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

Sheree E Armistead$^{1,2,3,*}$ Bruce M Eglington$^4$ Sally J Pehrsson$^1$

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 $\mu$ ($^{238}\text{U}/^{204}\text{Pb}$), time-integrated $\kappa$ ($^{232}\text{Th}/^{238}\text{U}$), 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.

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 (Vermeech 2018) and provenance (Vermeech, 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 $\mu$ ($\text{^{238}U}/\text{^{204}Pb}$) and time-integrated $\kappa$ ($\text{^{232}Th}/\text{^{238}U}$), 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, $\text{^{206}Pb}/\text{^{204}Pb}$, $\text{^{207}Pb}/\text{^{204}Pb}$, and $\text{^{208}Pb}/\text{^{204}Pb}$ 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 $\mu$ ($\text{^{238}U}/\text{^{204}Pb}$) and time-integrated $\kappa$ ($\text{^{232}Th}/\text{^{238}U}$). 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)), $x$ ($\text{^{206}Pb}/\text{^{204}Pb}$), $y$ ($\text{^{207}Pb}/\text{^{204}Pb}$) and $z$ ($\text{^{208}Pb}/\text{^{204}Pb}$) 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>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Default value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1</td>
<td>Model start time (Ma)</td>
<td>3700</td>
<td>Stacey and Kramers (1975)</td>
</tr>
<tr>
<td>X1</td>
<td>$\text{^{206}Pb}/\text{^{204}Pb}$ model starting composition</td>
<td>11.152</td>
<td>Stacey and Kramers (1975)</td>
</tr>
<tr>
<td>Y1</td>
<td>$\text{^{207}Pb}/\text{^{204}Pb}$ model starting composition</td>
<td>12.998</td>
<td>Stacey and Kramers (1975)</td>
</tr>
<tr>
<td>Z1</td>
<td>$\text{^{208}Pb}/\text{^{204}Pb}$ model starting composition</td>
<td>31.23</td>
<td>Stacey and Kramers (1975)</td>
</tr>
<tr>
<td>Mu1</td>
<td>$\text{^{238}U}/\text{^{204}Pb}$ model ($\mu_1$)</td>
<td>9.74</td>
<td>Stacey and Kramers (1975)</td>
</tr>
<tr>
<td>Ka1</td>
<td>$\text{^{232}Th}/\text{^{238}U}$ model ($\kappa_1$)</td>
<td>3.78</td>
<td>Stacey and Kramers (1975)</td>
</tr>
<tr>
<td>W1</td>
<td>$\text{^{232}Th}/\text{^{204}Pb}$ model ($\omega_1$)</td>
<td>36.84</td>
<td>Stacey and Kramers (1975)</td>
</tr>
<tr>
<td>L5</td>
<td>$\text{^{235}U}$ decay constant ($\lambda_5$)</td>
<td>9.8485 * $10^{-10}$</td>
<td>Jaffey et al. (1971)</td>
</tr>
<tr>
<td>L8</td>
<td>$\text{^{238}U}$ decay constant ($\lambda_8$)</td>
<td>1.55125 * $10^{-10}$</td>
<td>Jaffey et al. (1971)</td>
</tr>
<tr>
<td>L2</td>
<td>$\text{^{232}Th}$ decay constant ($\lambda_2$)</td>
<td>0.49475 * $10^{-10}$</td>
<td>Le Roux and Glendenin (n.d.)</td>
</tr>
<tr>
<td>U8U5</td>
<td>Present-day $\text{^{238}U}/\text{^{235}U}$ ratio</td>
<td>137.88</td>
<td>Stacey and Kramers (1975)</td>
</tr>
</tbody>
</table>

