# Package 'gaseous'

December 11, 2023

туре Раскаде
Title Greenhouse Gas Data Workflow Functions for the Margenot Lab
Version 0.1.0
Author Ezra Moses
Maintainer Ezra Moses <moses8@illinois.edu></moses8@illinois.edu>
<b>Description</b> Contains functions and a project template specifically designed for greenhouse gas data retrieved from the Gasmet. For use within the lab of Dr. Andrew Margenot at the University of Illinois Urbana-Champaign.
License MIT + file LICENSE
Encoding UTF-8
LazyData true
Imports conflicted,     dplyr,     purr,     stringr,     tibble,     cowplot,     ggpubr,     readxl  RoxygenNote 7.2.3
Roxygem tote 1.2.5
<pre>URL https://github.com/redseasoils/gaseous</pre>
BugReports https://github.com/redseasoils/gaseous/issues
R topics documented:
add_missing_rows       2         assumptions_plot_sub       3         attr_new_col       4         build_gas_lmer       5         build_manual       5         calculate_gas_loads       6         calib_optim       7         calib_range       7         chron_linear_interp       8
exclude_one_rep

2 add\_missing\_rows

exclude_outliers
f
gasmet_bind_check
gasmet_file_issues
get_latest_instructions
ghg_sum_stats
guess_prefix
hello
import_chamber_volume
impute_missing_values
include_n
is_outlier
make_preprocessing_report
mutate_levene_shapiro_p
mutate_residuals
negative_flux
noaa_temp_fig
ppm_seconds_lm
ppm_seconds_plot
qqplots
regression_fig
replace_gas_with_na
resplots
rm_random_fx
round_p
summary_boxplots_flux
summary_boxplots_loads
time series

add\_missing\_rows

Add rows to data frame to make missing values explicit

# Description

Add rows to data frame to make missing values explicit

```
add_missing_rows(
  data,
  site_var = site,
  plot_var = plot,
  date_var = Date,
  year_var = year,
  plots_unique_by = c(year, site),
  plots_unique_all = paste(treatment_key$year, treatment_key$site, treatment_key$plot),
  addl_id_vars = c(treatment, block)
)
```

assumptions\_plot\_sub 3

A data frame

#### **Arguments**

data

site_var	Name of column in data containing site names. Defaults to site.
plot_var	Name of column in data containing plot IDs. Defaults to plot.
date_var	Name of column in data containing sampling dates. Defaults to Date.
year_var	Name of column in data containing sampling year. Defaults to year.
plots_unique_by	
	Names of columns in data within which plot IDs are unique. Defaults to
	c(year, site).
plots_unique_al	1
	Vector of space-separated strings containing all unique plots preceded by their
	corresponding levels of plots_unique_by. Defaults to paste(treatment_key*year, treatment_l treatment_key*plot).
addl_id_vars	Additional names of ID columns (those not already listed in other arguments) in
	data. The values of these variables will be filled in added 'missing' rows in the

result. Set to NULL if there are no additional ID variables to be filled in. Defaults to c(treatment, block).

#### Value

data with additional rows of previously missing levels of specified variable combinations.

assumptions\_plot\_sub Make Plot Subtitle Containing Levene and Shapiro-Wilk Test p-values

## **Description**

Make Plot Subtitle Containing Levene and Shapiro-Wilk Test p-values

#### Usage

```
assumptions_plot_sub(
  data,
  var,
  trans_label,
  levene_label = "levene",
  shapiro_label = "shapiro",
  var_then_label = TRUE,
  sep = "_"
)
```

## **Arguments**

data	Data frame containing columns with Levene and Shapiro p values. There must be only one unique p-value for each test within the data frame or current group.
var	Column name of variable for which ANOVA assumptions are being tested. E.g. co2
trans_label	Optional. String describing data transformation performed on var prior to assumptions checks. E.g. 'log'.

4 attr\_new\_col

levene_label	String pattern which is appended on column names containing the Levene test p-value. If var_then_label is TRUE (the default), the name of the Levene p-value column should be paste0(var, sep, levene_label). Defaults to.
shapiro_label	String pattern which is appended on column names containing the Shapiro-Wilk test p-value. If var_then_label is TRUE (the default), the name of the Shapiro p-value column should be paste0(var, sep, shapiro_label). Defaults to "shapiro".
var_then_label	Logical. Are column names containing p-values formatted so that the name specified in var comes before the label specified in levene_label and shapiro_label, separated by sep? Defaults to TRUE.
sep	Character pattern separating var from levene_label or shapiro_label in names of columns containing p-values. Defaults to "_".

#### Value

A string that can be used as a formatted plot subtitle.

attr\_new\_col Data Attributes

#### **Description**

Data attributes are used in this workflow to record the reason(s) certain data points are marked for exclusion from modeling. These attributes are recorded for each gas in a single column, usually named attributes, created with attr\_new\_col(). attr\_update() is used to add attributes to this column. attr\_show\_codes() prints each unique attribute code and its meaning to the console.

#### Usage

```
attr_new_col(
  data,
  attr_var = attributes,
  prefixes = c("all", "co2", "n2o", "ch4", "nh3"),
  sep = ","
)
attr_show_codes()
attr_update(data, attr_var = attributes, prefix, attr_code, sep = ",")
```

# Arguments

data	A data frame
attr_var	Name of column in data where attributes are stored. Defaults to attributes.
prefixes	Character. Vector of prefixes to assign in new attribute column with attr_new_col(). Defaults to c('all', 'co2', 'n2o', 'ch4', 'nh3').
sep	String that separates attribute elements in attr_var. Defaults to ','.
prefix	$Character.\ Unique\ prefix\ preceding\ attribute\ codes\ to\ be\ updated\ with\ attr\_update().$
attr_code	Character. Attribute code to be appended with attr_update().

build\_gas\_lmer 5

#### Value

attr\_new\_col() and attr\_update() return a data frame with new or updated attr\_var, respectively. attr\_show\_codes() returns a message to the console.

