Package ‘isocalcR’

July 15, 2022

Type Package

Title Isotope Calculations in R

Version 0.1.0

Author Justin Mathias

Date 2022-07-14

Maintainer Justin Mathias <justin.m.mathias@gmail.com>

Description Perform common calculations based on published stable isotope theory, such as calculating carbon isotope discrimination and intrinsic water use efficiency from wood or leaf carbon isotope composition. See Farquhar, O'Leary, and Berry (1982) <doi:10.1071/PP9820121>.

License GPL-3

URL https://github.com/justinmathias/isocalcR

BugReports https://github.com/justinmathias/isocalcR/issues

Depends R (>= 4.0.0)

Imports

Encoding UTF-8

Language en-US

LazyData true

Suggests rmarkdown, knitr, testthat (>= 3.0.0), ggplot2, tidyr, dplyr

VignetteBuilder knitr

Config/testthat/edition 3

RoxygenNote 7.1.1

NeedsCompilation no

Repository CRAN

Date/Publication 2022-07-15 16:30:02 UTC
**R topics documented:**

CO2data ................................................................. 2  
custom.calc ......................................................... 3  
d13C.to.Cl ............................................................ 5  
d13C.to.ClCa ......................................................... 7  
d13C.to.D13C .......................................................... 9  
d13C.to.diffCaCi ..................................................... 10  
d13C.to.iWUE .......................................................... 12  
piru13C ............................................................... 15  

**Description**

Compiled records of atmospheric CO2 concentrations and stable carbon isotopes to reconstruct climate and derive plant ecophysiological indices from tree rings. Data are from Belmecheri, Lavergne, 2020, Dendrochronologia. Updated based on their methodology beyond C.E. 2019.

**Usage**

data(CO2data)

**Format**

A data frame with 2020 rows and 3 variables:

- **yr** Year of CO2 and d13CO2 measurement
- **Ca** Atmospheric CO2 concentration, in ppm
- **d13C.atm** Atmospheric d13CO2, in per mille, %

**Source**


**References**


**Examples**

data(CO2data)  
head(CO2data)
custom.calc

Description

Calculates D13C, Ci, CiCa, diffCaCi, or iWUE with user specified values of d13C.plant, d13CO2.atm, atmospheric CO2, temperature, and elevation. The user can also specify whether to calculate each physiological index using the 'simple', 'photorespiration', or 'mesophyll' formulation in all calculations where Ci is computed. Method defaults to 'simple' assuming 'leaf' tissue and incorporates an apparent fractionation by Rubisco, b, of 27 permille (Cernusak and Ubierna 2022). If 'wood' tissue is supplied as an argument in the 'simple' method, the apparent fractionation by Rubisco, b, is updated to 25.5 permille (Cernusak and Ubierna 2022).

Usage

custom.calc(
    d13C.plant,
    d13C.atm,
    frac = 0,
    outvar = "D13C",
    Ca = NULL,
    elevation = NULL,
    temp = NULL,
    method = "simple",
    tissue = "leaf"
)

Arguments

d13C.plant    Measured plant tissue carbon isotope signature, per mille (%)
d13C.atm     Atmospheric d13CO2, per mille (%)
frac         Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material, user should supply reasonable value if from wood (generally -1.9 - -2.1)
outvar        Variable of interest to calculate from the following: D13C, Ci, CiCa, diffCaCi, or iWUE. Defaults to D13C.
Ca            Atmospheric CO2 concentration (ppm).
elevation     Elevation (m.a.s.l.) of the sample, necessary to account for photorespiration processes
temp          Leaf temperature (°C)
method        Method to calculate iWUE (simple, photorespiration, or mesophyll). Defaults to 'simple'. See Lavergne et al. 2022, Ma et al. 2021, Gong et al. 2022.
tissue        Plant tissue of the sample (i.e. leaf or wood) used only during calculations using the simple formulation. Defaults to 'leaf'.
Value

One of the specified outvars: D13C (permille), Ci (ppm), CiCa (unitless), diffCaCi (ppm), or iWUE (micromol CO2 per mol H2O). Defaults to 'D13C'.

References


Examples

custom.calc(d13C.plant = -27, d13C.atm = -8.7)
**Description**

Calculates leaf intercellular CO2 concentration given plant tissue d13C signature. Defaults to the 'simple' formulation (See Lavergne et al. 2022) and 'leaf' tissue to calculate leaf Ci. Under the 'simple' formulation the apparent fractionation by Rubisco is 27 permille if from 'leaf' tissue and 25.5 permille if from wood tissue (Cernusak and Ubierna 2022).

