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. 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 complicated equations are implemented into simple R functions in the package PbIso. In addition, functions are provided for generating model curves, geochron lines, and time-dependent slopes. 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 application (https://shereearmistead.shinyapps.io/PbIsoApp/), which makes it easy for users without any R experience to use these calculations with their own data and to generate plots.

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1 Introduction

Pb isotopes are used in a range of science applications including ore geology, plate tectonics, studies of early Earth evolution and archaeometry. Despite their widespread applications, there are few tools readily available to users, to calculate and plot these data. In recent years, tools have been developed and adapted for various isotopic and geochemical datasets, including, IsoplotR (Vermeesch 2018) and provenance (Vermeesch, Resentini, and Garzanti 2016) in R, and pyrolite (Williams et al. 2020) in Python. Some of these have a linked graphic user interface (GUI), which allows users of various programming experience to use the tools. 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 the geosciences move toward big data analytics.

Typically Pb isotope calculations 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 impossible. 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 isotopes 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 flexibility by the optional input values depending on different starting model parameters.

1.1 Using `PbIso`

We introduce an R package `PbIso` which 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, geochron lines and y-intercepts, and time-dependent slopes. Using the package within R allows more 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.

Alternatively, we have implemented some of the basic features of `PbIso` into an online Shiny application (https://shereearmistead.shinyapps.io/PbIsoApp/), which requires no knowledge of R, making this very accessible for many 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 .csv 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 ($^{232}Th/^{238}U$). Four basic plots are automatically generated in the Shiny application based on the user data, and can be downloaded as .pdf figures.

All of 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. These values can be overridden in R if an alternative model (e.g. Stacey and Kramers (1975) 1st stage or others) is preferred.

Table 1: Default model parameters used in `PbIso` functions. These can be manually 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 (n.d.)
U8U5	Present-day $^{238}U/^{235}U$ ratio	137.88	Stacey and Kramers (1975)

1.1.1 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)
```

1.1.2 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 default parameters in all `PbIso` functions are based on the Stacey and Kramers (1975) 2nd stage model, however, we will show how these can be changed.

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

```
Calc64(2700)
```

```
## [1] 13.63662
```

The optional parameters, in this case, T1, X1, Mu1, which are the model starting parameters, can also be specified:

```
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 3 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.

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

Function	Required inputs	Optional inputs
Calc64()	t	T1, X1, Mu1, L8, model
Calc74()	t	T1, Y1, Mu1, U8U5, L5, model
Calc84()	t	T1, Z1, W1, L2, model
CalcModAge()	x, y	T1, X1, Y1, U8U5, L5, L8, model
CalcMu()	t, x, y	T1, X1, Y1, U8U5, L5, L8, model
CalcKa()	t, z, x	T1, X1, Z1, L2, L8, model
Calc64in()	t, x, y	T1, X1, Y1, U8U5, L5, L8, model
Calc74in()	t, x, y	T1, X1, Y1, U8U5, L5, L8, model
Calc84in()	t, x, y, z	T1, X1, Y1, Z1, U8U5, L5, L8, L2, model
modelcurve()	t:t	T1, X1, Y1, Z1, Mu1, W1, U8U5, L5, L8, L2, model

Function	Required inputs	Optional inputs
geochron76slope()	t	T1, X1, Y1, Mu1, U8U5, L5, L8, model
geochron76yint()	t	T1, X1, Y1, Mu1, U8U5, L5, L8, model
geochron86slope()	t	T1, X1, Z1, Mu1, W1, L8, L2, model
geochron86yint()	t	T1, X1, Z1, Mu1, W1, L8, L2, model

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

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

```
## [1] 12.98544
```

Alternatively, users may define their own models, which is particularly useful if this is needed for multiple calculations. To define your own model:

```
my_model <- list(T1 = 4000, X1 = 9, Y1 = 10, Z1 = 30, Mu1 = 8, W1 = 33)
Calc64(2700, model = my_model)
```

```
## [1] 11.71732
```

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 functions, it is best to include parameters required for all functions of interest.

Models that we have included as options are given in table 3.

Table 3: Predefined models that can be used in the functions by specifying model = SK1, for example

Model	R name	T1	X1	Y1	Z1	Mu1	W1
Stacey and Kramers (1975) single stage model	SK1	4570	9.307	10.294	29.487	7.19	33.21
Stacey and Kramers (1975) 2nd stage model	SK2	3700	11.152	12.998	31.23	9.74	36.84
Zartman and Doe (1981) mantle	ZDM	4000	10.32	12.12	30.56	8.316	29.211
Zartman and Doe (1981) upper crust	ZDUC	4000	10.32	12.12	30.56	13.301	45.34
Zartman and Doe (1981) lower crust	ZDLC	4000	10.32	12.12	30.56	6.364	37.403

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 isotopic compositions of the environments in which a mineral/rock formed. The abundance of the radiogenic isotopes increases with time (figure 1), so comparison of 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).