## **Examples**

```
attr_show_codes()
dat <- data.frame(x = rnorm(3))
dat <- attr_new_col(dat)
attr_update(dat, prefix = 'co2', attr_code = '02')</pre>
```

build\_gas\_lmer

Build linear mixed effect models for GHG data

## **Description**

Build lmer() models on multiple gas variables simultaneously.

#### Usage

```
build_gas_lmer(data, formula, gas_vars = c(co2, n2o, ch4, nh3))
```

#### **Arguments**

data A data frame

gas\_vars Names of columns in data containing gas data to be substituted in formula.

Each name should be an unquoted expression. Defaults to c(co2, n2o, ch4,

nh3).

## Value

A list of models

build\_manual

Build and Prep Manual for Export

## Description

For internal use only. Builds manual to inst/instructions and renames it to match version annotation of pptm instructions.

#### Usage

```
build_manual()
```

#### Value

Nothing in memory.

6 calculate\_gas\_loads

## Description

Calculate cumulative per-day gas loads after imputing gas data. This function calculates cumulative load using area under the curve ("AUC"). Each gas data point is assumed to be the hourly load for all days surrounding the measurement, up to one half of the distance between the measurement and its nearest preceding and following measurement.

Additional methods, like linear interpolation, may be added in the future as options in the method argument.

## Usage

```
calculate_gas_loads(
  data,
  gas_vars = c(co2_kg_ha_day_imputed, n2o_kg_ha_day_imputed, ch4_kg_ha_day_imputed,
        nh3_kg_ha_day_imputed),
  date_var = Date,
  site_var = site,
  plot_var = plot,
  method = "AUC",
  per_hour = FALSE
)
```

## **Arguments**

data	A data frame
gas_vars	Names of columns in data containing imputed (i.e. containing no NA values) gas data in mg kg $^{-1}$ . Defaults to c(co2_kg_ha_day_imputed, n2o_kg_ha_day_imputed, ch4_kg_h nh3_kg_ha_day_imputed).
date_var	Name of column in data containing sampling dates in YYYY-MM-DD format. Defaults to Date.
site_var	Name of column in data containing site names. Defaults to site.
plot_var	Name of column in data containing plot IDs. Defaults to plot.
method	Defaults to 'AUC' (area under the curve), currently the only option. Linear interpolation methods to be added.
per_hour	Logical. Are the units of gas_vars per hour (per_hour = TRUE) or per day

(per\_hour = FALSE). Defaults to FALSE.

## Value

data with new columns for gas loads

calib\_optim 7

	-	٠					٠	
ca		П	h	$\sim$	n	+	п	m
$\sim a$	_	_	v	·	v	ı	_	111

Optimization of Carbon Dioxide ppm per Second Models

#### **Description**

Finds optimum values of  $excl\_var$  column in data to make the  $R^2$  value of the lm() performed in  $ppm\_seconds\_lm\_optim()$  at least 0.98 while minimizing the amount of data points excluded from the model.

#### Usage

```
calib_optim(x, data, excl_var, min_n = 4)
```

#### **Arguments**

x Vector of 0s and 1s which will be randomly generated in calib\_range()

data Data frame containing CO<sub>2</sub> data

excl\_var Logical column in data which tracks observations that should be excluded from

the model

#### **Details**

See model\_co2() for details about the parameters and method of model optimization.

#### Value

Number of data points excluded from the model

#### See Also

```
model_co2(), calib_range()
```

calib\_range

Optimization of Carbon Dioxide ppm per Second Models

# Description

Generates random instances of the logical column specified in excl\_var, contained in data. In each random instance, existing TRUE observations are retained, and a random number of points at the head and tail of the column are replaced with TRUE. Maximum number of TRUE observations in the final instance is set at min\_n. Converts randomized vector to integer for compatibility with optim().

```
calib_range(data, excl_var, min_n = 4, x)
```

8 chron\_linear\_interp

#### **Arguments**

data	Data frame containing CO <sub>2</sub> data
excl_var	Logical column in data which tracks observations that should be excluded from the model
min_n	Integer. Minimum number of data points to retain in final model. Defaults to 4.
Х	Passed from calib_optim; not used in this function. Removing this parameter causes an error in optim, but it does not need to be explicitly specified when the function is called.

#### Value

Vector of 0s and 1s with the same length as data.

#### See Also

```
calib_optim, model_co2
```

chron\_linear\_interp Line

Linear interpolation of missing values between dates

#### **Description**

Linear interpolation of missing values between dates

## Usage

```
chron_linear_interp(
  data,
  gas_vars = c(co2_mg_kg_day, n2o_mg_kg_day, ch4_mg_kg_day, nh3_mg_kg_day),
  date_var = Date,
  site_var = site,
  year_var = year,
  plot_var = plot
)
```

## **Arguments**

data	A data frame
gas_vars	Names of columns in data containing gas data to be interpolated. Defaults to c(co2_mg_kg_day, n2o_mg_kg_day, ch4_mg_kg_day, nh3_mg_kg_day).
date_var	Name of column in data containing sampling dates of format "YYYY-MM-DD". Defaults to Date.
site_var	Name of column in data containing site names. Defaults to site.
year_var	Name of column in data containing year of sampling. Defaults to year.
plot_var	Name of column in data containing plot ID. Defaults to plot.

## Value

data with new columns containing interpolated data, named with suffix "\_interp".

exclude\_one\_rep 9

excl	ude	one	rep

Exclude observations in groups of length one

## Description

Exclude observations in groups of length one

## Usage

```
exclude_one_rep(
  data,
  excl_vars = c(co2_exclude, n2o_exclude, ch4_exclude, nh3_exclude),
  attr_var = attributes,
  prefixes = c("co2", "n2o", "ch4", "nh3"),
  by_vars = c(site, Date, treatment)
)
```

## **Arguments**

data	A data frame
excl_vars	Names of logical columns in data which should be changed to TRUE when the total instances of FALSE in the group (grouped by by_vars) is equal to one. Defaults to $c(co2\_exclude, n2o\_exclude, ch4\_exclude, nh3\_exclude)$ .
attr_var	Name of column in data containing data attributes. Defaults to attributes.
by_vars	Variables to group_by() when calculating totals where excl_vars == FALSE.

