Package: isocalcR (via r-universe)

September 18, 2024

Type Package

Title Isotope Calculations in R

Version 0.1.1

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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 Mathias and Hudiburg (2022) in Global Change Biology [<doi:10.1111/gcb.16407>](https://doi.org/10.1111/gcb.16407).

License GPL-3

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

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

Depends R $(>= 4.0.0)$ 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 7.2.1

Repository https://justinmathias.r-universe.dev

RemoteUrl https://github.com/justinmathias/isocalcr

RemoteRef HEAD

RemoteSha f07bcf5cc986e0b3cc1ff26a6a4c9a37c4a22663

Contents

CO2data *CO2data*

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 2023 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

https://www.sciencedirect.com/science/article/abs/pii/S1125786520300874

References

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.

```
data(CO2data)
head(CO2data)
tail(CO2data)
```


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"
\mathcal{L}
```
Arguments

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

References

Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. Rapid Commun. Mass Spectrom., 19, 1381–1391.

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.

Bernacchi, C.J., Singsaas, E.L., Pimentel, C., Portis Jr, A.R. & Long, S.P. (2001). Improved temperature response functions for models of Rubisco-limited photosynthesis. Plant, Cell Environ., 24, 253–259.

Craig, H. (1953). The geochemistry of the stable carbon isotopes. Geochim. Cosmochim. Acta, 3, 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 responses 291–310 (2022). doi:10.1007/978-3-030-92698-4_9.

Davies, J.A. & Allen, C.D. (1973). Equilibrium, Potential and Actual Evaporation from Cropped Surfaces in Southern Ontario. J. Appl. Meteorol., 12, 649–657.

Farquhar, G., O'Leary, M. & Berry, J. (1982). On the relationship between carbon isotope discrimination and the intercellular carbon dioxide concentration in leaves. Aust. J. Plant Physiol., 9, 121–137.

Frank, D.C., Poulter, B., Saurer, M., Esper, J., Huntingford, C., Helle, G., et al. (2015). Water-use efficiency and transpiration across European forests during the Anthropocene. Nat. Clim. Chang., 5, 579–583.

Gong, X. Y. et al. Overestimated gains in water-use efficiency by global forests. Glob. Chang. Biol. 1–12 (2022) doi:10.1111/gcb.16221.

Lavergne, A. et al. Global decadal variability of plant carbon isotope discrimination and its link to gross primary production. Glob. Chang. Biol. 28, 524–541 (2022).

Ma, W. T. et al. Accounting for mesophyll conductance substantially improves 13C-based estimates of intrinsic water-use efficiency. New Phytol. 229, 1326–1338 (2021).

Tsilingiris, P.T. (2008). Thermophysical and transport properties of humid air at temperature range between 0 and 100°C. Energy Convers. Manag., 49, 1098–1110.

Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C3 plants. Plant. Cell Environ., 37, 1494–1498.

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

```
d13C.to.Ci(
  d13C.plant,
  year,
  elevation,
  temp,
  method = "simple",
  tissue = "leaf",
  frac = \theta)
```
Arguments

Value

The concentration of leaf internal CO2 (ppm)

References

Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. Rapid Commun. Mass Spectrom., 19, 1381–1391.

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.

Bernacchi, C.J., Singsaas, E.L., Pimentel, C., Portis Jr, A.R. & Long, S.P. (2001). Improved temperature response functions for models of Rubisco-limited photosynthesis. Plant, Cell Environ., 24, 253–259.

Craig, H. (1953). The geochemistry of the stable carbon isotopes. Geochim. Cosmochim. Acta, 3, 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 responses 291–310 (2022). doi:10.1007/978-3-030-92698-4_9.

Davies, J.A. & Allen, C.D. (1973). Equilibrium, Potential and Actual Evaporation from Cropped Surfaces in Southern Ontario. J. Appl. Meteorol., 12, 649–657.

Farquhar, G., O'Leary, M. & Berry, J. (1982). On the relationship between carbon isotope discrimination and the intercellular carbon dioxide concentration in leaves. Aust. J. Plant Physiol., 9, 121–137.

Frank, D.C., Poulter, B., Saurer, M., Esper, J., Huntingford, C., Helle, G., et al. (2015). Water-use efficiency and transpiration across European forests during the Anthropocene. Nat. Clim. Chang., 5, 579–583.

Gong, X. Y. et al. Overestimated gains in water-use efficiency by global forests. Glob. Chang. Biol. 1–12 (2022) doi:10.1111/gcb.16221.

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Ma, W. T. et al. Accounting for mesophyll conductance substantially improves 13C-based estimates of intrinsic water-use efficiency. New Phytol. 229, 1326–1338 (2021).

Tsilingiris, P.T. (2008). Thermophysical and transport properties of humid air at temperature range between 0 and 100°C. Energy Convers. Manag., 49, 1098–1110.

Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C3 plants. Plant. Cell Environ., 37, 1494–1498.