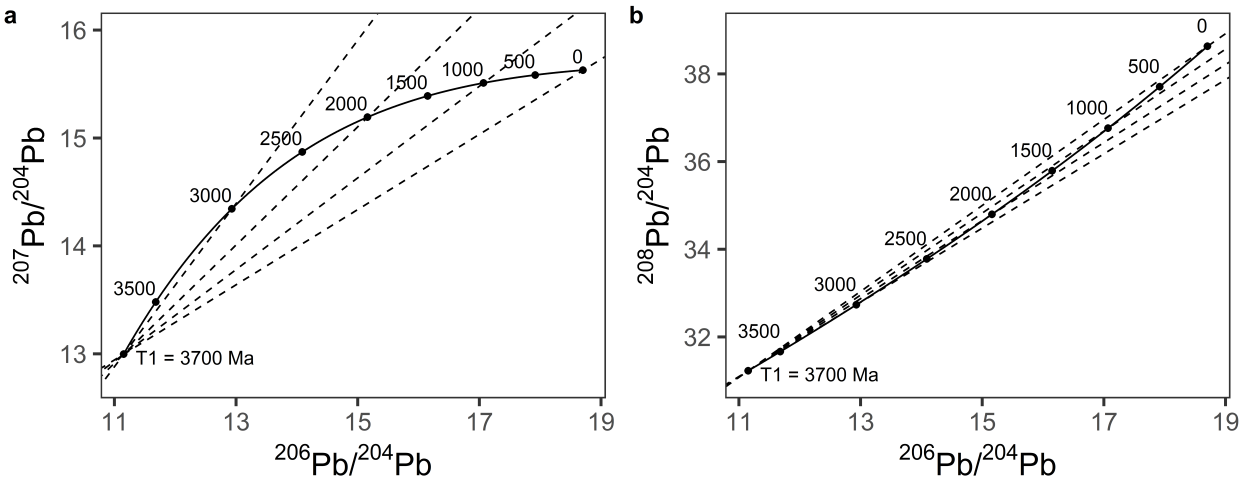

Figure 1: Pb isotopic evolution through time, a) evolution of $^{206}Pb/^{204}Pb$ and $^{207}Pb/^{204}Pb$; b) evolution of $^{206}Pb/^{204}Pb$ and $^{208}Pb/^{204}Pb$. Isochrons for 3000 Ma, 2000 Ma, 1000 Ma and 0 Ma shown as dashed lines in both plots. See section 3 for how to generate the model curves and isochron lines shown here.

1.3 The evolution of radiogenic Pb isotopes with time

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

$$\left(\frac{^{206}Pb}{^{204}Pb}\right)_t = \left(\frac{^{206}Pb}{^{204}Pb}\right)_{T_1} + \mu_1(e^{\lambda_8 T_1} - e^{\lambda_8 t}) \quad (1)$$

$$\left(\frac{^{207}Pb}{^{204}Pb}\right)_t = \left(\frac{^{207}Pb}{^{204}Pb}\right)_{T_1} + \frac{\mu_1}{137.88}(e^{\lambda_5 T_1} - e^{\lambda_5 t}) \quad (2)$$

$$\left(\frac{^{208}Pb}{^{204}Pb}\right)_t = \left(\frac{^{208}Pb}{^{204}Pb}\right)_{T_1} + \omega_1(e^{\lambda_2 T_1} - e^{\lambda_2 t}) \quad (3)$$

Note that ω ($^{232}Th/^{204}Pb$) in equaton (3) can also be expressed as $\mu * \kappa$ ($^{238}U/^{204}Pb$ * $^{232}Th/^{238}U$).

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.

E.g. 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 2 for the optional parameters for each of these functions to allow maximum flexibility.