**Usage**

```r
d13C.to.Ci(
    d13C.plant,
    year,
    elevation,
    temp,
    method = "simple",
    tissue = "leaf",
    frac = 0
)
```

**Arguments**

- `d13C.plant`: Measured plant tissue carbon isotope signature, per mille (%)
- `year`: Year to which the sample corresponds
- `elevation`: Elevation (m.a.s.l.) of the sample, necessary to account for photorespiration processes
- `temp`: Leaf temperature (°C)
- `method`: Method to calculate CiCa (simple, photorespiration, or mesophyll). See Lavergne et al. 2022, Ma et al. 2021, Gong et al. 2022
- `tissue`: Plant tissue of the sample (i.e. leaf or wood) used only during calculations using the simple formulation. Defaults to "leaf".
- `frac`: Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material, user should supply reasonable value if from wood (generally -1.9 - -2.1)

**Value**

The concentration of leaf internal CO2 (ppm)

**References**


Examples

d13C.to.Ci(d13C.plant = -27,
    year = 2015,
    elevation = 900,
    temp = 24,
    method = "simple",
    tissue = "leaf")

d13C.to.Ci(d13C.plant = -27,
    year = 2015,
    elevation = 900,
    temp = 24,
    method = "simple",
    tissue = "wood")
\texttt{d13C.to.CiCa(d13C.plant = -27,}
\texttt{ year = 2015,}
\texttt{ elevation = 900,}
\texttt{ temp = 24,}
\texttt{ method = "photorespiration")}

---

**Description**

Calculates the ratio of the concentration of leaf intercellular to atmospheric CO2, unitless. Defaults to the 'simple' formulation (See Lavergne et al. 2022) and 'leaf' tissue to calculate leaf Ci, and subsequently CiCa. Under the 'simple' formulation the apparent fractionation by Rubisco is 27 permille if from 'leaf' tissue and 25.5 permille if from wood tissue (Cernusak and Ubierna 2022).

**Usage**

\[
d13C.to.CiCa(d13C.plant, year, elevation, temp, method = "simple", tissue = "leaf", frac = 0)
\]

**Arguments**

- **d13C.plant**  
  Measured plant tissue carbon isotope signature, per mille (‰)
- **year**  
  Year to which the sample corresponds
- **elevation**  
  Elevation (m.a.s.l.) of the sample, necessary to account for photorespiration processes
- **temp**  
  Leaf temperature (°C)
- **method**  
  Method to calculate CiCa (simple, photorespiration, or mesophyll). See Lavergne et al. 2022, Ma et al. 2021, Gong et al. 2022
- **tissue**  
  Plant tissue of the sample (i.e. leaf or wood) used only during calculations using the simple formulation. Defaults to "leaf".
- **frac**  
  Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material, user should supply reasonable value if from wood (generally -1.9 - -2.1)
**Value**

The ratio of leaf intercellular to atmospheric CO2 (Ci/Ca), unitless

**References**


**Examples**

```r
d13C.to.CiCa(d13C.plant = -27,  
year = 2015,  
elevation = 900,  
temp = 24,  
method = "simple",```
d13C.to.D13C

tissue = "leaf")

d13C.to.CiCa(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "simple",
tissue = "wood")

d13C.to.CiCa(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "photorespiration")

---

d13C.to.D13C  d13C.to.D13C

Description

Calculates leaf carbon isotope discrimination given plant tissue d13C signature.

Usage

d13C.to.D13C(d13C.plant, year, frac = 0)

Arguments

- **d13C.plant**: Measured plant tissue carbon isotope signature, per mille (%).
- **year**: Year to which the sample corresponds.
- **frac**: Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material with no post-photosynthetic fractionation. User should supply reasonable value if leaf fractionation present or if samples are from wood (generally -1.9 - -2.1).

Value

Carbon isotope discrimination in units of per mille (%).

References


Examples

d13C.to.D13C(d13C.plant = -27, year = 2015)

Description

Calculates the difference between the atmospheric CO2 concentration and the leaf intercellular CO2 concentration in parts per mil (ppm). Defaults to the 'simple' formulation (See Lavergne et al. 2022) and 'leaf' tissue to calculate leaf Ci, and subsequently diffCaCi. Under the 'simple' formulation the apparent fractionation by Rubisco is 27 permille if from 'leaf' tissue and 25.5 permille if from wood tissue (Cernusak and Ubierna 2022).

Usage

d13C.to.diffCaCi(  
d13C.plant,  
year,  
elevation,  
temp,  
method = "simple",  
tissue = "leaf",  
frac = 0  
)
Arguments

d13C.plant  Measured plant tissue carbon isotope signature, per mille (%)
year       Year to which the sample corresponds
elevation  Elevation (m.a.s.l.) of the sample, necessary to account for photorespiration processes
temp       Leaf temperature (°C)
method     Method to calculate CiCa (simple, photorespiration, or mesophyll). See Lavergne et al. 2022, Ma et al. 2021, Gong et al. 2022
tissue     Plant tissue of the sample (i.e. leaf or wood) used only during calculations using the simple formulation. Defaults to “leaf”.
frac       Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material, user should supply reasonable value if from wood (generally -1.9 - -2.1)

Value

The difference between atmospheric and leaf intercellular CO2 concentrations (ppm).

References


Examples

