

Package: fluxfinder (via r-universe)

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Type Package

Title Parsing, Computation, and Diagnostics for Greenhouse Gas Measurements

Version 1.0.1

Description Parse static-chamber greenhouse gas measurement files generated by a variety of instruments; compute flux rates using multi-observation metadata; and generate diagnostic metrics and plots. Designed to be easy to integrate into reproducible scientific workflows.

URL <https://github.com/COMPASS-DOE/fluxfinder>

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Encoding UTF-8

LazyData true

Imports broom (≥ 1.0), jsonlite (≥ 1.8), lubridate (≥ 1.0), MASS (≥ 7.0)

Suggests gasfluxes, ggplot2, knitr, rmarkdown, testthat ($\geq 3.0.0$), withr (≥ 2.0)

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RoxygenNote 7.3.1

VignetteBuilder knitr

BugReports <https://github.com/COMPASS-DOE/fluxfinder/issues>

Config/pak/sysreqs libicu-dev

Repository <https://compass-doe.r-universe.dev>

RemoteUrl <https://github.com/compass-doe/fluxfinder>

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ffi_compute_fluxes	<i>Compute fluxes for multiple groups (measurements)</i>
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Description

Compute fluxes for multiple groups (measurements)

Usage

```
ffi_compute_fluxes(
  data,
  group_column,
  time_column,
  gas_column,
  dead_band = 0,
  normalize_time = TRUE,
  fit_function = ffi_fit_models,
  ...
)
```

Arguments

data	A data.frame (or tibble or data.table)
group_column	Name of the grouping column in data, character; pass NULL to run with no grouping
time_column	Name of the time column in data, character
gas_column	Name of the gas (concentration or quantity) column in data, character
dead_band	Length of dead band, the equilibration period at the beginning of the time series during which data are ignore, in seconds (numeric)

normalize_time Normalize the values so that first is zero? Logical
 fit_function Optional flux-fit function; default is [ffi_fit_models](#)
 ... Other parameters passed to fit_function

Value

A data.frame with one row per group_column value. It will always include the mean, minimum, and maximum values of time_column for that group, but other columns depend on what is returned by the fit_function.

See Also

[ffi_fit_models](#)

Examples

```
# No grouping
ffi_compute_fluxes(cars, group_column = NULL, "speed", "dist")
# With grouping
cars$Plot <- c("A", "B")
ffi_compute_fluxes(cars, "Plot", "speed", "dist")
# See the introductory vignette for a fully-worked example with real data
```

ffi_fit_models *Fit various models to gas concentration data*

Description

Fit various models to gas concentration data

Usage

```
ffi_fit_models(time, conc, area, volume)
```

Arguments

time Relative time of observation (typically seconds), numeric
 conc Greenhouse gas concentration (typically ppm or ppb), numeric
 area Area covered by the measurement chamber (typically cm²), numeric
 volume Volume of the system (chamber + tubing + analyzer, typically cm³), numeric

Details

If a linear model cannot be fit, NULL is returned. If the robust linear and/or polynomial models cannot be fit, then NA is returned for their particular statistics. The HM1981 approach is only valid for saturating (exponential) data and NA is returned otherwise.

Value

A wide-form `data.frame` with fit statistics for linear ("lin", `lm`), robust linear ("rob", `rlm`), polynomial ("poly"), and H&M1981 ("HM81", `ffi_hm1981`) models. The latter is based on an exponential model drawn from one-dimensional diffusion theory; see Hutchinson and Mosier (1981) and Nakano et al. (2004).

For each model type, the following columns are returned:

- Model statistics AIC, r.squared, RMSE, and p.value;
- Flux (slope) statistics `flux.estimate` and `flux.std.error`;
- Intercept statistics `int.estimate` and `int.std.error`;
- For the robust linear regression model only, a logical value `converged`.

Note

Normally this is not called directly by users, but instead via `ffi_compute_fluxes`.

References

Nakano, T., Sawamoto, T., Morishita, T., Inoue, G., and Hatano, R.: A comparison of regression methods for estimating soil-atmosphere diffusion gas fluxes by a closed-chamber technique, *Soil Biol. Biochem.*, 36, 107–113, 2004. doi:[10.1016/j.soilbio.2003.07.005](https://doi.org/10.1016/j.soilbio.2003.07.005)

Hutchinson, G. L. and Mosier, A. R.: Improved soil cover method for field measurement of nitrous oxide fluxes, *Soil Sci. Soc. Am. J.*, 45, 311-316, 1981. doi:[10.2136/sssaj1981.03615995004500020017x](https://doi.org/10.2136/sssaj1981.03615995004500020017x)

Examples

```
# Toy data - linear
ffi_fit_models(cars$speed, cars$dist)

# Toy data - nonlinear
ffi_fit_models(Puromycin$conc, Puromycin$rate)

# Real data
f <- system.file("extdata/TG10-01087.data", package = "fluxfinder")
dat <- ffi_read_LI7810(f)[1:75,] # isolate first observation
dat$SECONDS <- dat$SECONDS - min(dat$SECONDS) # normalize time to start at 0
plot(dat$SECONDS, dat$CO2)
ffi_fit_models(dat$SECONDS, dat$CO2)
```

ffi_hm1981

Compute flux using nonlinear Hutchinson and Mosier (1981) model

Description

Compute flux using nonlinear Hutchinson and Mosier (1981) model

Usage

```
ffi_hm1981(time, conc, h = 1)
```

Arguments

time	Time values, numeric
conc	Gas concentration values, numeric
h	Effective chamber height

Value

Flux estimate; see references for more information.

