes difficult and so these will simply be plotted as the same colour points. Optional lines and curves for different Pb isotopic models can be selected or deselected using the controls in the lower panel. The x and y axis limits can be specified either by typing a number or using the up/down arrows in the y min, y max, x min and x max fields. The two isotopic plots have the option of adding a 95% filled contour behind the data.

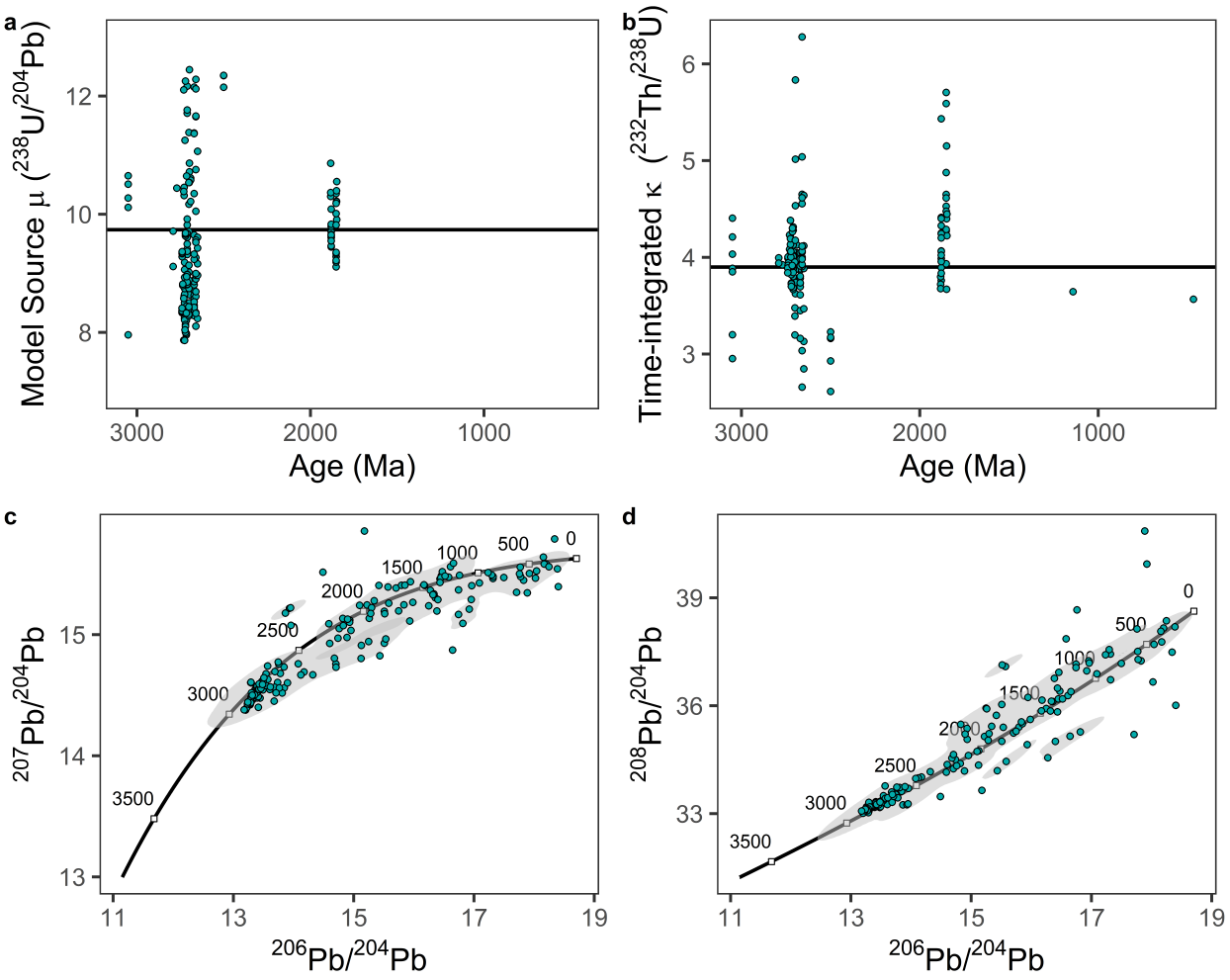


Figure 8: PbIso Shiny app plots that are produced based on user input data

8 Conclusion

We have provided a user-friendly R package for dealing with Pb isotope data. The functions allow flexibility in that they can be used in a very simple way accepting the default values for the Stacey and Kramers (1975) 2nd stage model, or the user can change individual parameters or apply a user-defined model. This toolset adds to the growing number of open-source software packages that help with processing and interpreting geological data. A preprint version of this manuscript is available through EarthArXiv (Armistead et al. (2021)). This package may continue to have features added beyond the publication of this manuscript, and all updates will be managed and maintained through: https://github.com/ShereeArmistead/PbIso.

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10 Code availability section

Name of the code/library: PbIso

Contact: sheree.armistead@utas.edu.au

Hardware requirements: …

Program language: R

Software required: R

Program size: 1MB

The source codes are available for downloading at the link: https://github.com/ShereeArmistead/PbIso

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