Package 'NEONiso'

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Type Package

Title Tools to Calibrate and Work with NEON Atmospheric Isotope Data

Version 0.5.1

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Depends R (>= 4.0.0)

Description Functions for downloading,
calibrating, and analyzing atmospheric isotope data bundled
into the eddy covariance data products of the National Ecological
Observatory Network (NEON) <https://www.neonscience.org>.
In this version, calibration tools are provided for only the
carbon isotope products. Tools for calibrating water isotope
products are under development. More details are found in Fiorella et al. (2021)
<doi:10.1029/2020JG005862>, and the readme
file at <https://github.com/SPATIAL-Lab/NEONiso>.

License GPL-3

BugReports https://github.com/SPATIAL-Lab/NEONiso/issues

URL https://github.com/SPATIAL-Lab/NEONiso

Encoding UTF-8

RoxygenNote 7.1.1

Imports dplyr, zoo, httr, lubridate, neonUtilities (>= 2.0.1),
magrittr, rhdf5 (>= 2.33.7), R.utils, tidyselect, data.table,
rlang, lifecycle

Suggests knitr, rmarkdown, testthat (>= 3.0.0)

VignetteBuilder knitr

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`calculate_12CO2` *calculate_12CO2*

Description

calculate_12CO2

Usage

```
calculate_12CO2(total_co2, delta13C, f = 0.00474)
```

Arguments

`total_co2`	Vector of CO2 mole fractions.
`delta13C`	Vector of d13C values.
`f`	Fraction of CO2 that is not 12CO2 or 13CO2. Assumed fixed at 0.00474

Value

Vector of 12CO2 mole fractions.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

Examples

```
calculate_12CO2(total_co2 = 410, delta13C = -8.5)
```

`calculate_13CO2` *calculate_13CO2*

Description

calculate_13CO2

Usage

```
calculate_13CO2(total_co2, delta13C, f = 0.00474)
```

Arguments

`total_co2`	Vector of CO2 mole fractions.
`delta13C`	Vector of d13C values.
`f`	Fraction of CO2 that is not 12CO2 or 13CO2. Assumed fixed at 0.00474

Value

Vector of 13CO2 mole fractions.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

Examples

```
calculate_13CO2(total_co2 = 410, delta13C = -8.5)
```

`calibrate_ambient_carbon_Bowling2003`
calibrate_ambient_carbon_Bowling2003

Description

calibrate_ambient_carbon_Bowling2003

Usage

```
calibrate_ambient_carbon_Bowling2003(
  amb_data_list,
  caldf,
  site,
  filter_data = TRUE,
  force_to_end = TRUE,
  force_to_beginning = TRUE,
  gap_fill_parameters = FALSE,
  r2_thres = 0.9
)
```

Arguments

`amb_data_list`	List containing an ambient d13C dataset. Will include all variables in 000_0x0_xxm. (character)
`caldf`	Calibration data frame containing gain and offset values for 12C and 13C isotopologues.
`site`	Four-letter NEON code corresponding to site being processed.
`filter_data`	Apply median absolute deviation filter from Brock 86 to remove impulse spikes? Inherited from `calibrate_ambient_carbon_Bowling2003()`
`force_to_end`	In given month, calibrate ambient data later than last calibration, using the last calibration? (default true)
`force_to_beginning`	In given month, calibrate ambient data before than first calibration, using the first calibration? (default true)
`gap_fill_parameters`	Should function attempt to 'gap-fill' across a bad calibration by carrying the last known good calibration forward? Implementation is fairly primitive currently, as it only carries the last known good calibration that's available forward rather than interpolating, etc. Default FALSE.
`r2_thres`	Minimum r2 value for calibration to be considered "good" and applied to ambient data.

Value

Depends on `write_to_file` argument. If true, returns nothing to environment; but returns calibrated ambient observations to the output file. If false, returns modified version of amb_data_list that include calibrated ambient data.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

Function called by `calibrate_carbon_bymoth()` to apply gain and offset parameters to the ambient datasets (000_0x0_09m and 000_0x0_30m). This function should generally not be used independently, but should be used in coordination with `calibrate_carbon_bymonth()`.