## Value

data with updated excl\_vars

exclude\_outliers

Mark outliers for exclusion

## Description

Determine outliers using is\_outlier() and mark them for exclusion from downstream processing.

```
exclude_outliers(
  data,
  gas_var,
  excl_var,
  attr_var = attributes,
  prefix,
  sep = ",",
  n_IQR = 3,
  datatable = FALSE
)
```

10

## **Arguments**

data	Data frame
gas_var	Name of column in data containing gas flux data to be screened for outliers.
excl_var	Name of logical column in data which is equal to TRUE when an observation of gas_var should be excluded from downstream processing and analysis.
attr_var	Passed to attr_update(). Name of column in data which records attributes. Defaults to attributes.
prefix	Unique prefix denoting attribute element in attr_var to be updated with attr_update(). If not specified, it will be inferred from gas_var.
sep	Passed to attr_update(). String that separates attribute elements in attr_var. Defaults to ','.
n_IQR	Integer. Passed to is_outlier. Number of interquartile ranges below 25 value will be considered an outlier. Defaults to 3.
datatable	Logical. Should a datatable (using datatable() of extracted negative flux values be printed? Defaults to FALSE.

## Value

data with updated excl\_var and attr\_var.

f Make formula with sprintf-style replacements

# Description

Shortcut for, e.g. as.formula(sprintf(%s  $\sim$  x, "y")). To be used inside a modeling function call.

## Usage

```
f(formula, repl, verbose = FALSE)
```

## Arguments

formula	String to be converted to formula, with instances of %s replaced by elements of repl
repl	character vector of replacements for each instance of %s in formula
1	T : 1 (1 11 1 16 11 1 1 1 1 1 1 1 1 1 1 1 1

verbose Logical. Should replaced formula be printed to the console? Defaults to FALSE.

## Value

A formula with specified replacements

gasmet\_bind\_check 11

#### **Examples**

```
x <- rnorm(20)
y1 <- rnorm(20)
y2 <- rnorm(20)

# Single replacement
formula <- '%s ~ x'
lm(f(formula, 'y1'))
lm(f(formula, 'y2'))

# Mutliple replacements
formula2 <- 'x ~ %s * %s'
lm(f(formula, c('y1', 'y2')))</pre>
```

gasmet\_bind\_check

Check that Gasmet data list is ready for binding

## **Description**

Performs several checks that evaluate if dfls is ready for binding with bind\_rows. Gives errors with specifics if binding will be unsuccessful. Otherwise, the output of the function is not useful.

#### Usage

```
gasmet_bind_check(dfls, issues_path = "gasmet_data_import_issues.txt")
```

## **Arguments**

dfls List of data frames to check before binding

issues\_path File path to .txt file generated with gasmet\_file\_issues(). Defaults to 'gas-

met\_data\_import\_issues.txt'

## Value

TRUE if data frames in dfls are ready for binding

#### **Description**

Detects issues in TXT files from the Gasmet such as missing columns, mismatches between dates in data columns and file/folder names, multiple dates contained in the same file, etc. Uses cat() to write a message with details about detected issues (and if they need to be resolved for processing to continue). Does not fix the issues - that must be done manually by the user.

12 get\_latest\_instructions

#### Usage

```
gasmet_file_issues(
  dfls,
  check_co2 = TRUE,
  check_n2o = TRUE,
  check_ch4 = TRUE,
  check_nh3 = TRUE,
  check_co = FALSE,
  ...
)
```

## **Arguments**

dfls	List of data frames, each list item containing data from a single site/date
check_co2	Logical. Whether or not to check issues in $\text{CO}_2$ related columns. Defaults to TRUE.
check_n2o	Logical. Whether or not to check issues in $\ensuremath{N_2}\ensuremath{O}$ related columns. Defaults to TRUE.
check_ch4	Logical. Whether or not to check issues in $\ensuremath{\text{CH}}_4$ related columns. Defaults to TRUE.
check_nh3	Logical. Whether or not to check issues in $\ensuremath{\text{NH}}_3$ related columns. Defaults to TRUE.
check_co	Logical. Whether or not to check issues in CO related columns. Defaults to FALSE.
	Passed to cat() in final message. Use file = 'file/path.txt' to write final message to a text file.

#### Value

Message with details about fatal and non-fatal issues. Writes to the console by default. When file is specified, writes to that file.

```
get_latest_instructions
```

Get Latest Version of PowerPoint Package Instructions

# Description

Get Latest Version of PowerPoint Package Instructions

# Usage

```
get_latest_instructions(directory = "instructions")
```

## **Arguments**

directory String. Directory in which to copy PowerPoint file. Defaults to "instructions".

ghg\_sum\_stats 13

#### Value

Nothing in memory. Copies latest instructions to directory if the latest version is not already contained there. If the latest version is already present, a message is printed to the console.

ghg\_sum\_stats

Summary Statistics for GHG Data

## **Description**

Shortcut function to get calculate mean, median, min, max, standard deviation, standard error, and count for sum\_vars. Best used in combination with group\_by(). See examples.

## Usage

```
ghg_sum_stats(.data, ..., showDT = TRUE)
```

## **Arguments**

... A data frame containing GHG data
... Variable(s) in .data to be summarized
showDT Logical. Do you want to print an HTML data table of results made with datatable()?
Defaults to TRUE

## Details

Columns in results will have the format ".col\_.fn" where ".col" is the original column name in data and ".fn" is the function that has been performed in the summary. See examples.

## Value

A data frame of summary statistics

#### **Examples**

```
data <- data.frame(
  co2 = rnorm(100, mean = 1000),
  n2o = rnorm(100, mean = 1000),
  treatment = rep(1:4, 25),
  site = rep(1:2, each = 50)
)
data %>% group_by(treatment, site) %>% ghg_sum_stats(co2, n2o, showDT = FALSE)
```

guess\_prefix

Infer prefix from a gas column name

## Description

Infer prefix from a gas column name

#### Usage

```
guess_prefix(based_on)
```

## Arguments

based\_on

Name of gas column

#### Value

Prefix compatible with attributes

hello

Hello, World!

