NO_x data correction and flagging

Davide Putero –

d.putero@isac.cnr.it

IR0000032 – ITINERIS, Italian Integrated Environmental Research Infrastructures System
(D.D. n. 130/2022 - CUP B53C22002150006) Funded by EU - Next Generation EU PNRR-Mission 4 “Education and Research” - Component 2: “From research to business” - Investment 3.1: “Fund for the realisation of an integrated system of research and innovation infrastructures”

Finanziato dall'Unione europea NextGenerationEU
Ministero dell'Università e della Ricerca
Italiadomani

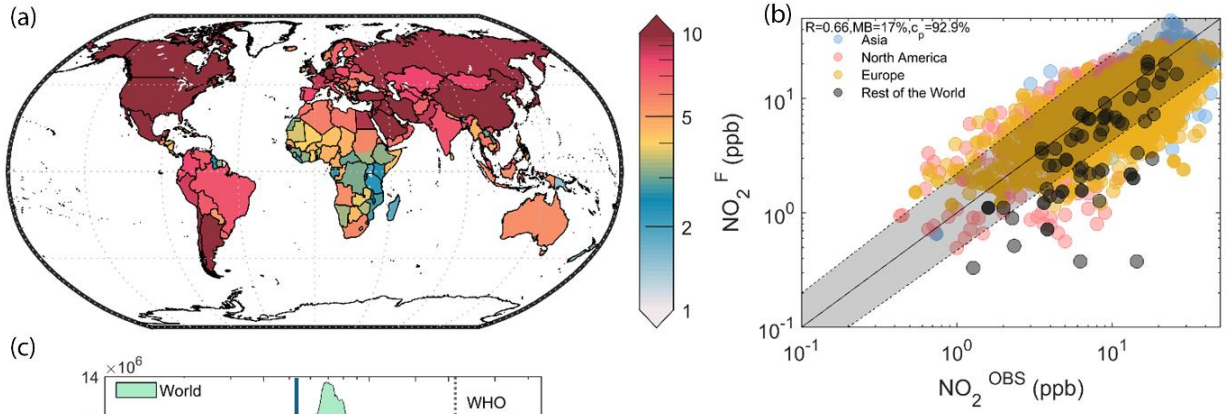
Outline

- **Measurements of NO_x**
  - Introduction
  - Calibration
  - Interferences by ozone and relative humidity, zero offset correction
- **NO_x data preparation and submission**
  - Data levels
  - Workflow
  - lev0 and lev1 templates
- **Overview of the automatic procedures at CNR-ISAC**
- **Assignment**

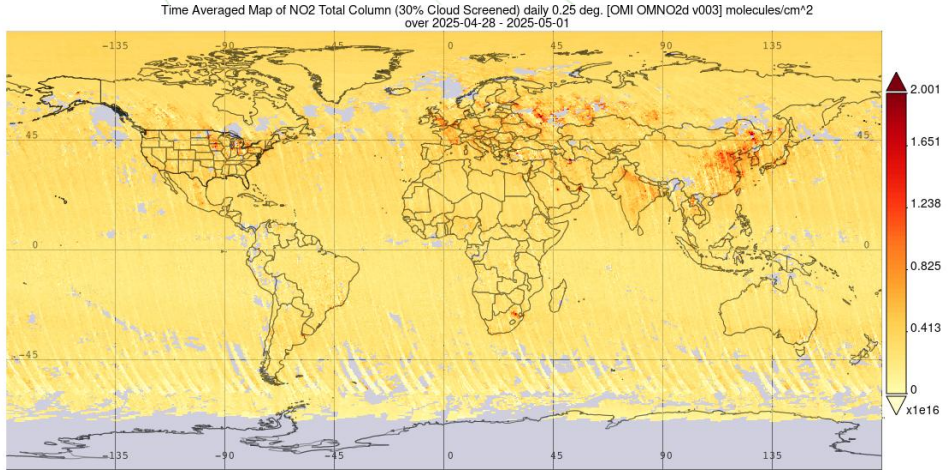
Introduction on NO and NO_2 (NO_x)

NO Nitric oxide
NO_2 Nitrogen dioxide
} NO_x

Lifetime of hours (NO), hours to days (NO_2)
Health effects: respiratory irritation, aggravation of asthma, respiratory infections
Environmental effects: NO_x react with VOCs to produce O_3, control OH, acid rain



Chowdhury et al. (2021)