`calibrate_ambient_carbon_linreg`

calibrate_ambient_carbon_linreg

Description

calibrate_ambient_carbon_linreg

Usage

```
calibrate_ambient_carbon_linreg(
  amb_data_list,
  caldf,
  outname,
  site,
  file,
  filter_data = TRUE,
  force_to_end = TRUE,
  force_to_beginning = TRUE,
  gap_fill_parameters = FALSE,
  r2_thres = 0.9
)
```

Arguments

`amb_data_list`	List containing an ambient d13C dataset. Will include all variables in 000_0x0_xxm. (character)
`caldf`	Calibration data frame containing gain and offset values for 12C and 13C isotopologues.
`outname`	Output variable name. Inherited from `calibrate_ambient_carbon_linreg`
`site`	Four-letter NEON code corresponding to site being processed.
`file`	Output file name. Inherited from `calibrate_ambient_carbon_linreg`

filter_data — Apply median absolute deviation filter from Brock 86 to remove impulse spikes? Inherited from calibrate_ambient_carbon_linreg

force_to_end — In given month, calibrate ambient data later than last calibration, using the last calibration? (default true)

force_to_beginning — In given month, calibrate ambient data before than first calibration, using the first calibration? (default true)

gap_fill_parameters — Should function attempt to 'gap-fill' across a bad calibration by carrying the last known good calibration forward? Implementation is fairly primitive currently, as it only carries the last known good calibration that's available forward rather than interpolating, etc. Default FALSE.

r2_thres — Minimum r2 value for calibration to be considered "good" and applied to ambient data.

Value

Nothing to environment; returns calibrated ambient observations to the output file. This function is not designed to be called on its own, and is not exported to the namespace.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

Function called by calibrate_ambient_carbon_linreg to apply gain and offset parameters to the ambient datasets (000_0x0_09m and 000_0x0_30m). This function should generally not be used independently, but should be used with calibrate_ambient_carbon_linreg.

---

calibrate_carbon *calibrate_carbon*

Description

[Experimental] This function drives a workflow that reads in NEON carbon isotope data of atmospheric CO2, calibrates it to the VPDB scale, and (optionally) writes the calibrated data to a new HDF5 file. Two different approaches are possible: a) a calibration on 12CO2 and 13CO2 isotopologues independently, after Bowling et al. 2003 (Agr. For. Met.), or b) a direct calibration of d13C and CO2 values using linear regression. The vast majority of the time the results generated from either method are extremely similar to each other. Wen et al. 2013 compared several different carbon isotope calibration techniques and found this to be the superior method under most circumstances. We also found this to be the case for NEON data (Fiorella et al. 2021; JGR-Biogeosciences).

Usage

```
calibrate_carbon(
  inname,
  outname,
  site,
  method = "Bowling_2003",
  calibration_half_width = 0.5,
  force_cal_to_beginning = TRUE,
  force_cal_to_end = TRUE,
  gap_fill_parameters = FALSE,
  filter_ambient = TRUE,
  r2_thres = 0.95,
  correct_refData = TRUE,
  write_to_file = TRUE
)
```

Arguments

inname	Input file(s) that are to be calibrated. If a single file is given, output will be a single file per site per month. If a list of files corresponding to a timeseries at a given site is provided, will calibrate the whole time series.
outname	Name of the output file. (character)
site	Four letter NEON site code for site being processed. (character)
method	Are we using the Bowling et al. 2003 method ("Bowling_2003") or direct linear regression of d13C and CO2 mole fractions ("linreg")?
calibration_half_width	Determines the period (in days) from which reference data are selected (period is 2*calibration_half_width).
force_cal_to_beginning	Extend first calibration to the beginning of the file? (default true)
force_cal_to_end	Extend last calibration to the end of the file? (default true)
gap_fill_parameters	Should function attempt to 'gap-fill' across a bad calibration by carrying the last known good calibration forward? Implementation is fairly primitive currently, as it only carries the last known good calibration that's available forward rather than interpolating, etc. Default FALSE.
filter_ambient	Apply the median absolute deviation filter (Brock 86) to remove impulse spikes in output ambient data? (logical; default true)
r2_thres	Minimum r2 threshold of an "acceptable" calibration. Acts to remove calibration periods where a measurement error makes relationship nonlinear. Default = 0.95
correct_refData	NEON has indicated there are a few instances where reported d13C or CO2 reference values are wrong. If set to true, correct known incorrect values. This argument will (hopefully, eventually) go away after NEON has fixed the reference database. Users will be warned prior to removal of this argument.
write_to_file	Write calibrated ambient data to file? (Mostly used for testing)

Details

The 'linreg' method simply takes measured and reference d13C and CO2 values and generates a transfer function between them using `lm()`. For the gain-and-offset method, d13C and CO2 values are converted to 12CO2 and 13CO2 mole fractions. Gain and offset parameters are calculated for each isotopologue independently, and are analogous to regression slope and intercepts, but jointly correct for CO2 concentration dependence and place d13C values on the VPDB scale. The gain and offset parameters are defined by:

$$G = (X_{2,ref} - X_{1,ref})/(X_{2,meas} - X_{1,meas})$$

$$O = X_{2,ref} - GX_{2,meas}$$

Calibrated ambient isotopologues are then given as:

$$X_{cal} = X_{meas}G + O$$

Measurements of reference materials were considered "good" if the following conditions were met:

- Measured CO2 concentrations were within 10 ppm of known "reference" concentrations.
- Variance of the CO2 concentration in standard peak was < 5 ppm.
- Measured d13C value must be within 5 per mil of known "reference" d13C value.