1.4 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 2, 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:

$$\frac{\frac{^{207}Pb}{^{204}Pb}_{t_{sample}} - \frac{^{207}Pb}{^{204}Pb}_{T_1}}{\frac{^{206}Pb}{^{204}Pb}_{t_{sample}} - \frac{^{206}Pb}{^{204}Pb}_{T_1}} = \frac{1}{137.88} * \frac{e^{\lambda_5 T_1} - e^{\lambda_5 t_{sample}}}{e^{\lambda_8 T_1} - e^{\lambda_8 t_{sample}}} \tag{4}$$

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
```

The model age is sensitive to the starting composition used. In general we advise against using the model age, especially if independent age constraints are available, as the calculation is very sensitive to radiogenic samples and the model parameters used (e.g. Stacey and Kramers (1975) used here). Nevertheless, the model age can provide important information when comparing samples from similar regions or when absolute ages are not available.

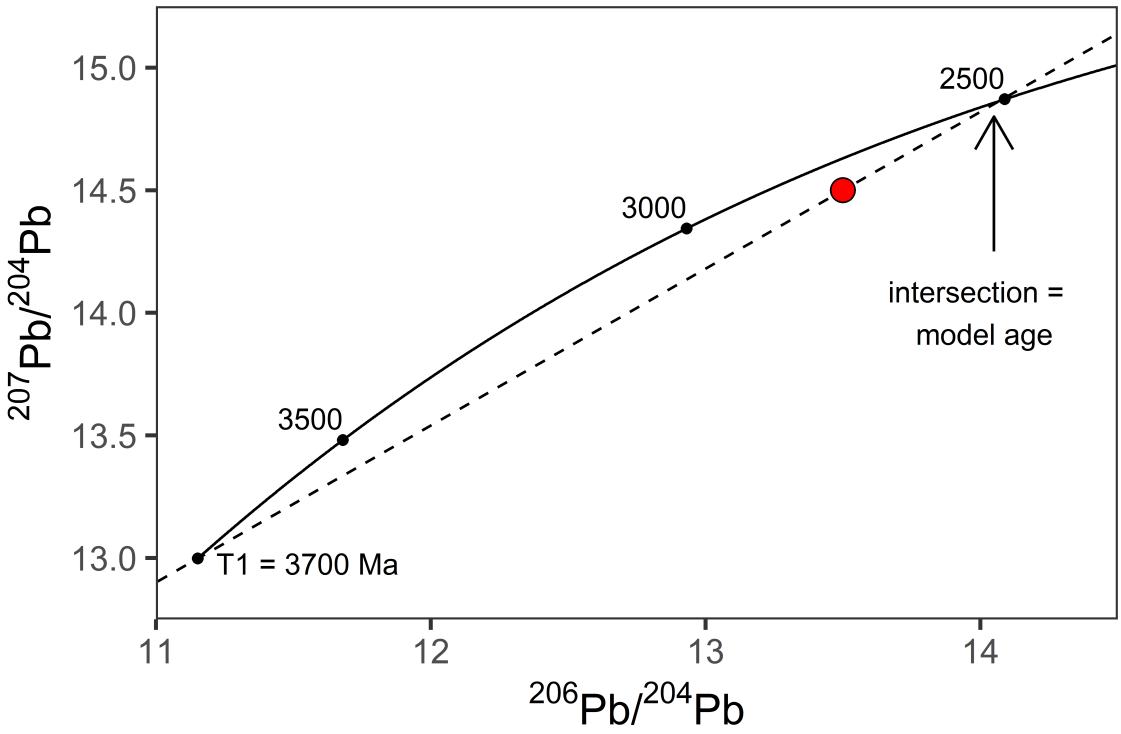

Figure 2: Hypothetical sample (red circle) showing that a line connected between a model starting composition and the sample composition, will project onto the Stacey and Kramers (1975) model curve at the corresponding model age

1.5 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's often more useful to compare the model source μ ($^{238}U/^{204}Pb$) rather than the Pb isotope ratios, as it 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 a line on a $^{206}Pb/^{204}Pb$ vs $^{207}Pb^{204}Pb$ plot (red line in figure 3). The least radiogenic samples