#### **Description**

Prints 'Hello, world!'.

## Usage

hello()

## **Examples**

hello()

 ${\tt import\_chamber\_volume} \ \ {\it Import\ Chamber\ Volume\ Data}$ 

## Description

Imports and cleans up chamber volume Excel spreadsheets contained in path.

## Usage

```
import_chamber_volume(path = "data/00_raw/chamber_volume")
```

## Arguments

path

File path in which to look for chamber volume files. Defaults to "data/00\_raw/chamber\_volume".

#### Value

A data frame of all chamber volume data.

impute\_missing\_values Impute missing gas data

#### **Description**

Replaces gas\_vars with NA according to excl\_vars. Then fills NAs with imputed values using the procedure described in **Details**.

#### Usage

```
impute_missing_values(
  data,
  gas_vars = c(co2_kg_ha_day, n2o_kg_ha_day, ch4_kg_ha_day, nh3_kg_ha_day),
  excl_vars = NULL,
  site_var = site,
  date_var = Date,
  plot_var = plot,
  keep_all_cols = FALSE
)
```

#### **Arguments**

data	A data frame		
gas_vars	Names of columns in data containing gas data to be imputed. Defaults to c(co2_kg_ha_day, n2o_kg_ha_day, ch4_kg_ha_day,nh3_kg_ha_day).		
excl_vars	Names of logical columns in data which are TRUE when the corresponding gas_vars should be replaced with NA and then imputed. The order of names should match those in gas_vars (i.e. the first column specified in gas_vars is imputed when the first column specified in excl_vars is TRUE. Defaults to c(co2_exclude, n2o_exclude, ch4_exclude, nh3_exclude).		
site_var	Name of column in data containing site names. Defaults to site.		
date_var	Name of column in data containing sampling dates. Defaults to Date.		
plot_var	Name of column in data containing plot IDs. Defaults to plot.		
keep_all_cols	Logical. Should intermediate columns used in imputation calculations be retained in the output?		

## **Details**

Imputation is performed using the following procedure:

- 1. Data are arranged by site\_var, plot\_var, and date\_var so that each unique plot's samplings appear in chronological order in data.
- 2. Columns are added that fill NAs with the nearest non-NA observation before AND after each missing value.
- 3. The distance between the missing values and each of the values it was filled with is calculated (i.e. how many samplings between the missing value and the nearest non-NA values before and after, chronologically?)

include\_n

4. If the minimum distance between the missing value and a non-NA value is 2 or less, the missing value is replaced with the mean of the previous non-NA value and the next non-NA value chronologically.

5. If the minimum distance is greater than 2, the missing value is replaced with the grand mean of all non-NA observations for the plot.

#### Value

data with new columns for imputed values. When keep\_all\_cols is TRUE, intermediate columns generated for imputation calculations (e.g. grand means by plot) are retained in the output.

include\_n

Count Observations Not Yet Excluded from Processing

## **Description**

Count Observations Not Yet Excluded from Processing

#### Usage

```
include_n(data, excl_var)
```

#### **Arguments**

data A data frame containing a logical column tracking processing exclusions by

observation.

excl\_var Name of logical column which tracks processing exclusions. Defaults to exclude\_obs.

#### Value

Integer count of rows in data where exclude is FALSE.

#### **Examples**

```
dat <- data.frame(
x = rnorm(10),
exclude_obs = sample(c(TRUE, FALSE), 10, replace = TRUE)
)
include_n(dat)</pre>
```

is\_outlier 17

is\_outlier

Detect outliers

#### **Description**

Intended for use inside mutate() or filter(). Detects outliers in column or grouped column x as values less than the 25 ranges or greater than the 75 Returns TRUE for outliers and FALSE for non outliers.

# Usage

```
is\_outlier(x, n\_IQR = 3)
```

#### **Arguments**

n\_IQR Integer. Number of interquartile ranges below 25 above 75 to 3.

gas\_var Gas flux column in which to detect outliers

#### Value

A logical vector the same length as x (or current group)

```
make_preprocessing_report
```

Perform Preprocessing Steps and Make HTML Reports

## Description

Perform Preprocessing Steps and Make HTML Reports

```
make_preprocessing_report(
  data,
  date_var = Date,
  site_var = site,
  rmd_file = "code/110_preprocessing.Rmd",
  output_data_dir,
  output_report_dir,
  output_file,
  parent = rstudioapi::getActiveDocumentContext()$path,
  overwrite = FALSE,
  verbose = TRUE
)
```

#### **Arguments**

data	A data frame containing a single unique date and site of sampling	
date_var	Name of column in data containing the date of sampling. Defaults to Date.	
site_var	Name of column in data containing the site of sampling. Defaults to site.	
rmd_file	RMarkdown file from which to generate reports using render(). Defaults to "code/110_preprocessing.Rmd".	
output_data_di	ir	
	Optional. Directory in which to store data outputs. If not specified, data outputs will be stored in "data/01_converted_to_flux_rate/site_var_1", where site_var_1 is replaced with the name of the single unique site in data\$site_var. The directory will be created if it does not already exist.	
output_report_dir		
	Optional. Directory in which to store HTML report outputs. If not specified, reports will be stored in "data/01_converted_to_flux_rate/site_var_1/html_reports", where site_var_1 is replaced with the name of the single unique site in data\$site_var. The directory will be created if it does not already exist.	
output_file	Optional. Name of file outputs. If not specified, files will be named "YYYYMMDD_preprocessing", where "YYYYMMDD" is replaced with the single unique date in data\$date_var.	
overwrite	Logical. Should render() be performed if output_file.html already exists at output_report_dir? Defaults to FALSE.	
verbose	Logical. Should messages be printed to the console? Defaults to TRUE.	