References

Hutchinson, G. L. and Mosier, A. R.: Improved soil cover method for field measurement of nitrous oxide fluxes, Soil Sci. Soc. Am. J., 45, 311-316, 1981. doi:[10.2136/sssaj1981.03615995004500020017x](https://doi.org/10.2136/sssaj1981.03615995004500020017x)

Examples

```
# If data are approximately linear, then NA is returned
ffi_hm1981(cars$speed, cars$dist)
# If data are nonlinear (saturating) then flux based on gas diffusion theory
ffi_hm1981(Puromycin$conc, Puromycin$rate)
```

ffi_metadata_match	<i>Match metadata info with a vector of data timestamps</i>
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Description

Match metadata info with a vector of data timestamps

Usage

```
ffi_metadata_match(data_timestamps, start_dates, start_times, obs_lengths)
```

Arguments

data_timestamps	Data timestamps, either character (YYYY-MM-DD HH:MM:SS) or <code>POSIXct</code>
start_dates	Metadata measurement dates, either character (YYYY-MM-DD) or <code>POSIXct</code>
start_times	Metadata measurement start time entries, either character (HH:MM:SS) or <code>period</code>
obs_lengths	Observation lengths in seconds, numeric; must be same length as <code>start_dates</code> . This should include both the intended measurement period as well as any dead band time at the beginning

Value

A numeric vector equal in length to `data_timestamps`, with each entry indicating the metadata entry that should be used for that observation. NA is returned if a timestamp has no match in the metadata (i.e., does not fall within any window defined by the `start_dates`, `start_times`, and observation length parameters).

Note

If `data_timestamps` or `start_dates` cannot be parsed as YYYY-MM-DD, the preferred format, then MM/DD/YYYY (used by U.S. versions of Microsoft Excel when saving CSV files, for example) will be tried.

Examples

```
# Data timestamps
d_t <- c("2024-01-01 13:00:05", "2024-01-01 13:00:10",
"2024-01-01 13:05:05", "2024-01-01 13:10:00")
# Metadata start dates and times: two measurements, starting 5 minutes apart
s_d <- c("2024-01-01", "2024-01-01")
s_t <- c("13:00:00", "13:05:00")
ol <- c(60, 60) # Observation lengths
ffi_metadata_match(d_t, s_d, s_t, ol)
# Returns {1, 1, 2, NA} indicating that the first and second data timestamps
# correspond to metadata entry 1, the third to entry 2, and the fourth
# has no match

# This generates an error because of overlapping timestamps:
## Not run:
s_t <- c("13:00:00", "13:01:00")
ffi_metadata_match(d_t, s_d, s_t, ol)

## End(Not run)
```

ffi_qaqc

Generate a QA/QC document

Description

Generate a QA/QC document

Usage

```
ffi_qaqc(
  flux_data,
  group_column,
  output_file = "qaqc.html",
  output_dir = getwd(),
  open_output = TRUE
)
```

Arguments

flux_data	A data frame from <code>ffi_compute_fluxes</code> or similar
group_column	Name of the grouping label column in flux_data, character; pass NULL to run with no grouping
output_file	Name of the output file
output_dir	Name of the output directory; default is current working directory
open_output	Automatically open the output HTML file?

Value

The path of the output file.

Examples

```
# Toy data
cars$Plot <- c("A", "B")
fd <- ffi_compute_fluxes(cars, "Plot", "speed", "dist")
x <- ffi_qaqc(fd, group_column = "Plot")
file.remove(x) # clean up
# See the introductory vignette for a fully-worked example with real data
```

ffi_read_EGM4	<i>Read an EGM-4 data file</i>
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Description

Read an EGM-4 data file

Usage

```
ffi_read_EGM4(file, year, tz = "UTC")
```

Arguments

file	Filename to read, character
year	Four-digit year of the data (EGM-4 output files have month, day, hour, and minute, but not year), numeric or character
tz	Time zone of the file's time data, character (optional)

Value

A `data.frame` with the parsed data.

Examples

```
f <- system.file("extdata/EGM4-data.dat", package = "fluxfinder")
dat <- ffi_read_EGM4(f, 2023)
dat <- ffi_read_EGM4(f, 2023, tz = "EST") # specify time zone
```

ffi_read_LGR915	<i>Read a LGR 915-0011 data file</i>
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Description

Read a LGR 915-0011 data file

Usage

```
ffi_read_LGR915(file, date_format = "DMY", tz = "UTC")
```

Arguments

file	Filename to read, character
date_format	Date format, character: "MDY" (month-day-year) "DMY" (day-month-year), or "YMD" (year-month-day)
tz	Time zone of the file's time data, character (optional)

Details

The LGR 915-0011 was an Ultra-Portable Greenhouse Gas Analyzer made by Los Gatos Research. The date in its output files can appear in different formats, which is why the `date_format` parameter is needed.

