

## Supplementary material

S1 Code section. Configuration file settings used in the example with one month of data (January 2021).

```
[import]

src = [
    "indata/2021/**/*.*.dat"
]

timestamp_col = "EPOCH_TIME"

[import.columns]
EPOCH_TIME = "float64"
solenoid_valves = "float16"
ALARM_STATUS = "int8"
CO2 = "float32"
N2O_dry = "float32"
CH4_dry = "float32"

[filters.__TIMESTAMP__]
min_value = "2021-01-01 00:00:01"
max_value = "2021-01-31 23:59:59"

[filters.ALARM_STATUS]
allow_only = [0, 4]
disallow = []

[measurements]
chamber_col = "solenoid_valves"
max_gap = 10 # 10 seconds
min_duration = "00:19:30"
max_duration = "00:24:30"

[chamber_labels]
1 = "RAS 1"
2 = "RAS 2"
3 = "RAS 3"
4 = "RAS 4"
5 = "RAS 5"
6 = "RAS 6"
7 = "RAS 7"
8 = "RAS 8"
9 = "RAS 9"
10 = "RAS 10"
11 = "RAS 11"
12 = "RAS 12"
13 = "RAS 13"
14 = "RAS 14"
15 = "RAS 15"

[fluxes]
gases = ["N2O_dry", "CH4_dry", "CO2"]
t0_delay = "00:06:10"
t0_margin = "00:02:00"
A = 0.25
```

Q = 4.16e-6

V = 50e-3

Figure S1. Fragment of the output data after calculating the volumetric flux with fluxes command.

data_start	t0	chamber_val	chamber_lab	gas	c0	vol_flux
27:27,4	33:37,4	7	RAS 7	N2O_dry	0,3300338	1,64E-06
27:27,4	33:37,4	7	RAS 7	CH4_dry	2,4132714	-1,69E-06
27:27,4	33:37,4	7	RAS 7	CO2	424,77641	0,0041118
51:26,5	57:36,5	9	RAS 9	N2O_dry	0,3269602	2,51E-06
51:26,5	57:36,5	9	RAS 9	CH4_dry	2,3178809	-6,88E-06
51:26,5	57:36,5	9	RAS 9	CO2	417,94748	0,0102696
15:26,8	21:36,8	10	RAS 10	N2O_dry	0,3310946	9,11E-07
15:26,8	21:36,8	10	RAS 10	CH4_dry	2,1703534	-4,07E-06
15:26,8	21:36,8	10	RAS 10	CO2	422,54909	0,0141031
39:25,1	45:35,1	11	RAS 11	N2O_dry	0,3286364	2,84E-06
39:25,1	45:35,1	11	RAS 11	CH4_dry	2,198592	9,68E-07
39:25,1	45:35,1	11	RAS 11	CO2	433,04235	0,0083728
03:26,1	09:36,1	12	RAS 12	N2O_dry	0,3233077	4,44E-06
03:26,1	09:36,1	12	RAS 12	CH4_dry	2,2650669	-1,70E-06
03:26,1	09:36,1	12	RAS 12	CO2	435,01125	0,0057738
27:27,1	33:37,1	13	RAS 13	N2O_dry	0,3162934	3,16E-06
27:27,1	33:37,1	13	RAS 13	CH4_dry	2,3414638	-3,28E-07
27:27,1	33:37,1	13	RAS 13	CO2	426,89046	0,0092592
51:26,3	57:36,3	14	RAS 14	N2O_dry	0,3330736	-1,72E-06
51:26,3	57:36,3	14	RAS 14	CH4_dry	2,3197139	5,29E-06
51:26,3	57:36,3	14	RAS 14	CO2	427,14597	9,85E-05
15:24,9	21:34,9	15	RAS 15	N2O_dry	0,3275981	1,84E-06
15:24,9	21:34,9	15	RAS 15	CH4_dry	2,4127424	-1,22E-06
15:24,9	21:34,9	15	RAS 15	CO2	433,2103	0,0103378
39:25,2	45:35,2	1	RAS 1	N2O_dry	0,3338425	-1,45E-06
39:25,2	45:35,2	1	RAS 1	CH4_dry	2,1740399	-6,14E-07
39:25,2	45:35,2	1	RAS 1	CO2	418,95824	0,00112
03:24,7	09:34,7	2	RAS 2	N2O_dry	0,3240874	2,48E-06

S2 Code section. The commands in the command prompt for importing and transforming data into fluxes in Picarrito.

```
(venv) C:\>picarrito import
INFO          Reading database from 'picarrito\database.feather' (0.3 MiB).
Reading source files          [#####] 522/522
INFO          Database updated:
          Size in memory (MB)          Rows
Before                  0.0              0
New data                 48.9          2,229,120
After                   48.9          2,229,120

INFO          Saved database to 'picarrito\database.feather' (40.6 MiB).

(venv) C:\>picarrito fluxes
INFO          Reading database from 'picarrito\database.feather' (40.6 MiB).
INFO          Database has 2,229,120 rows.
INFO          Data excluded by filters:
          Number rejected  Share rejected
__TIMESTAMP__              2,117          0.1%
ALARM_STATUS                619          0.0%
```

```

All filters combined                2,736                0.1%
INFO      Filtered database has 2,226,384 rows.
INFO
Number of chunks  Average duration  Total duration
All chunks        4,966            00:06:17        21 days 15:31:32
Rejected chunks   3,839            00:01:05         2 days 21:38:29
Final measurements 1,127            00:23:57        18 days 17:53:03

Analyzing measurements [#####] 1127/1127
INFO      Estimated 3381 fluxes (N20_dry, CH4_dry, CO2) in 1127 measurements.
INFO      Saved fluxes to 'picarrito\fluxes.csv'.

```

**(venv) C:\>picarrito plot flux-fits**

```

INFO      Reading database from 'picarrito\database.feather' (40.6 MiB).
INFO      Database has 2,229,120 rows.
INFO      Data excluded by filters:
Number rejected Share rejected
__TIMESTAMP__      2,117                0.1%
ALARM_STATUS        619                0.0%
All filters combined 2,736                0.1%
INFO      Filtered database has 2,226,384 rows.
INFO
Number of chunks  Average duration  Total duration
All chunks        4,966            00:06:17        21 days 15:31:32
Rejected chunks   3,839            00:01:05         2 days 21:38:29
Final measurements 1,127            00:23:57        18 days 17:53:03
Plotting measurements [#####] 1127/1127

```

## Supplementary Materials S1. Solution to the differential equation.

Calculation of the first equation estimating the theoretical concentration profile derived using a mass balance:

$$Q'c_0 + FA = Qc(t) + V \frac{dc}{dt}.$$

With  $Q'c_0 + FA$  as the total input in the chamber when adding up the that goes out of the chamber to the analyzer  $Qc(t)$  and the accumulation  $V \frac{dc}{dt}$  of the gas over time.

Approximating  $Q' = Q$  and rearranging terms, we obtain a first-order ordinary differential equation:

$$\frac{dc}{dt} = \frac{Q}{V} (c_0 - c(t)) + F \frac{A}{V}.$$

Solving it and enforcing the initial condition where  $c(t_0) = c_0$  the solution is

$$c(t) = c_0 + F \frac{A}{Q} (1 - e^{-\frac{Q}{V}(t-t_0)}).$$