# Value

Nothing in R memory. Exports reports and data files to specified directories.

```
\begin{tabular}{ll} mutate\_levene\_shapiro\_p \\ Add\ levene\ and\ shapiro\ p\ values\ to\ model\ data \end{tabular}
```

# Description

Add levene and shapiro p values to model data

```
mutate_levene_shapiro_p(
  data,
  formula,
  gas_vars = c(co2, n2o, ch4, nh3),
  resid_vars = NULL
)
```

mutate\_residuals 19

#### **Arguments**

data A data frame

gas\_vars Names of columns in data containing gas data to be substituted in formula.

Each name should be an unquoted expression. Defaults to c(co2, n2o, ch4,

nh3).

resid\_vars Unquoted expressions. Names of columns in data containing model residuals.

Order should correspond with gas\_vars. If NULL, gas\_vars will be appended

with "\_resid" to deduce the residual variable names.

#### Value

data with length(gas\_vars) \* 2 new columns

mutate\_residuals

Add model residuals to data

## **Description**

Add model residuals to data frame used in modeling. Typically used after build\_gas\_lmer.

#### Usage

```
mutate_residuals(data, models, suffix = "_resid")
```

#### **Arguments**

data A data frame

models List of models generated with build\_gas\_lmer.

suffix String. By default, names of new columns containing residuals will be based on

the names of the models in models (usually gas variable names), plus a suffix of

"\_resid". A different suffix can be specified with this argument.

#### Value

data with length(models) new columns.

negative\_flux

Replace or Exclude Negative Values

## Description

Replace or Exclude Negative Values

20 noaa\_temp\_fig

#### Usage

```
negative_flux(
  data,
  gas_var,
  excl_var,
  method = c("excl", "zero"),
  attr_var = attributes,
  prefix,
  sep = ",",
  datatable = FALSE
)
```

## **Arguments**

data	A data frame
gas_var	Name of column in data containing gas flux data to be screened for negative values
excl_var	Name of logical column in data which is equal to TRUE when an observation of gas_var should be excluded from downstream processing and analysis.
method	Character. Method of handling negative values: exclusion or replacement with 0. Options are "excl" or "zero".
attr_var	Passed to attr_update(). Name of column in data which records attributes. Defaults to attributes.
prefix	Passed to attr_update(). Character. Unique prefix denoting attribute element in attr_var to be updated. If not specified, it will be inferred from gas_var.
sep	Passed to attr_update(). String that separates attribute elements in attr_var. Defaults to ','.
datatable	Logical. Should a datatable (using datatable() of extracted negative flux values be printed? Defaults to FALSE.

#### Value

data with, if method = "excl", updated excl\_var and attr\_var, or, if method = "zero", updated gas\_var.

noaa\_temp\_fig

Daily Minimum and Maximum Air Temperatures Barplot

## Description

Daily Minimum and Maximum Air Temperatures Barplot

```
noaa_temp_fig(
  data,
  date_var = Date,
  tmax = NOAA_airtemp_c_max,
  tmin = NOAA_airtemp_c_min,
```

ppm\_seconds\_lm 21

```
site_var = NULL,
sample_dates,
bar_fill_colors = c("#D2B4DE", "#AED6F1", "#A569BD", "#3498DB"),
date_breaks = "1 month",
date_labels = "%b %Y",
text_size = 14,
x_lab = "Date",
y_lab = "Daily Minimum and Maximum\nAir Temperature (°C)"
)
```

#### **Arguments**

data A data frame containing one row per calendar day Name of column in data containing dates in "YYYY-MM-DD" format. Defaults to date\_var Date. tmax Name of column in data containing daily maximum air temperature. Defaults to NOAA\_airtemp\_c\_max. tmin Name of column in data containing daily minimum air temperature. Defaults to NOAA\_airtemp\_c\_min. Name of column in data containing site names. If provided, it will be used in site\_var the rows argument of facet\_grid(). Defaults to NULL. Vector of all unique dates of sampling. By default, bars on these dates will be sample\_dates darker than non-sampling-date bars. bar\_fill\_colors Vector of length 4 specifying colors for, respectively, daily max temp on a nonsampling date, daily min temp on a non-sampling date, daily max temp on a sampling date, and daily min temp on a sampling date. Defaults to c('#D2B4DE', '#AED6F1', '#A569BD', '#3498DB'). date\_breaks String. Passed to scale\_x\_date(). Defaults to '1 month'. text\_size Integer. Size of text on plots. Defaults to 14.  $x_1ab$ String or expression. X-axis label. Defaults to "Date".

String or expression. Y-axis label. Defaults to "Daily Minimum and Maximum\nAir

#### Value

y\_lab

A ggplot object

ppm_seconds_lm	Model Gas ppm per Second
• •	** *

Temperature (°C)".

#### Description

Create a model of gas ppm per second, with or without use of an optimization algorithm to remove endpoints attributable to Gasmet warm-up or cool-down.

When optimization = TRUE, the function uses calib\_optim() and calib\_range() to model  $CO_2$  data with optimization as described in **Details**. Returns data with optimized excl\_var column,

22 ppm\_seconds\_lm

updated attr\_var, and additional columns:  $co2\_rsq$ ,  $co2\_intercept$ , and  $co2\_slope$ , which correspond to the  $R^2$ , intercept, and slope of the final model, respectively.

When optimization = FALSE (the default), the function creates a linear model of gas\_var  $\sim$  seconds\_var excluding observations where excl\_var == TRUE. If the model  $R^2$  is at least 0.1, the function adds the model coefficients and  $R^2$  value in new columns in data. Otherwise, the same columns are added but with all entries NA. Attributes are updated in data as needed (see ?attr\_show\_codes for details). A logical column is added to track exclusions of the specific gas being modeled.

Typically, this function should be run first on  $CO_2$  data with optimization = TRUE, then on other gases with optimization = FALSE.