Value

A [data.frame](#) with the parsed data.

Note

Some LGR 915 files can have a PGP block at the end; this is ignored.

Examples

```
f <- system.file("extdata/LGR-data.csv", package = "fluxfinder")
dat <- ffi_read_LGR915(f, date_format = "MDY")
dat <- ffi_read_LGR915(f, date_format = "MDY", tz = "EST") # specify time zone
```

ffi_read_LI7810	<i>Read a LI-7810 data file</i>
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Description

Read a LI-7810 data file

Usage

```
ffi_read_LI7810(file)
```

Arguments

file	Filename to read, character
------	-----------------------------

Details

Currently LI-7810 and LI-7820 files are handled identically.

Value

A [data.frame](#) with the parsed data.

Examples

```
f <- system.file("extdata/TG10-01087.data", package = "fluxfinder")
dat <- ffi_read_LI7810(f)
```

ffi_read_LI7820	<i>Read a LI-7820 data file</i>
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Description

Read a LI-7820 data file

Usage

```
ffi_read_LI7820(file)
```

Arguments

file	Filename to read, character
------	-----------------------------

Details

Currently LI-7810 and LI-7820 files are handled identically.

Value

A `data.frame` with the parsed data.

Examples

```
f <- system.file("extdata/TG20-01182.data", package = "fluxfinder")
dat <- ffi_read_LI7820(f)
```

<code>ffi_read_LI850</code>	<i>Read a LI-850 data file</i>
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Description

Read a LI-850 data file

Usage

```
ffi_read_LI850(file, tz = "UTC")
```

Arguments

<code>file</code>	Filename to read, character
<code>tz</code>	Time zone of the file's time data, character (optional)

Value

A `data.frame` with the parsed data, including a `TIMESTAMP` column.

Examples

```
f <- system.file("extdata/LI850.txt", package = "fluxfinder")
dat <- ffi_read_LI850(f)
dat <- ffi_read_LI850(f, tz = "EST") # specify time zone
```

<code>ffi_read_LIsmartchamber</code>	<i>Read a LI-8200-01S (smart chamber) data file</i>
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Description

Read a LI-8200-01S (smart chamber) data file

Usage

```
ffi_read_LIsmartchamber(file, concentrations = TRUE)
```

Arguments

`file` Filename to read, character
`concentrations` Return concentration data (the default), or just summary information? Logical

Value

A `data.frame` with the parsed data.

Note

These files are in **JSON** format. See also <https://www.licor.com/env/products/soil-flux/smart-chamber>.

Author(s)

Ben Bond-Lamberty

Examples

```
f <- system.file("extdata/LI8200-01S.json", package = "fluxfinder")
dat <- ffi_read_LIsmartchamber(f) # returns 240 rows
ffi_read_LIsmartchamber(f, concentrations = FALSE) # only 4 rows
```

`ffi_read_PicarroG2301` *Read a Picarro G2301 data file*

Description

Read a Picarro G2301 data file

Usage

```
ffi_read_PicarroG2301(file, tz = "UTC")
```

Arguments

`file` Filename to read, character
`tz` Time zone of the file's time data, character (optional)

Value

A `data.frame` with the parsed data.

References

https://www.picarro.com/environmental/products/g2301_gas_concentration_analyzer

Examples

```
f <- system.file("extdata/PicarroG2301-data.dat", package = "fluxfinder")
dat <- ffi_read_PicarroG2301(f)
dat <- ffi_read_PicarroG2301(f, tz = "EST") # specify time zone
```

ideal-gas-law

Convert gas concentration to quantity using the Ideal Gas Law

Description

Convert gas concentration to quantity using the Ideal Gas Law

Usage

```
ffi_ppm_to_umol(ppm, volume, temp, atm)
```

```
ffi_ppb_to_nmol(ppb, volume, temp, atm)
```

Arguments

ppm	Gas concentration (ppmv), numeric
volume	System volume (chamber + tubing + analyzer, m3), numeric
temp	Optional chamber temperature (degrees C), numeric
atm	Optional atmospheric pressure (Pa), numeric
ppb	Gas concentration (ppbv), numeric

Value

The quantity value, in micromoles (for `ffi_ppm_to_umol`) or nanomoles (for `ffi_ppb_to_nmol`).

Note

If `temp` and/or `atm` are not provided, the defaults are NIST normal temperature and pressure.

References

Steduto et al.: Automated closed-system canopy-chamber for continuous field-crop monitoring of CO₂ and H₂O fluxes, *Agric. For. Meteorol.*, 111:171-186, 2002. doi:[10.1016/S01681923\(02\)00023-0](https://doi.org/10.1016/S01681923(02)00023-0)

Examples

```
ffi_ppm_to_umol(400, 0.1)
ffi_ppb_to_nmol(400, 0.1)
```

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