NASA/GSFC/HSL

2021: the WHO reduced the guideline to 10 µg m^{-3}

→ **Most of the World's population lives in unhealthy conditions**

Sources:

Biogenic	22 Tg/y
Lightning	10-20 Tg/y
Biomass Burning	18 Tg/y
Anthropogenic	72 Tg/y

Müller (1992)

Measurements of NO_x by chemiluminescence

The **chemiluminescence** occurs when NO is exposed to O_3. It is a two-step process.
First, the NO and O_3 molecules collide and react to produce O_2 and one molecule of NO_2. Part of this reaction gives excited NO_2

$$NO + O_3 \rightarrow NO_2 + O_2$$
$$NO + O_3 \rightarrow NO_2^* + O_2$$

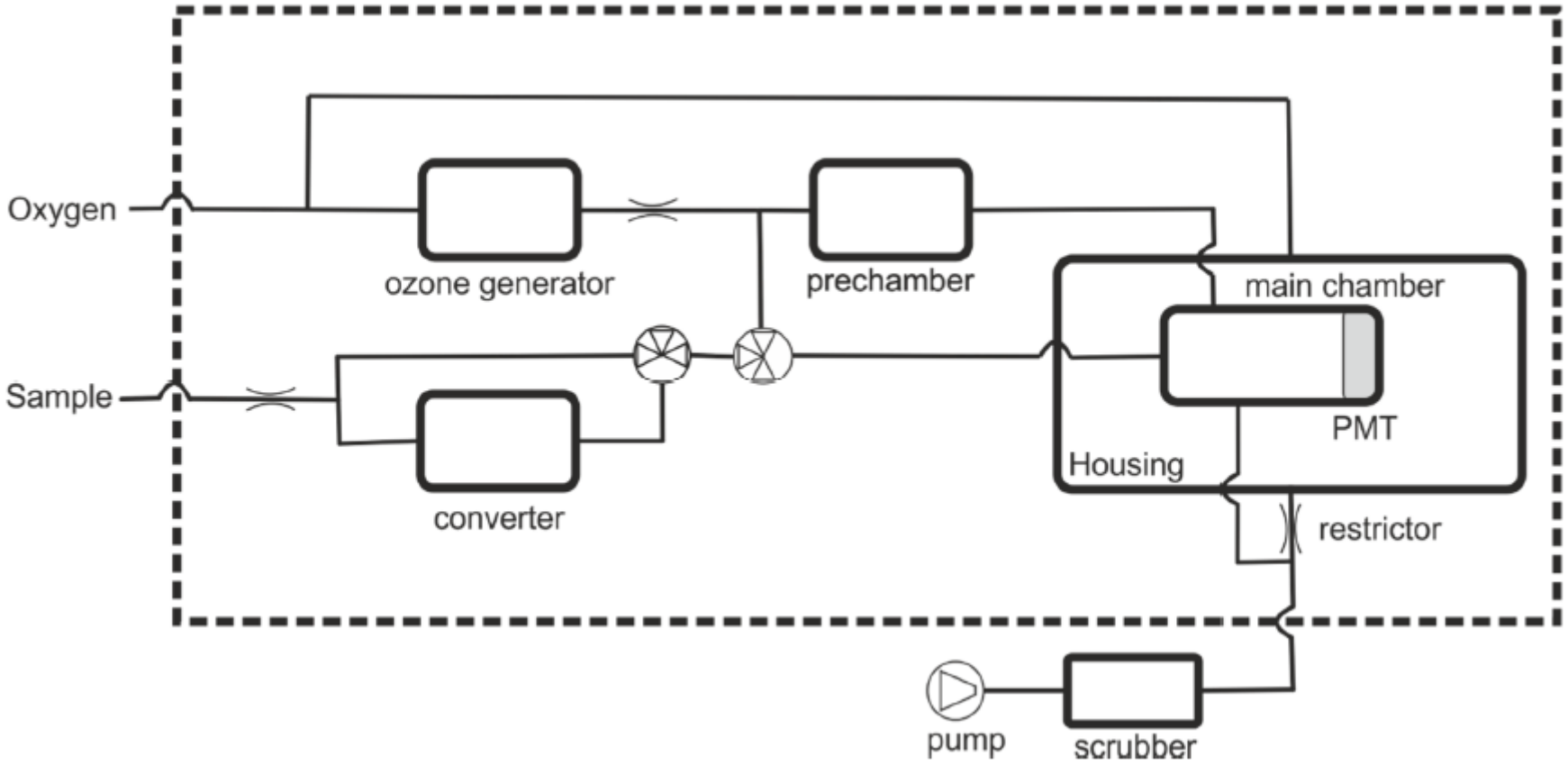
The excited NO_2 can be quenched by other molecules, or can quickly return to its ground state, **releasing excess energy**, in the form of a quantum of light

$$NO_2^* + M \rightarrow NO_2 \quad , \mathrm{M} = \mathrm{N_2}, \mathrm{O_2}, \mathrm{H_2O}, \mathrm{Ar}$$
$$NO_2^* \rightarrow NO_2 + h\upsilon_{1200nm}$$