```r
d13C.to.diffCaCi(d13C.plant = -27,
    year = 2015,
    elevation = 900,
    temp = 24,
    method = "simple",
    tissue = "leaf")
```

```r
d13C.to.diffCaCi(d13C.plant = -27,
    year = 2015,
    elevation = 900,
    temp = 24,
    method = "simple",
    tissue = "wood")
```

```r
d13C.to.diffCaCi(d13C.plant = -27,
    year = 2015,
    elevation = 900,
    temp = 24,
    method = "photorespiration")
```

Description

Calculates leaf intrinsic water use efficiency given plant tissue d13C signature. Defaults to the 'simple' formulation (See Lavergne et al. 2022) and 'leaf' tissue to calculate leaf Ci, and subsequently iWUE. Under the 'simple' formulation the apparent fractionation by Rubisco is 27 permille if from 'leaf' tissue and 25.5 permille if from wood tissue (Cernusak and Ubierna 2022).
Usage

d13C.to.iWUE(
  d13C.plant,
  year,
  elevation,
  temp,
  method = "simple",
  tissue = "leaf",
  frac = 0
)

Arguments

d13C.plant  Measured plant tissue carbon isotope signature, per mille (‰)
year        Year to which the sample corresponds
Elevation (m.a.s.l.)  of the sample, necessary to account for photorespiration
processes
temp        Leaf temperature (°C)
method      Method to calculate iWUE (simple, photorespiration, or mesophyll). See Lavergne et al. 2022, Ma et al. 2021, Gong et al. 2022
tissue      Plant tissue of the sample (i.e. leaf or wood) used only during calculations using
            the simple formulation. Defaults to "leaf".
frac        Post-photosynthetic fractionation factor, defaults to 0 assuming leaf material,
            user should supply reasonable value if from wood (generally -1.9 - -2.1)

Value

Intrinsic water use efficiency in units of micromol CO2 per mol H2O.

References

fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. Rapid
Belmecheri, S. & Lavergne, A. (2020). Compiled records of atmospheric CO2 concentrations and
stable carbon isotopes to reconstruct climate and derive plant ecophysiological indices from tree
rings. Dendrochronologia, 63, 125748.
perature response functions for models of Rubisco-limited photosynthesis. Plant, Cell Environ., 24,
253–259.
53–92.
Cernusak, L. A. & Ubierna, N. Carbon Isotope Effects in Relation to CO2 Assimilation by Tree
Canopies. in Stable Isotopes in Tree Rings: inferring physiological, climatic, and environmental


Examples

d13C.to.iWUE(d13C.plant = -27, 
  year = 2015, 
  elevation = 900, 
  temp = 24, 
  method = "simple", 
  tissue = "leaf")

d13C.to.iWUE(d13C.plant = -27, 
  year = 2015, 
  elevation = 900, 
  temp = 24, 
  method = "simple", 
  tissue = "wood")

d13C.to.iWUE(d13C.plant = -27, 
  year = 2015, 
  elevation = 900, 
  temp = 24, 
  method = "photorespiration")
Description

Usage
data(piru13C)

Format
A data frame with 223 rows and 6 variables:

- **Year** Year of sample
- **Site** Study location name
- **wood.d13C** Measured tree ring (i.e. wood) d13C, in per mille, %
- **MGT_C** Mean growing season temperature, °C
- **Elevation_m** Elevation of study location, meters
- **frac** Leaf-to-wood fractionation factor

Source

References

Examples

data(piru13C)
head(piru13C)
Index

* datasets
  CO2data, 2
  piru13C, 15

CO2data, 2
custom.calc, 3

d13C.to.Ci, 5
d13C.to.CiCa, 7
d13C.to.D13C, 9
d13C.to.diffCaCi, 10
d13C.to.iWUE, 12

piru13C, 15