## Usage

```
ppm_seconds_lm(
 data,
 gas_var,
 excl_var = exclude_obs,
 min_n = 4,
  seconds_var = seconds,
  attr_var = attributes,
 prefix,
 optimization = FALSE
)
ppm_seconds_lm_optim(
 data,
 gas_var = Carbon.dioxide.CO2,
 excl_var = exclude_obs,
 min_n = 4,
  seconds_var = seconds,
 attr_var = attributes,
 prefix = "all",
 optimization = TRUE
ppm_seconds_lm_asis(
 data,
 gas_var,
 min_n = 4,
 excl_var = exclude_obs,
  seconds_var = seconds,
  attr_var = attributes,
 prefix,
  optimization = FALSE
```

#### **Arguments**

data	Data frame containing CO <sub>2</sub> data
gas_var	Name of column in data containing gas ppm data to be modeled. Defaults to Carbon.dioxide.CO2 when optimization = TRUE.
excl_var	Logical column in data which is equal to TRUE when an observation of gas_var should be excluded from modeling and downstream analyses. Defaults to exclude obs.

ppm\_seconds\_lm 23

min_n	Integer. Minimum number of data points for optimization algorithm to retain in final model. Passed to calib_optim() and calib_range(). Defaults to 4.
seconds_var	Name of column in data containing seconds since start of gas measurement. Defaults to seconds.
attr_var	Name of column in data where attributes are stored. Defaults to attributes.
prefix	Passed to attr_update(). Defaults to "all" when optimization = TRUE. If missing when optimization = FALSE, it will attempt to be inferred from gas_var.
optimization	Logical. Whether or not to perform optimization algorithm descibed in <b>Details</b> . Defaults to FALSE.

#### **Details**

When optimization = TRUE, the optimization proceeds as follows:

- If data has less than min\_n observations where excl\_var == FALSE, modeling is not performed and '02' is added to data\$attr\_var for all gases. New columns are added with all values NA.
- 2. Otherwise, optim() is called:
  - Random instances of data\$excl\_var are generated using calib\_range():
    - Existing observations where data\$excl\_var == TRUE are retained
    - n observations at the head  $(n_{\rm head})$  and/or tail  $(n_{\rm tail})$  of data\$excl\_var are replaced with TRUE, where n = 0 m, and m is a dynamic integer which keeps the sum of  $n_{\rm head}$  and  $n_{\rm tail}$  less than nrow(data) min\_n (i.e. the number of observations included remains  $\geq \min_n$ )
  - Each random instance of data\$excl\_var is fed to calib\_optim() which executes the following scheme:
    - A model of CO<sub>2</sub> per second, excluding observations marked for exclusion in the random instance, is generated
    - If the model  $R^2$  value is  $\geq 0.98$ , the result fed to optim is the number of observations excluded from the model (this is the value we want to minimize)
    - If the model R<sup>2</sup> value is < 0.98, an arbitrary, extremely large value is returned to discourage optim() from choosing that model
    - The previous three steps are repeated 1000 or nrow(data) \* 10 times, whichever is larger.
- 3. If there is never a model with  $R^2 \geq 0.98$  in any iteration, the modeling is considered a failure case, all values in data $excl_var$  are updated to TRUE, '03' is added to dataatributes, and new columns are added with all values NA.
- 4. Otherwise, the model is considered a success case and the resulting data frame contains the values of data\$excl\_var used in the final model, and new columns with model coefficients.

#### Value

data with new columns containing model coefficients and updated attr\_var.

#### See Also

```
ppm_seconds_plot(), calib_optim(), calib_range()
```

24 ppm\_seconds\_plot

ppm\_seconds\_plot Create ggplot for ppm Gas per Second Linear Models

#### **Description**

Create side-by-side ggplots of pre- and post-optimization models of gas ppm per second, or a plot displaying a failure message when models do not meet quality control parameters.

## Usage

```
ppm_seconds_plot(
   data,
   gas_var,
   gas_name = c("co2", "n2o", "ch4", "nh3"),
   excl_var = paste0(gas_name, "_exclude"),
   rsq_var = paste0(gas_name, "_rsq"),
   co2_excl_var = exclude_obs,
   co2_rsq_var = co2_rsq,
   plot_var = plot,
   seconds_var = seconds
)
```

## **Arguments**

data	A data frame
gas_var	Name of column in data containing gas data to be plotted
gas_name	Character. Name of gas that should be used in messages on plots. Options are 'co2', 'n2o', 'ch4', and 'nh3'. Should correspond to gas_var.
excl_var	Name of logical column in data which tracks observations of gas_var which were excluded from ppm per second modeling. Defaults to paste0(gas_name, "_excl").
rsq_var	Name of column containing R-squared values for the model of gas_var $\sim$ seconds_col. Defaults to paste0(gas_name, "_rsq").
co2_rsq_var	Name of column containing R-squared value for CO2 ppm ~ seconds model. If model_co2() was used, this should be co2_rsq. Defaults to co2_rsq.
plot_var	Name of column containing plot IDs. Defaults to plot.
seconds_var	Name of column containing number seconds since the start of the gas measurement in the plot. Defaults to seconds.

#### **Details**

data should contain data for a single plot on a single sampling date.

## Value

A plot

#### See Also

```
model_co2()
```

qqplots 25

qqplots

Make Normal Quantile-Quantile Plots for Multiple Gases

#### **Description**

Make Normal Quantile-Quantile Plots for Multiple Gases

## Usage

```
qqplots(
  data,
  gas_vars = c(co2, n2o, ch4, nh3),
  resid_vars = NULL,
  one_plot = TRUE
)
```

#### **Arguments**

data A data frame

gas\_vars Unquoted expressions. Names of columns in data containing gas data.

resid\_vars Unquoted expressions. Names of columns in data containing model residuals.

Order should correspond with gas\_vars. If NULL, gas\_vars will be appended

with "\_resid" to deduce the residual variable names.

one\_plot Logical. Should plots be arranged on a single grid in the output? If FALSE, a list

of plots is returned.