All things being constant (i.e., T, P, amount of O_3, …), the relation between NO and the amount of light emitted is **very linear**. If more NO is present, more IR light is produced. By measuring the amount of IR light produced with a sensor sensitive in the infra-red spectrum, the amount of NO present can be determined.

Measurements of NO_x by chemiluminescence

The NO **chemiluminescence** detector (CLD) has been invented in 1970 (Fontijn et al., 1970)



By altering both the converter mode and the chamber mode, a measurement cycle consists of **4 steps**

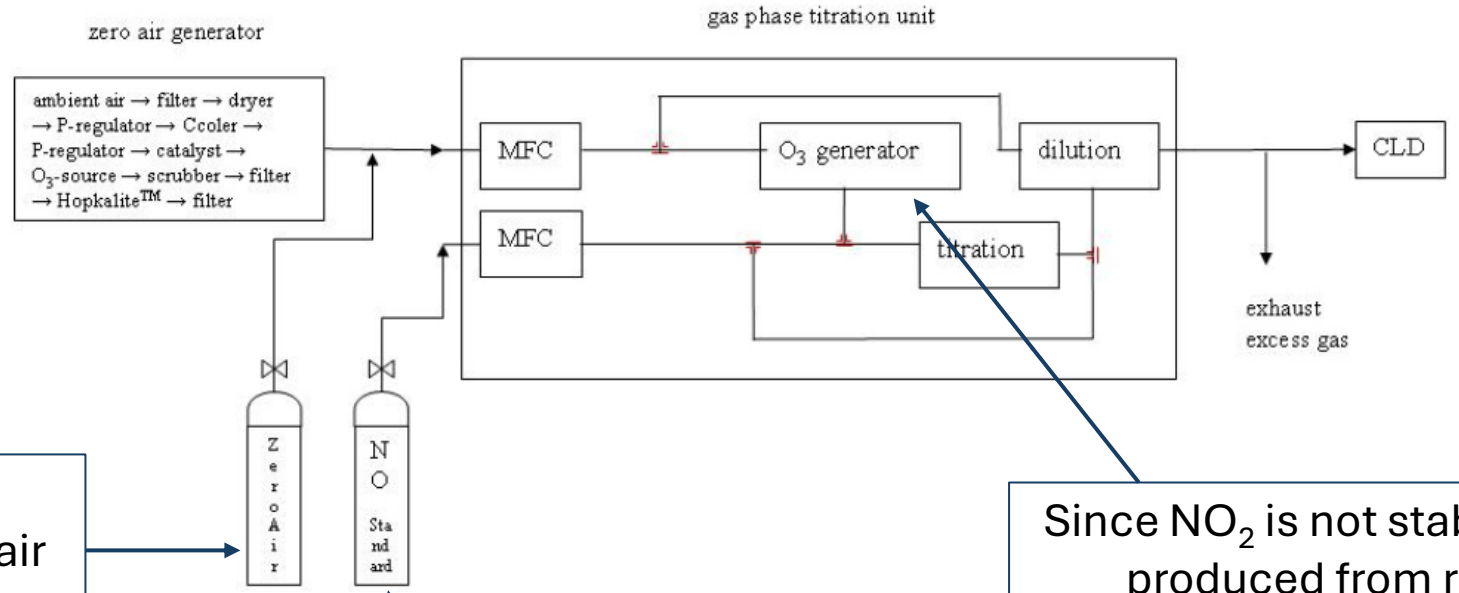
Raw data files

- Daily raw files
- 1-min time resolution
- NO, NO_2, NO_x concentrations as well as ancillary parameters
- Instrument status and warning

```
#date time daydec NO[ppb] NO2[ppb] NOx[ppb] Pre Pre_low Pre_High T_int ReactCellT[C] T_Cooler PMT_V T_NO2_conv ReactCellP[incHg] O3_flow[cc/m] SampleFlow[cc/m] status warning
2025-05-14 00:00:00 133.000000 0.031 0.065 0.096 -999 -999 -999 31.925 39.997 4.655 520.525 0.000 2.417 59.099 774.527 SAMPLE 00100000000
2025-05-14 00:01:00 133.000694 0.032 0.049 0.082 -999 -999 -999 31.930 39.996 4.658 520.525 0.000 2.418 59.122 774.476 SAMPLE 00100000000
2025-05-14 00:02:00 133.001389 0.031 0.035 0.066 -999 -999 -999 31.932 39.995 4.657 520.533 0.000 2.421 59.115 773.654 SAMPLE 00100000000
2025-05-14 00:03:00 133.002083 0.035 0.029 0.064 -999 -999 -999 31.935 39.998 4.657 520.509 0.000 2.427 59.146 779.451 SAMPLE 00100000000
2025-05-14 00:04:00 133.002778 0.038 0.041 0.079 -999 -999 -999 31.935 39.996 4.656 520.533 0.000 2.426 59.133 779.469 SAMPLE 00100000000
2025-05-14 00:05:00 133.003472 0.042 0.040 0.082 -999 -999 -999 31.937 39.995 4.656 520.525 0.000 2.420 59.156 775.047 SAMPLE 00100000000
2025-05-14 00:06:00 133.004167 0.036 0.047 0.083 -999 -999 -999 31.931 39.996 4.658 520.533 0.000 2.421 59.101 774.518 SAMPLE 00100000000
2025-05-14 00:07:00 133.004861 0.025 0.057 0.082 -999 -999 -999 31.926 39.997 4.657 520.541 0.000 2.422 59.088 774.479 SAMPLE 00100000000
2025-05-14 00:08:00 133.005556 0.037 0.055 0.091 -999 -999 -999 31.927 39.997 4.657 520.517 0.000 2.423 59.106 778.475 SAMPLE 00100000000