The first two criteria are intended to filter out periods where there is a clear issue with the gas delivery system (i.e., nearly empty gas tank, problem with a valve in the manifold, etc.); the third criterion was adopted after visual inspection of data timeseries revealed that often the first standard measurement following an instrument issue had higher-than-expected error. This criterion clips clearly poor values. Selection of these criteria will become a function argument, and therefore customizable, in a future release.

The behavior of this function will be a bit different depending on what is supplied as `inname`. If a single file is provided, the output will be monthly. However, a list of files corresponding to a site can also be provided, and then a single output file per site will be generated.

Value

Returns nothing to the environment, but creates a new output HDF5 file containing calibrated carbon isotope values.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

Examples

```
## Not run: fin <- system.file('extdata',
         'NEON.D15.ONAQ.DP4.00200.001.nsae.2019-05.basic.20201020T211037Z.packed.h5',
         package = 'NEONiso', mustWork = TRUE)
calibrate_carbon_bymonth(inname = fin, outname = 'out.h5',
         site = 'ONAQ', write_to_file = FALSE)
calibrate_carbon_bymonth(inname = fin, outname = 'out.h5',
         site = 'ONAQ', method = 'linreg', write_to_file = FALSE)
## End(Not run)
```

calibrate_carbon_bymonth
calibrate_carbon_bymonth

Description

[Stable] This function drives a workflow that reads in NEON carbon isotope data of atmospheric CO2, calibrates it to the VPDB scale, and (optionally) writes the calibrated data to a new HDF5 file. Two different approaches are possible: a) a calibration on 12CO2 and 13CO2 isotopologues independently, after Bowling et al. 2003 (Agr. For. Met.), or b) a direct calibration of d13C and CO2 values using linear regression. The vast majority of the time the results generated from either method are extremely similar to each other. Wen et al. 2013 compared several different carbon isotope calibration techniques and found this to be the superior method under most circumstances. We also found this to be the case for NEON data (Fiorella et al. 2021; JGR-Biogeosciences).

Usage

```
calibrate_carbon_bymonth(
  inname,
  outname,
  site,
  method = "Bowling_2003",
  calibration_half_width = 0.5,
  force_cal_to_beginning = TRUE,
  force_cal_to_end = TRUE,
  gap_fill_parameters = FALSE,
  filter_ambient = TRUE,
  r2_thres = 0.95,
  correct_refData = TRUE,
  write_to_file = TRUE
)
```

Arguments

inname	Name of the input file. (character)
outname	Name of the output file. (character)
site	Four letter NEON site code for site being processed. (character)
method	Are we using the Bowling et al. 2003 method ("Bowling_2003") or direct linear regression of d13C and CO2 mole fractions ("linreg")?
calibration_half_width	Determines the period (in days) from which reference data are selected (period is 2*calibration_half_width).
force_cal_to_beginning	Extend first calibration to the beginning of the file? (default true)
force_cal_to_end	Extend last calibration to the end of the file? (default true)

`gap_fill_parameters`
: Should function attempt to 'gap-fill' across a bad calibration by carrying the last known good calibration forward? Implementation is fairly primitive currently, as it only carries the last known good calibration that's available forward rather than interpolating, etc. Default FALSE.

`filter_ambient`
: Apply the median absolute deviation filter (Brock 86) to remove impulse spikes in output ambient data? (logical; default true)

`r2_thres`
: Minimum r2 threshold of an "acceptable" calibration. Acts to remove calibration periods where a measurement error makes relationship nonlinear. Default = 0.95

`correct_refData`
: NEON has indicated there are a few instances where reported d13C or CO2 reference values are wrong. If set to true, correct known incorrect values. This argument will (hopefully, eventually) go away after NEON has fixed the reference database. Users will be warned prior to removal of this argument.