#### Value

If one\_plot = TRUE, a single plot. If one\_plot = FALSE, a list of ggplots.

regression\_fig

Scatterplot Figure with Regression Line, Equation, and Stats

## Description

Scatterplot Figure with Regression Line, Equation, and Stats

```
regression_fig(
  data,
  x_var,
  y_var,
  group_var,
  facet_rows_var = gas,
  facet_cols_var = site,
  labeller = "label_value",
  group_colors,
  x_lab = "",
```

26 regression\_fig

```
y_lab = "",
color_lab = "",
text_size = 14,
point_shape = 16,
point_alpha = 0.5,
legend_position = "top",
eqn_x = 0,
eqn_y = Inf,
eqn_vjust = 1.5,
rr_x = 0,
rr_y = Inf,
rr_vjust = 1
```

#### **Arguments**

data A data frame. Should contain one row per experimental unit. Name of column in data to be used as the x variable. x\_var Name of column in data to be used as the y variable. y\_var Optional. Name of column in data to be used as a grouping variable. One group\_var regression line will appear per group. Optional. Name of column in data to be used as rows argument in facet\_grid(). facet\_rows\_var Set to NULL to remove facet rows. Defaults to gas. Optional. Name of column in data to be used as cols argument in facet\_grid(). facet\_cols\_var Set to NULL to remove facet columns. Defaults to site. labeller Passed to facet\_grid(). A labeller object containing specifications to be used in labeller(). See ?labeller for details. Defaults to "label\_value". group\_colors Optional. Color palette for group\_var. If group\_var is provided but group\_colors is missing, brewer.pal()'s 'Set3' will be used as the color palette. x\_lab String. X axis label. Defaults to empty. y\_lab String. Y axis label. Defaults to empty. color\_lab String. Color legend title. Defaults to empty. text\_size Size of text on plot. Defaults to 14. Integer. Shape of points. Defaults to 16. point\_shape point\_alpha Numeric 0-1. Opacity of points. Defaults to 0.5. legend\_position String. Position of legend on plot. Options 'top', 'left', 'right', 'bottom', or 'none'. Defaults to 'top'. Numeric. X axis position of regression equation. Defaults to 0. eqn\_x Numeric. Y axis position of regression equation. Defaults to Inf. eqn\_y Numeric. Vertical justification of regression equation. Defaults to 1.5. eqn\_vjust Numeric. X axis position of  $\mathbb{R}^2$  and p-value. Defaults to  $\emptyset$ . rr\_x Numeric. Y axis position of R<sup>2</sup> and p-value. Defaults to Inf. rr\_y

Numeric. Vertical justification of R<sup>2</sup> and p-value. Defaults to 1.

#### Value

A plot

rr\_vjust

replace\_gas\_with\_na 27

replace_gas_w	۷i	th_	na
---------------	----	-----	----

Replace gas variable entries with NA based on their corresponding exclusion tracking columns

#### **Description**

Replace gas variable entries with NA based on their corresponding exclusion tracking columns

## Usage

```
replace_gas_with_na(
 data,
 gas_vars = c(co2_kg_ha_day, n2o_kg_ha_day, ch4_kg_ha_day, nh3_kg_ha_day),
 excl_vars = c(co2_exclude, n2o_exclude, ch4_exclude, nh3_exclude)
```

#### **Arguments**

data A data frame gas\_vars Names of columns in data containing gas data to be replaced with NA when the corresponding variable in excl\_vars is TRUE. Defaults to c(co2\_kg\_ha\_day, n2o\_kg\_ha\_day, ch4\_kg\_ha\_day, nh3\_kg\_ha\_day). excl\_vars Names of logical columns in data which are TRUE when the corresponding gas\_vars should be replaced with NA. The order of names should match those in gas\_vars (i.e. the first column specified in gas\_vars is replaced with NA

when the first column specified in excl\_vars is TRUE. Defaults to c(co2\_exclude, n2o\_exclude, ch4\_exclude, nh3\_exclude).

#### Value

data with updated gas\_vars columns

resplots

Make Model Residual Plots for Multiple Gases

#### **Description**

Make Model Residual Plots for Multiple Gases

```
resplots(
  data,
  gas_vars = c(co2, n2o, ch4, nh3),
 resid_vars = NULL,
  one_plot = TRUE
)
```

28 round\_p

#### **Arguments**

data A data frame

gas\_vars Unquoted expressions. Names of columns in data containing gas data.

resid\_vars Unquoted expressions. Names of columns in data containing model residuals.

Order should correspond with gas\_vars. If NULL, gas\_vars will be appended

with "\_resid" to deduce the residual variable names.

one\_plot Logical. Should plots be arranged on a single grid in the output? If FALSE, a list

of plots is returned.

#### Value

A list of ggplots

rm\_random\_fx

Remove random effects from lmer-type model formula

#### **Description**

Convenience function to remove random effects from lmer type model formulas, which is sometimes necessary for model checking functions like Levene's test.

#### Usage

```
rm_random_fx(formula)
```

## **Arguments**

formula String.

String. Formula of the type " $y \sim x + (1|block)$ ".

#### Value

String containing only fixed effects from formula

round\_p

Round P Values for Plot Labels

## Description

Rounds p to three decimal places. If the rounded value is less than 0.001, the output is "< 0.001". Otherwise, the output is "= 0.000" where 0.000 is the rounded p.

## Usage

round\_p(p)

#### **Arguments**

р

Numeric. P value to be rounded

#### Value

Character "< 0.001" or "= p" where p is rounded to 3 decimal places.