will fall near the lower left end of this line, while more radiogenic samples will fall near the upper right end. One way to calculate a rock's age is to define a line joining multiple sample analyses. The slope of this line is directly related to its 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:

$$m_{sample} = \frac{e^{\lambda_5 t_{sample}} - 1}{137.88(e^{\lambda_8 t_{sample}} - 1)} \tag{5}$$

This is implemented in `PbIso` by the function `mslope()`, which takes the argument t and additional optional arguments (see documentation). Substituting equation (5) into the following equation gives us the model source μ ($^{238}U/^{204}Pb$):

$$\mu = \frac{m_{sample}(X_1 - X_{sample}) + Y_{sample} - Y_1}{\frac{e^{\lambda_5 T_1} - e^{\lambda_5 t_{sample}}}{137.88} - m_{sample}(e^{\lambda_8 T_1} - e^{\lambda_8 t_{sample}})} \tag{6}$$

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 known age 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 3. The intersection of the age dependent slope (m_{sample}; red line in figure 3), the geochron associated with the sample age (2700 Ma in this case), and the model source μ curve of 8.43 (blue curve in figure 3), 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 1.7 for calculating initial Pb isotope ratios, and section 3 for generating the model curves and geochron lines shown in figure 3.

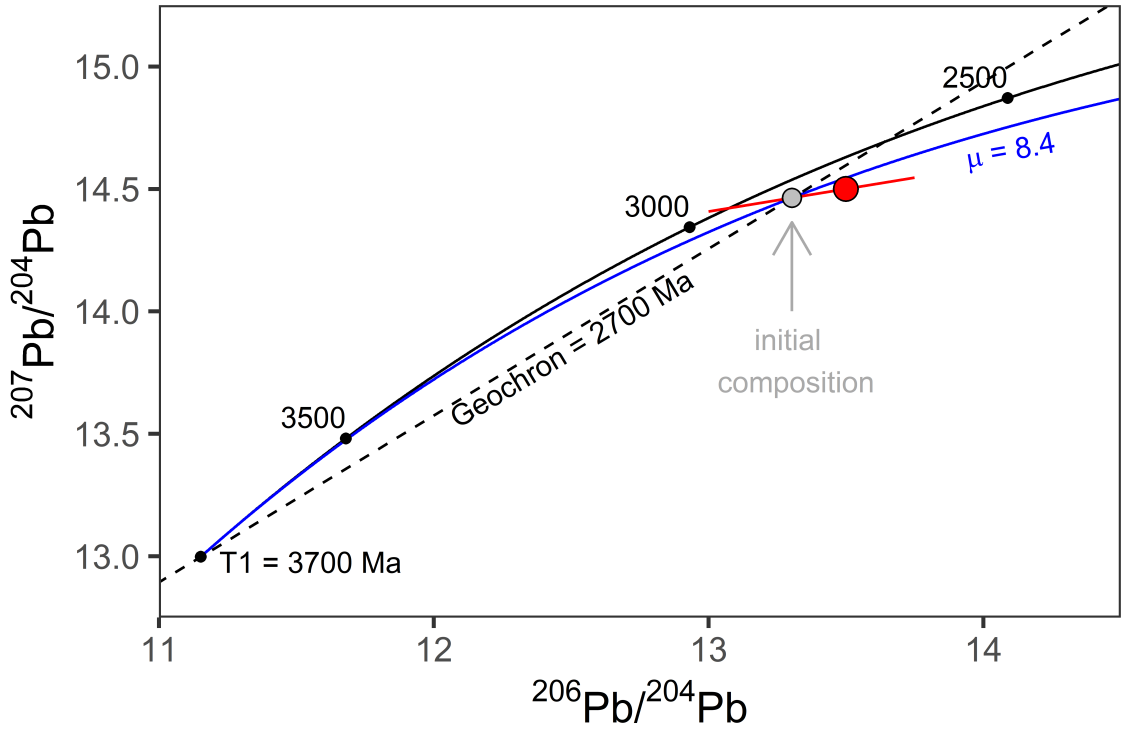

Figure 3: The same sample as the previous plot, but this time with additional parameters that can be calculated when the sample age is known.