2025-05-14 00:09:00 133.006250 0.034 0.058 0.092 -999 -999 -999 31.920 39.996 4.656 520.359 0.000 2.427 59.137 780.192 SAMPLE 00100000000
2025-05-14 00:10:00 133.006944 0.021 0.068 0.089 -999 -999 -999 31.918 39.996 4.658 520.525 0.000 2.429 59.095 779.342 SAMPLE 00100000000
2025-05-14 00:11:00 133.007639 0.008 0.069 0.077 -999 -999 -999 31.915 39.997 4.657 520.533 0.000 2.425 59.088 773.522 SAMPLE 00100000000
2025-05-14 00:12:00 133.008333 0.014 0.058 0.072 -999 -999 -999 31.915 39.994 4.656 520.549 0.000 2.420 59.128 774.288 SAMPLE 00100000000
2025-05-14 00:13:00 133.009028 0.007 0.075 0.083 -999 -999 -999 31.915 39.998 4.655 520.517 0.000 2.415 59.112 775.220 SAMPLE 00100000000
2025-05-14 00:14:00 133.009722 -0.000 0.079 0.079 -999 -999 -999 31.919 39.996 4.654 520.541 0.000 2.418 59.114 775.773 SAMPLE 00100000000
2025-05-14 00:15:00 133.010417 -0.001 0.086 0.086 -999 -999 -999 31.927 40.000 4.654 520.541 0.000 2.417 59.101 780.043 SAMPLE 00100000000
2025-05-14 00:16:00 133.011111 -0.011 0.121 0.110 -999 -999 -999 31.929 39.997 4.656 520.533 0.000 2.418 59.101 774.360 SAMPLE 00100000000
2025-05-14 00:17:00 133.011806 -0.017 0.137 0.120 -999 -999 -999 31.939 39.994 4.656 520.533 0.000 2.411 59.051 774.232 SAMPLE 00100000000
2025-05-14 00:18:00 133.012500 -0.004 0.128 0.124 -999 -999 -999 31.940 39.991 4.656 520.533 0.000 2.414 59.097 774.290 SAMPLE 00100000000
2025-05-14 00:19:00 133.013194 -0.002 0.134 0.131 -999 -999 -999 31.937 39.995 4.656 520.541 0.000 2.423 59.101 774.350 SAMPLE 00100000000
2025-05-14 00:20:00 133.013889 -0.013 0.133 0.120 -999 -999 -999 31.943 39.997 4.657 520.454 0.000 2.424 59.108 780.034 SAMPLE 00100000000
2025-05-14 00:21:00 133.014583 -0.024 0.148 0.124 -999 -999 -999 31.943 39.992 4.655 520.533 0.000 2.423 59.143 777.995 SAMPLE 00100000000
2025-05-14 00:22:00 133.015278 -0.024 0.162 0.138 -999 -999 -999 31.939 39.996 4.654 520.336 0.000 2.416 59.106 775.373 SAMPLE 00100000000
```

Calibration by gas phase titration (GPT)

The chemiluminescence method is not an absolute method, therefore **periodic calibration** of the instrument is required. Sensitivity depends on parameters like cell temperature or pressure, photon count efficiency of the PMT, contamination or degradation of optical components, etc. which can change with time.