#### **Examples**

```
round_p(0.000025038)
round_p(0.424610370)
```

summary\_boxplots\_flux Summary Boxplots of Daily Flux Data

## Description

Summary Boxplots of Daily Flux Data

#### Usage

```
summary_boxplots_flux(
  data,
  x_{var} = treatment,
  y_vars = c(co2_kg_ha_day, n2o_kg_ha_day, ch4_kg_ha_day, nh3_kg_ha_day),
  by = c(site, Date),
  x_lab = "Treatment",
 y_{abs} = c("Carbon Dioxide\n(kg CO2-C/ha/day)", "Nitrous Oxide\n(kg N2O-N/ha/day)",
    "Methane\n(kg\ CH4-C/ha/day)", "Ammonia\n(kg\ NH3-N/ha/day)"),
  box_color = "sienna2",
  box_fill = "transparent",
  box_alpha = 1,
  point_shape = 21,
  point_alpha = 0.5,
  point_color = "black",
  point_fill = "gray",
  plot_var = plot,
  facet_scales = "free_y"
)
```

# Arguments

data	A data frame
x_var	Name of column in data that should be plotted as the $\boldsymbol{x}$ variable. Defaults to treatment.
y_vars	Name(s) of column(s) in data that should be plotted as the y variable(s). If mulliple names are given, plots will be faceted so that there is one facet per y variable. See facet_grid() for details.
by	Split the data by these variables and make a plot for each. Defaults to c(site, Date). Set to NULL to generate a single plot.
x_lab	String. Label that will appear on the x axis. Defaults to 'Treatment'.
y_labs	String. Label(s) that will appear on the y axis or facet labels. Order should correspond to y_vars.

```
box_color
                  String. Outline color of boxes in boxplots. Defaults to 'sienna2'.
box_fill
                  String. Fill color of boxes in boxplots. Defaults to "transparent".
                  Numeric 0-1. Opacity of boxes in boxplots. Defaults to 1.
box_alpha
point_shape
                  Integer. Shape of points on boxplots. Defaults to 21.
point_alpha
                  Numeric 0-1. Opacity of points on boxplots. Defaults to 0.5.
point_color
                  String. Outline color of points on boxplots. Defaults to 'black'.
point_fill
                  String. Fill color of points on boxplots. Defaults to "gray".
plot_var
                  Name of column in data containing plot IDs. Defaults to plot.
                  String. Passed to scales arg of facet_grid(). Defaults to "free_y".
facet_scales
```

#### Value

A single boxplot if by is NULL, or else a list of boxplots.

```
summary_boxplots_loads
```

Summary Boxplots of Cumulative Gas Load Data

## Description

Summary Boxplots of Cumulative Gas Load Data

```
summary_boxplots_loads(
 data,
 x_{var} = treatment,
 y_vars = c(co2_kg_ha_load, n2o_kg_ha_load, ch4_kg_ha_load, nh3_kg_ha_load),
 by = site,
 x_lab = "Treatment",
 y_{abs} = c("Carbon Dioxide Load\n(kg CO2-C/ha)", "Nitrous Oxide Load\n(kg N2O-N/ha)",
    "Methane Load\n(kg CH4-C/ha)", "Ammonia Load\n(kg NH3-N/ha)"),
 box_color = "sienna2",
 box_fill = "transparent",
 box_alpha = 1,
 point_shape = 21,
 point_alpha = 0.5,
 point_color = "black",
 point_fill = "gray",
 plot_var = plot,
 date_var = Date,
  facet_scales = "free_y"
)
```

time\_series 31

# Arguments

data	A data frame
x_var	Name of column in data that should be plotted as the $\boldsymbol{x}$ variable. Defaults to treatment.
y_vars	Name(s) of column(s) in data that should be plotted as the y variable(s). If mutliple names are given, plots will be faceted so that there is one facet per y variable. See facet_grid() for details.
by	Split the data by these variables and make a plot for each. Defaults to c(site, Date). Set to NULL to generate a single plot.
x_lab	String. Label that will appear on the x axis. Defaults to 'Treatment'.
y_labs	String. Label(s) that will appear on the y axis or facet labels. Order should correspond to y_vars.
box_color	String. Outline color of boxes in boxplots. Defaults to 'sienna2'.
box_fill	String. Fill color of boxes in boxplots. Defaults to "transparent".
box_alpha	Numeric 0-1. Opacity of boxes in boxplots. Defaults to 1.
point_shape	Integer. Shape of points on boxplots. Defaults to 21.
point_alpha	Numeric 0-1. Opacity of points on boxplots. Defaults to 0.5.
point_color	String. Outline color of points on boxplots. Defaults to 'black'.
point_fill	String. Fill color of points on boxplots. Defaults to "gray".
plot_var	Name of column in data containing plot IDs. Defaults to plot.
date_var	Name of column in data containing sampling date. Defaults to Date.
facet_scales	String. Passed to scales arg of facet_grid(). Defaults to "free_y".

## Value

A single boxplot if by is NULL, or else a list of boxplots.

time_series	Time Series of Gas Data	

# Description

Time Series of Gas Data

```
time_series(
  data,
  date_var = Date,
  mean_var = gas_value,
  se_var = se,
  lines_group_var = treatment,
  facet_rows_var = gas,
  facet_cols_var = site,
  labeller = "label_value",
  line_colors,
```

32 time\_series

```
x_lab = "Date",
y_lab = "",
color_lab = "Treatment",
date_breaks = "1 month",
date_labels = "%b %Y",
text_size = 14
)
```

# Arguments

data	A data frame. Should be summarized (in most cases, by site/Date/treatment).
date_var	Name of column in data containing sampling date in "YYYY-MM-DD" format. Defaults to Date.
mean_var	Name of column in data containing mean gas value to be used as the y variable. Defaults to gas_value.
se_var	Name of column in data containing standard error of the mean gas value to be used in error bars. Defaults to se.
lines_group_var	•
	Name of column in data to use as grouping variable for lines. Defaults to treatment. Set to 1 to plot a single line.
facet_rows_var	Name of column in data to be used in faceting rows using facet_grid(). Defaults to gas. Set to NULL to remove row faceting.
facet_cols_var	Name of column in data to be used in faceting columns using facet_grid(). Defaults to site. Set to NULL to remove column faceting.
labeller	Passed to labeller(). A labeller object containing specifications to be used in facet_grid(). See ?facet_grid for details.
line_colors	Vector of colors to be used for lines. Length must match length of unique levels of lines_group_var in data. If not specified, the function will use 'Set3' from brewer.pal().
x_lab	Label for the x axis. Defaults to 'Date'.
y_lab	Label for the y axis. Defaults to empty.
color_lab	Label for color legend. Defaults to "Treatment".
date_breaks	Passed to scale_color_manual(). Defaults to '1 month'.
text_size	Size of text on plot. Defaults to 14.

# Value

A plot