### 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

<table>
<thead>
<tr>
<th>Function</th>
<th>Required inputs</th>
<th>Optional inputs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calc64()</td>
<td>t</td>
<td>T1, X1, Mu1, L8, model</td>
</tr>
<tr>
<td>Calc74()</td>
<td>t</td>
<td>T1, Y1, Mu1, U8U5, L5, model</td>
</tr>
<tr>
<td>Calc84()</td>
<td>t</td>
<td>T1, Z1, W1, L2, model</td>
</tr>
<tr>
<td>CalcModAge()</td>
<td>x, y</td>
<td>T1, X1, Y1, U8U5, L5, L8, model</td>
</tr>
<tr>
<td>CalcMu()</td>
<td>t, x, y</td>
<td>T1, X1, Y1, U8U5, L5, L8, model</td>
</tr>
<tr>
<td>CalcKa()</td>
<td>t, z, x</td>
<td>T1, X1, Z1, L2, L8, model</td>
</tr>
<tr>
<td>Calc64in()</td>
<td>t, x, y</td>
<td>T1, X1, Y1, U8U5, L5, L8, model</td>
</tr>
<tr>
<td>Calc74in()</td>
<td>t, x, y</td>
<td>T1, X1, Y1, U8U5, L5, L8, model</td>
</tr>
<tr>
<td>Calc84in()</td>
<td>t, x, y, z</td>
<td>T1, X1, Y1, Z1, U8U5, L5, L8, L2, model</td>
</tr>
<tr>
<td>modelcurve()</td>
<td>t:t</td>
<td>T1, X1, Y1, Z1, Mu1, W1, U8U5, L5, L8, L2, model</td>
</tr>
</tbody>
</table>
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>
<thead>
<tr>
<th>Model</th>
<th>R name</th>
<th>T1</th>
<th>X1</th>
<th>Y1</th>
<th>Z1</th>
<th>Mu1</th>
<th>W1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stacey and Kramers (1975) single stage model</td>
<td>SK1</td>
<td>4570</td>
<td>9.307</td>
<td>10.294</td>
<td>29.487</td>
<td>7.19</td>
<td>33.21</td>
</tr>
<tr>
<td>Stacey and Kramers (1975) 2nd stage model</td>
<td>SK2</td>
<td>3700</td>
<td>11.152</td>
<td>12.998</td>
<td>31.23</td>
<td>9.74</td>
<td>36.84</td>
</tr>
<tr>
<td>Zartman and Doe (1981) mantle</td>
<td>ZDM</td>
<td>4000</td>
<td>10.32</td>
<td>12.12</td>
<td>30.56</td>
<td>8.316</td>
<td>29.211</td>
</tr>
<tr>
<td>Zartman and Doe (1981) upper crust</td>
<td>ZDUC</td>
<td>4000</td>
<td>10.32</td>
<td>12.12</td>
<td>30.56</td>
<td>13.301</td>
<td>45.34</td>
</tr>
<tr>
<td>Zartman and Doe (1981) lower crust</td>
<td>ZDLC</td>
<td>4000</td>
<td>10.32</td>
<td>12.12</td>
<td>30.56</td>
<td>6.364</td>
<td>37.403</td>
</tr>
</tbody>
</table>

1.2 Pb isotope systematics

The decay of $^{238}\text{U}$ to $^{206}\text{Pb}$; $^{235}\text{U}$ to $^{207}\text{Pb}$ and $^{232}\text{Th}$ to $^{208}\text{Pb}$ and the non-radiogenic $^{204}\text{Pb}$ 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 $^{206}\text{Pb}/^{204}\text{Pb}$, $^{207}\text{Pb}/^{204}\text{Pb}$, and $^{208}\text{Pb}/^{204}\text{Pb}$ ratios. To allow easy comparison of samples across broad time periods, the model source $\mu$ ($^{238}\text{U}/^{204}\text{Pb}$) and $\kappa$ ($^{232}\text{Th}/^{238}\text{U}$) 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).
1.3 The evolution of radiogenic Pb isotopes with time

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

\[
\frac{^{206}\text{Pb}}{^{204}\text{Pb}}_t = \left( \frac{^{206}\text{Pb}}{^{204}\text{Pb}} \right)_{T_1} + \mu_1 (e^{\lambda_8 T_1} - e^{\lambda_8 t})
\]

\[
\frac{^{207}\text{Pb}}{^{204}\text{Pb}}_t = \left( \frac{^{207}\text{Pb}}{^{204}\text{Pb}} \right)_{T_1} + \frac{\mu_1}{137.88} (e^{\lambda_5 T_1} - e^{\lambda_5 t})
\]

\[
\frac{^{208}\text{Pb}}{^{204}\text{Pb}}_t = \left( \frac{^{208}\text{Pb}}{^{204}\text{Pb}} \right)_{T_1} + \omega_1 (e^{\lambda_2 T_1} - e^{\lambda_2 t})
\]

Note that \( \omega (^{232}\text{Th}/^{204}\text{Pb}) \) in equation (3) can also be expressed as \( \mu \cdot \kappa (^{238}\text{U}/^{204}\text{Pb} \cdot ^{232}\text{Th}/^{238}\text{U}) \).