```
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")
```
d13C.to.CiCa 7

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

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 = \theta\lambda
```
Arguments

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

References

Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. Rapid Commun. Mass Spectrom., 19, 1381–1391.

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.

Bernacchi, C.J., Singsaas, E.L., Pimentel, C., Portis Jr, A.R. & Long, S.P. (2001). Improved temperature response functions for models of Rubisco-limited photosynthesis. Plant, Cell Environ., 24, 253–259.

Craig, H. (1953). The geochemistry of the stable carbon isotopes. Geochim. Cosmochim. Acta, 3, 53–92.

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Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C3 plants. Plant. Cell Environ., 37, 1494–1498.

```
d13C.to.CiCa(d13C.plant = -27,year = 2015,
elevation = 900,
temp = 24,
method = "simple",
```
d13C.to.D13C 9

```
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 = <math>0</math>)
```
Arguments

Value

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

References

Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. Rapid Commun. Mass Spectrom., 19, 1381–1391.

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.

Craig, H. (1953). The geochemistry of the stable carbon isotopes. Geochim. Cosmochim. Acta, 3, 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 responses 291–310 (2022). doi:10.1007/978-3-030-92698-4_9.

Farquhar, G., O'Leary, M. & Berry, J. (1982). On the relationship between carbon isotope discrimination and the intercellular carbon dioxide concentration in leaves. Aust. J. Plant Physiol., 9, 121–137.

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Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C3 plants. Plant. Cell Environ., 37, 1494–1498.

Examples

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

d13C.to.diffCaCi *d13C.to.diffCaCi*

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 = \theta)
```
d13C.to.diffCaCi 11

Arguments

Value

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

References

Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. Rapid Commun. Mass Spectrom., 19, 1381–1391.

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.

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Tsilingiris, P.T. (2008). Thermophysical and transport properties of humid air at temperature range between 0 and 100°C. Energy Convers. Manag., 49, 1098–1110.

Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C3 plants. Plant. Cell Environ., 37, 1494–1498.

Examples

```
d13C.to.diffCaCi(d13C.plant = -27,
year = 2015,elevation = 900,
temp = 24,
method = "simple",
tissue = "leaf")
d13C.to.diffCaCi(d13C.plant = -27,
year = 2015,
elevation = 900,
temp = 24,
method = "simple",
tissue = "wood")
d13C.to.diffCaci(d13C.plant = -27,year = 2015,
elevation = 900,
temp = 24,
method = "photorespiration")
```
d13C.to.iWUE *d13C.to.iWUE*

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).

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Usage

```
d13C.to.iWUE(
  d13C.plant,
  year,
  elevation,
  temp,
  method = "simple",
  tissue = "leaf",
  frac = \theta)
```
Arguments

Value

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

References

Badeck, F.-W., Tcherkez, G., Nogués, S., Piel, C. & Ghashghaie, J. (2005). Post-photosynthetic fractionation of stable carbon isotopes between plant organs—a widespread phenomenon. Rapid Commun. Mass Spectrom., 19, 1381–1391.

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.

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Tsilingiris, P.T. (2008). Thermophysical and transport properties of humid air at temperature range between 0 and 100°C. Energy Convers. Manag., 49, 1098–1110.

Ubierna, N. & Farquhar, G.D. (2014). Advances in measurements and models of photosynthetic carbon isotope discrimination in C3 plants. Plant. Cell Environ., 37, 1494–1498.

```
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

Accompanying tree ring carbon isotope signature data for "Mathias, J.M. & Thomas, R.B. Disentangling the effects of acidic air pollution, atmospheric CO2, and climate change on recent growth of red spruce trees in the Central Appalachian Mountains. Glob. Chang. Biol. 24, 3938–3953 (2018).".

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

https://onlinelibrary.wiley.com/doi/full/10.1111/gcb.14273

References

Mathias, J.M. & Thomas, R.B. Disentangling the effects of acidic air pollution, atmospheric CO2, and climate change on recent growth of red spruce trees in the Central Appalachian Mountains. Glob. Chang. Biol. 24, 3938–3953 (2018).

Examples

data(piru13C) head(piru13C)

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