1.6 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:

$$\kappa = \frac{Z_{sample} - Z_1}{X_{sample} - X_1} \div \frac{e^{\lambda_2 T_1} - e^{\lambda_2 t_{sample}}}{e^{\lambda_8 T_1} - e^{\lambda_8 t_{sample}}} \tag{7}$$

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.

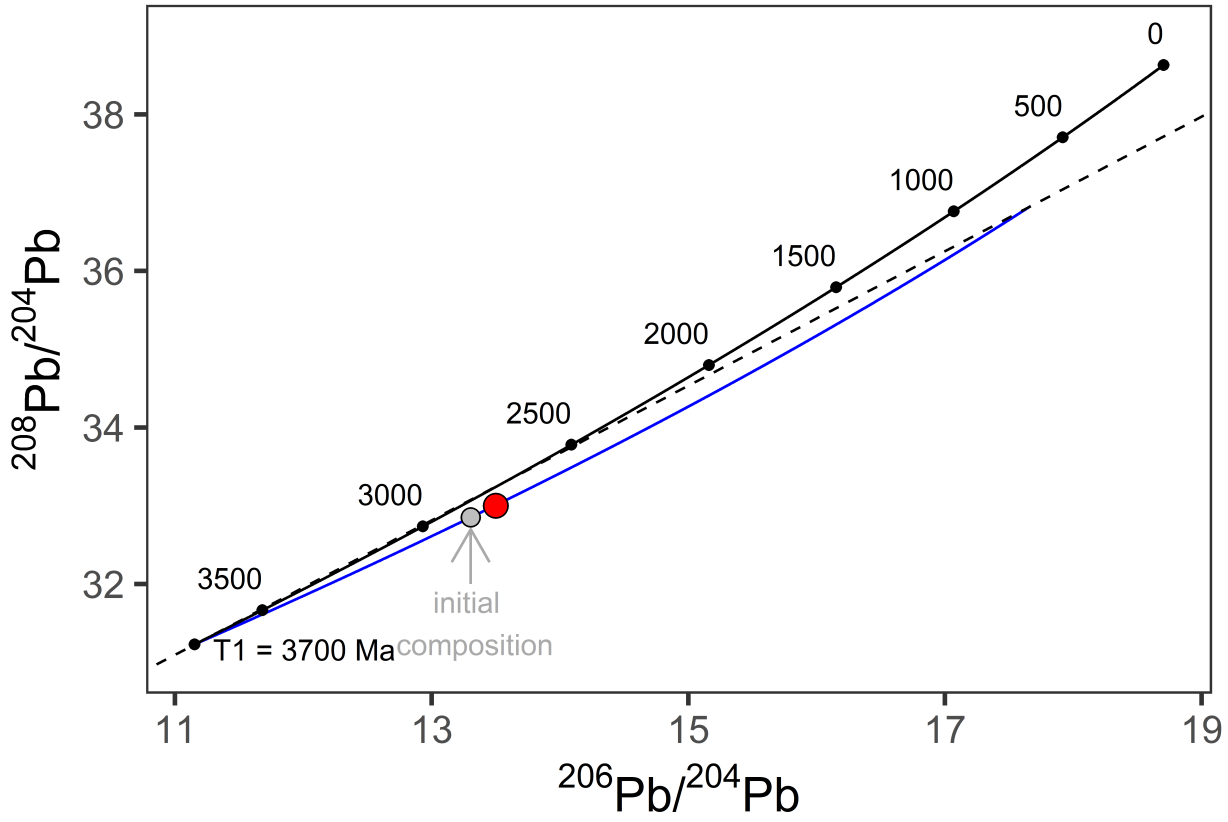

Figure 4: Plot of $^{208}Pb/^{204}Pb$ vs $^{206}Pb/^{204}Pb$ with the same hypothetical sample as previous plots, with the 2700 Ma isochron (dashed line), corresponding kappa curve (blue) and initial isotope composition (grey circle)

1.7 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.

$$\left(\frac{^{206}Pb}{^{204}Pb}\right)_{initial} = \left(\frac{^{206}Pb}{^{204}Pb}\right)_{T_1} + \mu_{sample}(e^{\lambda_8 T_1} - e^{\lambda_8 t}) \quad (8)$$

$$\left(\frac{^{207}Pb}{^{204}Pb}\right)_{initial} = \left(\frac{^{207}Pb}{^{204}Pb}\right)_{T_1} + \frac{\mu_{sample}}{137.88}(e^{\lambda_5 T_1} - e^{\lambda_5 t}) \quad (9)$$

$$\left(\frac{^{208}Pb}{^{204}Pb}\right)_{initial} = \left(\frac{^{208}Pb}{^{204}Pb}\right)_{T_1} + \omega_{sample}(e^{\lambda_2 T_1} - e^{\lambda_2 t}) \quad (10)$$

The above equations are identical to the Pb isotope equations in section 1.3, so we could use the same functions, but substitute the sample μ in. However, for simplicity we have added the functions `Calc64in()`, `Calc74in()` and `Calc84in()` to calculate the initial Pb isotope ratios directly. So 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
```