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 \( ^{206}\text{Pb}/^{204}\text{Pb}, ^{207}\text{Pb}/^{204}\text{Pb} \) and \( ^{208}\text{Pb}/^{204}\text{Pb} \) 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
## [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:

\[
\frac{^{207}Pb}{^{204}Pb}_{t_{sample}} - \frac{^{207}Pb}{^{204}Pb}_{T1} = \frac{1}{137.88} \left( e^{\lambda_5 T1} - e^{\lambda_5 t_{sample}} \right) - \frac{^{206}Pb}{^{204}Pb}_{T1} - \frac{^{207}Pb}{^{204}Pb}_{t_{sample}}
\]

(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 \texttt{uniroot()} function in the \texttt{stats} package in R. This is implemented in \texttt{PbIso} using the \texttt{CalcModAge()} function. Only the \(^{206}\text{Pb}/^{204}\text{Pb}\) (x) and \(^{207}\text{Pb}/^{204}\text{Pb}\) (y) ratios are needed to solve for the model age.

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

\texttt{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 $\mu$ ($^{238}\text{U}/^{204}\text{Pb}$)

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 $\mu$ ($^{238}\text{U}/^{204}\text{Pb}$) 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 $^{206}\text{Pb}/^{204}\text{Pb}$ vs $^{207}\text{Pb}/^{204}\text{Pb}$ 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 ($t_{\text{sample}}$) is defined by:

$$m_{\text{sample}} = \frac{e^{\lambda_{t}t_{\text{sample}}} - 1}{137.88(e^{\lambda_{t}t_{\text{sample}}} - 1)}$$

(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 $\mu$ ($^{238}\text{U}/^{204}\text{Pb}$):

$$\mu = \frac{m_{\text{sample}}(X_{1} - X_{\text{sample}}) + Y_{\text{sample}} - Y_{1}}{e^{\lambda_{t}T_{1} - e^{\lambda_{t}t_{\text{sample}}}} - m_{\text{sample}}(e^{\lambda_{t}T_{1}} - e^{\lambda_{t}t_{\text{sample}}})}$$

(6)
This is implemented in PbIso by the function CalcMu(), using the sample age (t) in Ma, $^{206}\text{Pb}/^{204}\text{Pb}$ (x) and $^{207}\text{Pb}/^{204}\text{Pb}$ (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; $^{206}\text{Pb}/^{204}\text{Pb} = 13.5$, and $^{207}\text{Pb}/^{204}\text{Pb} = 14.5$, and accepting the default Stacey and Kramers (1975) model values, we can calculate the model source $\mu$ 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 ($m_{\text{sample}}$; red line in figure 3), the geochron associated with the sample age (2700 Ma in this case), and the model source $\mu$ 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 $\kappa$ ($^{232}\text{Th}/^{238}\text{U}$)

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

The time-integrated $\kappa$ ($^{232}\text{Th}/^{238}\text{U}$) is given by:
\[ \kappa = \frac{Z_{\text{sample}} - Z_1}{X_{\text{sample}} - X_1} \cdot \frac{e^{\lambda_2 T_1} - e^{\lambda_2 t_{\text{sample}}}}{e^{\lambda_8 T_1} - e^{\lambda_8 t_{\text{sample}}}} \]  

(7)

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

\[ \text{CalcKa}(2700, 33, 13.5) \]