`write_to_file`
: Write calibrated ambient data to file? (Mostly used for testing)

Details

The 'linreg' method simply takes measured and reference d13C and CO2 values and generates a transfer function between them using `lm()`. For the gain-and-offset method, d13C and CO2 values are converted to 12CO2 and 13CO2 mole fractions. Gain and offset parameters are calculated for each isotopologue independently, and are analogous to regression slope and intercepts, but jointly correct for CO2 concentration dependence and place d13C values on the VPDB scale. The gain and offset parameters are defined by:

$$G = (X_{2,ref} - X_{1,ref})/(X_{2,meas} - X_{1,meas})$$

$$O = X_{2,ref} - GX_{2,meas}$$

Calibrated ambient isotopologues are then given as:

$$X_{cal} = X_{meas}G + O$$

Measurements of reference materials were considered "good" if the following conditions were met:

- Measured CO2 concentrations were within 10 ppm of known "reference" concentrations.
- Variance of the CO2 concentration in standard peak was < 5 ppm.
- Measured d13C value must be within 5 per mil of known "reference" d13C value.

The first two criteria are intended to filter out periods where there is a clear issue with the gas delivery system (i.e., nearly empty gas tank, problem with a valve in the manifold, etc.); the third criterion was adopted after visual inspection of data timeseries revealed that often the first standard measurement following an instrument issue had higher-than-expected error. This criterion clips clearly poor values. Selection of these criteria will become a function argument, and therefore customizable, in a future release.

Value

Returns nothing to the environment, but creates a new output HDF5 file containing calibrated carbon isotope values.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

Examples

```
## Not run: fin <- system.file('extdata',
         'NEON.D15.ONAQ.DP4.00200.001.nsae.2019-05.basic.20201020T211037Z.packed.h5',
         package = 'NEONiso', mustWork = TRUE)
calibrate_carbon_bymonth(inname = fin, outname = 'out.h5',
         site = 'ONAQ', write_to_file = FALSE)
calibrate_carbon_bymonth(inname = fin, outname = 'out.h5',
         site = 'ONAQ', method = 'linreg', write_to_file = FALSE)
## End(Not run)
```

`calibrate_standards_carbon` *calibrate_standards_carbon*

Description

calibrate_standards_carbon

Usage

```
calibrate_standards_carbon(
  cal_df,
  ref_df,
  f = 0.00474,
  r2_thres = 0.95,
  correct_bad_refvals = FALSE,
  site,
  refGas
)
```

Arguments

`cal_df`	Data.frame containing calibration parameters
`ref_df`	Data.frame containing reference gas measurements
`f`	Fraction of CO2 isotopologues that are not 12CO2 or 13CO2. Inherited from script calling this function.
`r2_thres`	Threshold for calibration regression to be used to calibrate standards data. Default is 0.95. Calibrated reference gas measurements occurring during calibration periods with r2 values less than `r2_thres` will be marked NA.
`correct_bad_refvals`	Should we correct known/suspected incorrect reference values in the NEON HDF5 files? (Default = `FALSE`).

site	Four letter NEON site code. Only used if correct_bad_refvals = TRUE.
refGas	One of "low", "med", or "high." Only used if correct_bad_refvals = TRUE.

Value

A data.frame having the same number of rows of cal_df, with additional columns added for calibrated CO2 mole fractions and d13C values.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

---

correct_carbon_ref_cval

correct_carbon_ref_cval

Description

This ugly function is present out of necessity, and will only exist for as long as it is necessary. It is an internal correction within the NEONiso calibration routines that is required as there are some mismatches between the 'true' isotope reference values and those in the NEON HDF5 files. NEON is working on correcting this, and after it has been corrected, this function has no need to exist and will be immediately deprecated. As a result, this function is fairly messy but there is little incentive to improve it.

Usage

```
correct_carbon_ref_cval(std_frame, site)
```

Arguments

std_frame	Standard data frame to perform swap on.
site	NEON four letter site code.

Value

A data.frame, based on std_frame, where NEON-supplied reference values have been corrected if a mismatch has previously been identified.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

delta_to_R *delta_to_R*

Description

delta_to_R

Usage

```
delta_to_R(delta_values, element)
```

Arguments

delta_values	A vector of isotope ratios in delta notation.
element	Which element to return R values - carbon, oxygen, or hydrogen.

Value

Vector of isotope ratios (R values).

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

Examples

```
delta_to_R(delta_values = 0, element = 'oxygen') # returns 2005.2e-6 for VSMOW.
```

filter_median_Brock86 *filter_median_Brock86*

Description

Median absolute deviation filter of Brock 1986.