2 Applying `PbIso` functions to a dataset

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 random subset of 200 samples from the DepIso databse (http://thera2.usask.ca:8092/). We briefly document below how to apply functions to this dataset.

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 4.

Table 4: First six rows of sample data input with sample information and measured Pb isotope ratios

DepositName	age	Pb64	Pb74	Pb84
Buchans - Oriental	465	17.823	15.491	37.610
Hood River - Gondor	2668	13.441	14.538	33.274
Tasmania - Fossey	500	18.383	15.612	38.223
Mattagami - Orchan	2725	13.130	14.324	32.996
Tasmania - Elliott Bay	500	18.085	15.600	37.945
Buchans - Lucky Strike	465	17.815	15.489	37.606

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:

```
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 now shown in table 5:

Table 5: First six rows of dataframe after the `PbIso` functions have been applied

DepositName	age	Pb64	Pb74	Pb84	Mu	Ka	Pb64in	Pb74in	Pb84in	ModAge
Buchans - Oriental	465	17.823	15.491	37.610	9.4	3.8	17.975	15.484	37.494	384
Hood River - Gondor	2668	13.441	14.538	33.274	8.7	3.9	13.710	14.537	33.269	2663
Tasmania - Fossey	500	18.383	15.612	38.223	9.7	3.8	17.918	15.586	37.777	207
Mattagami - Orchan	2725	13.130	14.324	32.996	7.7	3.9	13.579	14.312	32.937	2652
Tasmania - Elliott Bay	500	18.085	15.600	37.945	9.8	3.8	17.918	15.592	37.803	407
Buchans - Lucky Strike	465	17.815	15.489	37.606	9.3	3.8	17.975	15.482	37.493	386

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

3 Plotting parameters

In addition to plotting sample data, there are also several plotting features that are usually plotted such as model curves and geochron lines.

3.1 Model curves

The data for model curves can be produced using the `modelcurve()` function in `PbIso`. This function takes the arguments for time (t), as well as optional arguments for model starting composition, μ_1, ω_1 values and decay constants (see package documentation for further details). 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 (1), (2) and (3) in section 1.3.

To generate a simple (Stacey and Kramers 1975) 2nd stage model curve, only the time (t) is needed in the function `modelcurve()`. The dataframe 'SKcurve' is used to produce the solid black curves in 1. The 'SKcurve' dataframe will have 3701 rows of data, each corresponding to a 1 Ma time interval (table 6).

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

Table 6: First six 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

The `modelcurve()` function can be used to produce model curves with different model parameters. For example the blue curve in figure 3, which corresponds to a model μ of 8.43 is generated by the following:

```
bluecurve <- modelcurve(0:3700, Mu1 = 8.43)
```

The `modelcurve()` function can be used to produce model curves over different time ranges with optional arguments (see `PbIso` documentation for more information). For example, in the code below, 'mc1' is the (Stacey and Kramers 1975) 1st stage model from 4570 Ma to 3700 Ma, 'm2' is the (Stacey and Kramers 1975) 2nd stage model from 3700 Ma to present, and 'mc3' is a hypothetical model using (Stacey and Kramers 1975) 2nd stage starting composition but with a μ_1 of 8. These three curves are shown in figure 5.

```
mc1 <- modelcurve(3700:4570, model = SK1)
mc2 <- modelcurve(0:3700)
mc3 <- modelcurve(0:3700, Mu1 = 8)
```

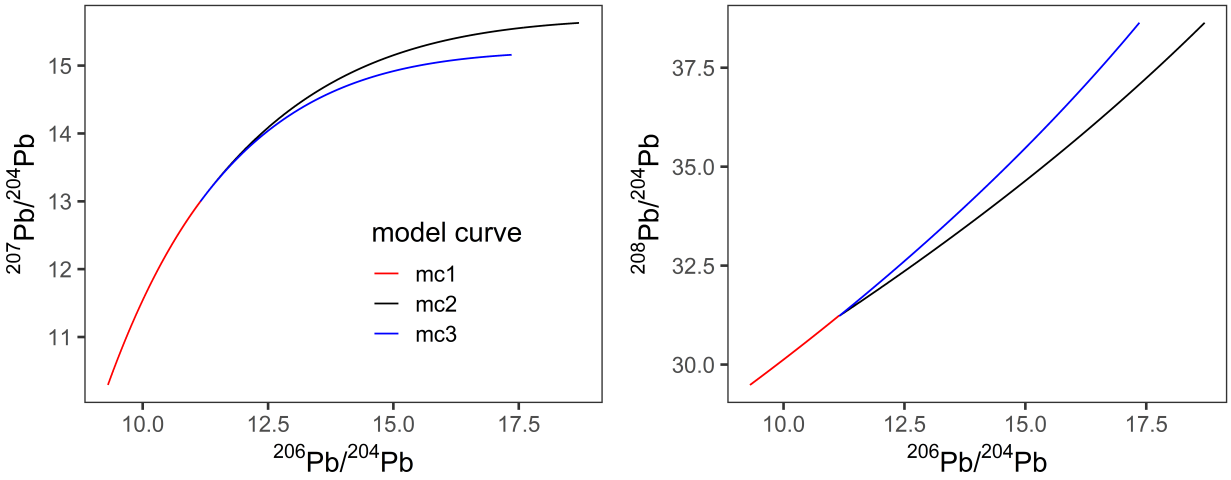

Figure 5: Model curves generated using the `modelcurve()` function for (Stacey and Kramers 1975) 1st stage (mc1), (Stacey and Kramers 1975) 2nd stage (mc2) and a hypothetical sample with Mu=8 (mc3)

3.2 Geochron lines

To generate geochron lines for a given time (t), the slope and y-intercept are needed. To calculate the slope of a geochron line on a $^{206}Pb/^{204}Pb$ vs. $^{207}Pb/^{204}Pb$ plot, the function `geochron76slope()` is used, which takes the argument t as well as optional arguments (see documentation). The associated y-intercept for that geochron is given by the function `geochron76yint()`. These can then be used to plot the geochron line along with a model curve. Similarly, to calculate the geochron slope and y-intercept on a $^{206}Pb/^{204}Pb$ vs. $^{208}Pb/^{204}Pb$ plot, the functions `geochron86slope()` and `geochron86yint()` can be used. Geochron lines in figure 1 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 geochron lines, or the function can be called directly, for example by using `abline(a = geochron76yint(2700), b = geochron76slope(2700))` in base R plotting, or `geom_abline(slope = geochron76slope(2700), intercept = geochron76yint(2700))` in ggplot. To use this function to generate the slope and y-intercept of a geochron at time 2700 Ma:

```
geochron76slope(2700)
```

```
## [1] 0.681
```

```
geochron76yint(2700)
```

```
## [1] 5.4
```

```
geochron86slope(2700)
```

```
## [1] 0.86
```

```
geochron86yint(2700)
```

```
## [1] 21.6
```

4 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 the capabilities of `PbIso`, we have deployed the `PbIso` package into a Shiny application (https://shereearmistead.shinyapps.io/PbIsoApp/). 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. We advise caution before modifying these values unless there are good model constraints available.

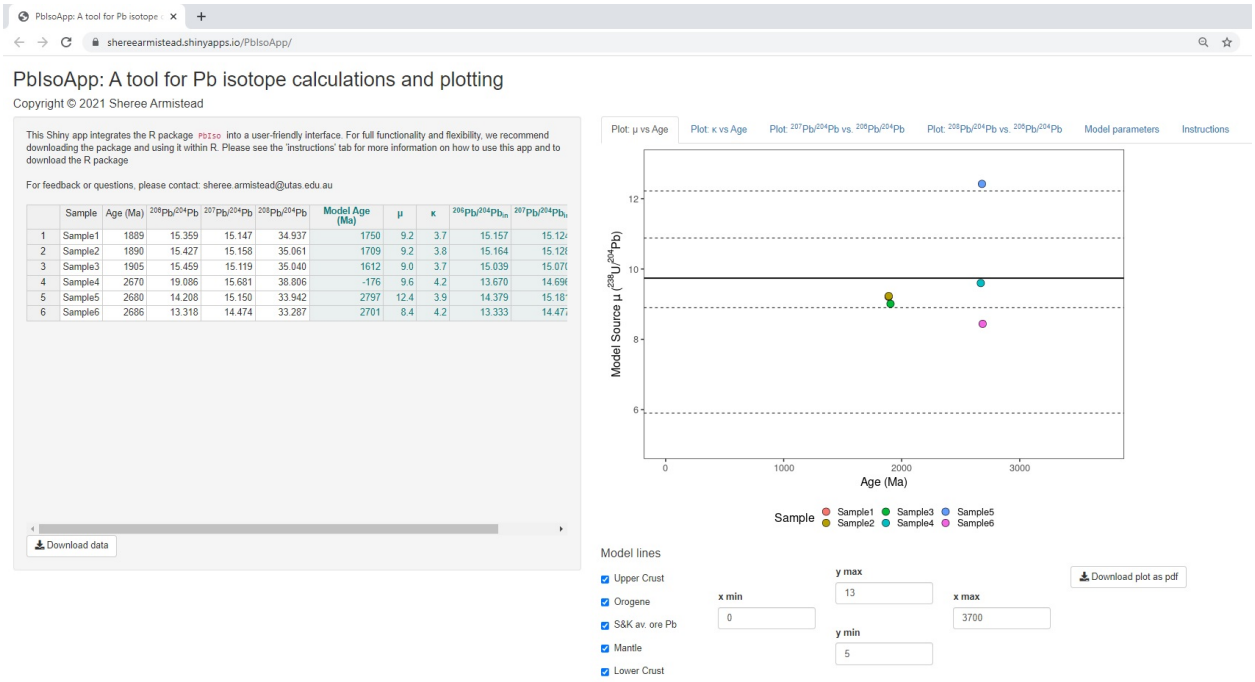

Figure 6: Screenshot of the PbIso shiny application. Left side is where the user can copy and paste data, and values are subsequently calculated. The right side has a series of tabs that include four commonly used Pb isotope plots and a tab for modifying the model parameters