## 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.
\[
\left( \frac{^{206}Pb}{^{204}Pb} \right)_{initial} = \left( \frac{^{206}Pb}{^{204}Pb} \right)_{T_i} + \mu_{sample} (e^{\lambda_3 T_i} - e^{\lambda_{84} T_i}) \tag{8}
\]

\[
\left( \frac{^{207}Pb}{^{204}Pb} \right)_{initial} = \left( \frac{^{207}Pb}{^{204}Pb} \right)_{T_i} + \frac{\mu_{sample}}{137.88} (e^{\lambda_5 T_i} - e^{\lambda_{84} T_i}) \tag{9}
\]

\[
\left( \frac{^{208}Pb}{^{204}Pb} \right)_{initial} = \left( \frac{^{208}Pb}{^{204}Pb} \right)_{T_i} + \omega_{sample} (e^{\lambda_2 T_i} - e^{\lambda_{84} T_i}) \tag{10}
\]

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 $\mu$ 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:

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

## [1] 13.304

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


```r
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 $\mu$ ($^{238}$U/$^{204}$Pb), time-integrated $\kappa$ ($^{232}$Th/$^{238}$U) and initial Pb isotope ratios. However, usually we will want to apply these calculations to an entire dataset rather than 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 database (http://thera2.usask.ca:8092/). We briefly document below how to apply functions to this dataset.

Import the SampleData.csv file:

```r
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

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

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.

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

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

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

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

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, \( \mu_1 \), \( \omega_1 \) 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, \( ^{206}\text{Pb}/^{204}\text{Pb} \), \( ^{207}\text{Pb}/^{204}\text{Pb} \) and \( ^{208}\text{Pb}/^{204}\text{Pb} \), 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).

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

Table 6: First six rows of the ‘SKcurve’ dataframe produced using the `modelcurve()` function.

<table>
<thead>
<tr>
<th>t</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>18.703</td>
<td>15.629</td>
<td>38.631</td>
</tr>
<tr>
<td>1</td>
<td>18.702</td>
<td>15.629</td>
<td>38.629</td>
</tr>
<tr>
<td>2</td>
<td>18.700</td>
<td>15.629</td>
<td>38.627</td>
</tr>
<tr>
<td>3</td>
<td>18.699</td>
<td>15.629</td>
<td>38.625</td>
</tr>
<tr>
<td>4</td>
<td>18.697</td>
<td>15.629</td>
<td>38.623</td>
</tr>
<tr>
<td>5</td>
<td>18.696</td>
<td>15.629</td>
<td>38.621</td>
</tr>
</tbody>
</table>

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 \( \mu \) of 8.43 is generated by the following:

```r
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 \( \mu_1 \) of 8. These three curves are shown in figure 5.

```r
mc1 <- modelcurve(3700:4570, model = SK1)
m2 <- 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 $^{206}\text{Pb}/^{204}\text{Pb}$ vs. $^{207}\text{Pb}/^{204}\text{Pb}$ 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 $^{206}\text{Pb}/^{204}\text{Pb}$ vs. $^{208}\text{Pb}/^{204}\text{Pb}$ plot, the functions `geochron86slope()` and `geochron86yint()` can be used. Geochron lines in figure 1 are plotted using the below functions for $t = 3000 \text{ Ma}$, $t = 2000 \text{ Ma}$, $t = 1000 \text{ Ma}$ and $t = 0 \text{ Ma}$. 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:

```r
geochron76slope(2700)
```

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

```r
geochron76yint(2700)
```

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

```r
geochron86slope(2700)
```

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

```r
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 $\mu_{\text{(U/Pb)}}$, time-integrated $\kappa_{\text{(Th/U)}}$ and the three initial Pb isotope ratios. The app also plots these data onto a series of standard plots. These include: 1) model source $\mu_{\text{(U/Pb)}}$ vs. age; 2) time-integrated $\kappa_{\text{(Th/U)}}$ vs. age; 3) $^{206}\text{Pb} /^{204}\text{Pb}$ vs. $^{207}\text{Pb} /^{204}\text{Pb}$; and 4) $^{206}\text{Pb} /^{204}\text{Pb}$ vs. $^{208}\text{Pb} /^{204}\text{Pb}$. 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.

![Shiny Application Screenshot](https://shereearmistead.shinyapps.io/PbIsoApp/)

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.
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

References