Usage

```
filter_median_Brock86(data, width = 7, threshold = 5)
```

Arguments

data	Vector to filter.
width	Width of filter, in rows.
threshold	Only filter values that are abs(threshold) away from median

Value

Returns filtered vector.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

`fit_carbon_regression` *fit_carbon_regression*

Description

fit_carbon_regression

Usage

```
fit_carbon_regression(ref_data, method, calibration_half_width)
```

Arguments

`ref_data`	Reference data.frame from which to estimate calibration parameters.
`method`	Are we using the Bowling et al. 2003 method ("Bowling_2003") or direct linear regression of d13C and CO2 mole fractions ("linreg")?
`calibration_half_width`	Determines the period (in days) from which reference data are selected (period is 2*calibration_half_width).

Value

Returns a data.frame of calibration parameters. If `method == "Bowling_2003"`, then data.frame includes gain and offset parameters for 12CO2 and 13CO2, and r^2 values for each regression. If `method == "linreg"`, then data.frame includes slope, intercept, and r^2 values for d13C and CO2 values.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

get_Rstd *get_Rstd*

Description

get_Rstd

Usage

```
get_Rstd(element)
```

Arguments

element	Which element to return standard ratio - carbon, oxygen, or hydrogen.

Value

Heavy-to-light isotope ratio of most common stable isotope standard. VSMOW for water, VPDB for carbon.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

---

manage_local_EC_archive *manage_local_EC_archive*

Description

Utility function to help retrieve new EC data and/or prune duplicates, as NEON provisions new data or re-provisions data for an existing site and month.

Usage

```
manage_local_EC_archive(
  file_dir,
  get = TRUE,
  unzip_files = TRUE,
  trim = FALSE,
  dry_run = TRUE,
  sites = "all"
)
```

Arguments

file_dir	Specify the root directory where the local EC store is kept.
get	Pull down data from NEON API that does not exist locally?
unzip_files	NEON gzips the hdf5 files, should we unzip any gzipped files within file_dir? (Searches recursively)
trim	Search through local holdings, and remove older file where there are duplicates?
dry_run	List files identified as duplicates, but do not actually delete them? Default true to prevent unintended data loss.
sites	Which sites to retrieve data from? Default will be all sites with available data, but can specify a single site or a vector here.

Value

Returns nothing to the environment, but will download new NEON HDF5 files for selected sites (if get = TRUE), unzip them in the local file directory (if unzip_files = TRUE), and identify and remove suspected duplicate files (if trim = TRUE and dry_run = FALSE).

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

NEONiso — *NEONiso: A package for calibrating NEON atmospheric isotope observations.*

Description

This package provides functions for retrieving, calibrating, and generating diagnostic plots of NEON atmospheric isotope data.

R_to_delta — *R_to_delta*

Description

R_to_delta

Usage

```
R_to_delta(R_values, element)
```

Arguments

R_values	A vector of isotope ratios (e.g., R values).
element	Which element to return delta values - carbon, oxygen, or hydrogen.

Value

Vector of isotope ratios in delta notation.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

Examples

```
R_to_delta(R_values = 2005.20e-6, element = 'oxygen') # returns 0.
```

`select_daily_reference_data` *select_daily_reference_data*

Description

select_daily_reference_data

Usage

```
select_daily_reference_data(standard_df, analyte, min_nobs = NA)
```

Arguments

`standard_df`	Input reference data.frame.
`analyte`	Are we calibrating CO2 and H2O? (Use argument 'co2' or 'h2o', or else function will throw error)
`min_nobs`	Minimum number of high-frequency observations to define a peak. If not supplied, defaults are 200 for `analyte = 'co2'` or 30 for `analyte = 'h2o'`

Value

Smaller data.frame where only the reference data selected to use in the calibration routines is returned. Assumes that we are calibrating on a daily basis, and not on a longer time scale. Data are selected based on two criteria: cannot be missing, and must be at least a certain number of high-frequency observations in order to qualify as a valid measurement. For the water system, this function also keeps only the last three injections for each reference water per day.

terrestrial_core_sites *terrestrial_core_sites*

Description

terrestrial_core_sites

Usage

```
terrestrial_core_sites()
```

Value

A vector listing NEON core terrestrial sites.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

Examples

```
terrestrial_core_sites()
```

terrestrial_relocatable_sites *terrestrial_relocatable_sites*

Description

terrestrial_relocatable_sites

Usage

```
terrestrial_relocatable_sites()
```

Value

A vector listing NEON core terrestrial sites.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

Examples

```
terrestrial_relocatable_sites()
```

validate_analyte *validate_analyte*

Description

validate_analyte

Usage

```
validate_analyte(analyte)
```

Arguments

analyte	Co2 or H2o?

Value

Standardized string for the water ('H2o') or carbon ('Co2') systems to make sure strings are standardized across package functions.

Author(s)

Rich Fiorella <rich.fiorella@utah.edu>

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