The spreadsheet with newly calculated values can be exported as a .csv file by clicking the 'Download data' button. 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.

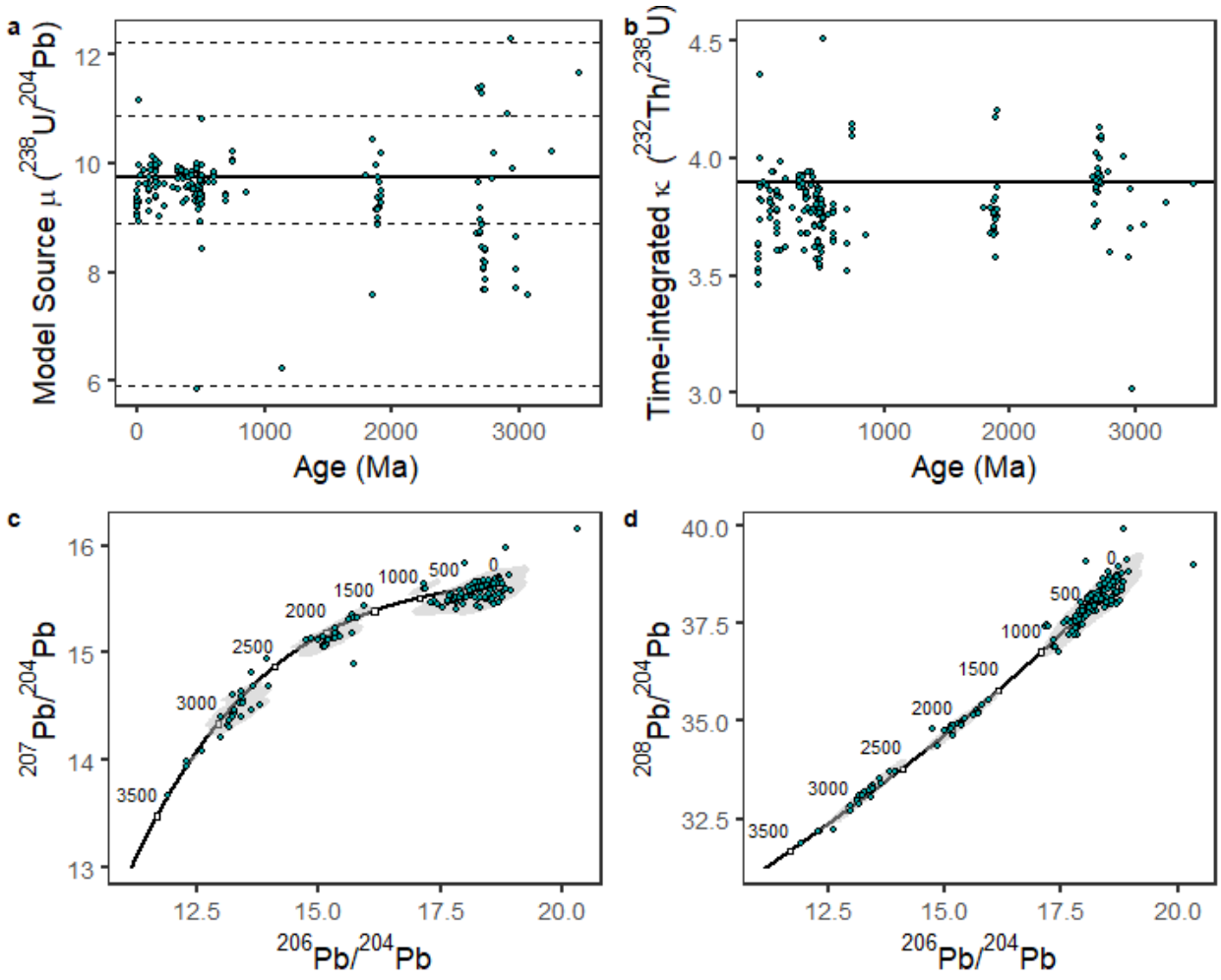

Figure 7: PbIso Shiny app plots that are produced based on user input data

5 Conclusion

We have provided a user-friendly R package for dealing with Pb isotope data. The functions allow maximum 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. 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 .

6 Acknowledgments

- Metal Earth publication number ####TBA
- Ryan Ickert and Michael Anenburg are thanked for feedback that improved the Shiny Application

7 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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