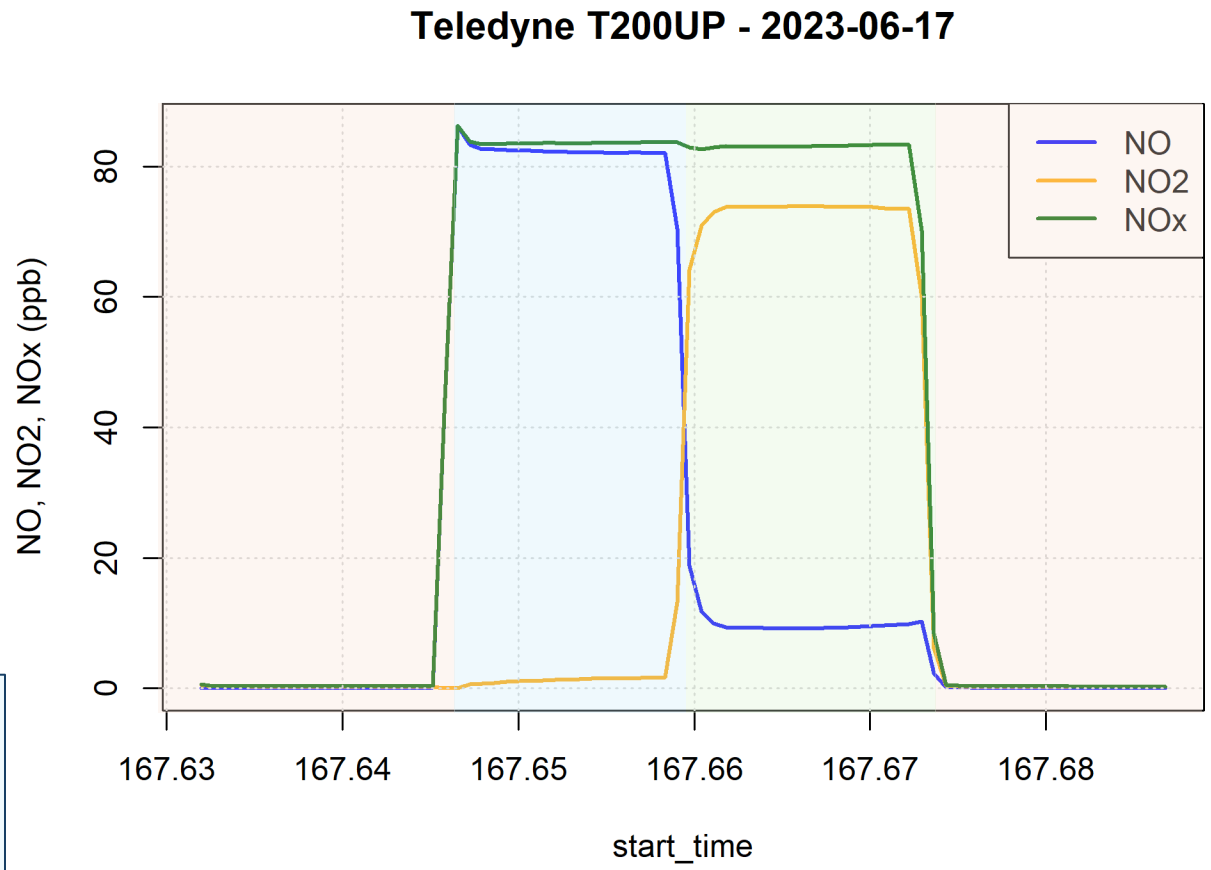


Zero air (from cylinder/generator), i.e., air without significant amounts of NO in it

Since NO_2 is not stable in cylinders, it is produced from reaction with O_3

Calibration standard from the CCL (Central Calibration Lab), with NO stable in the ppm range, diluted before entering the CLD

Calibration by gas phase titration (GPT)



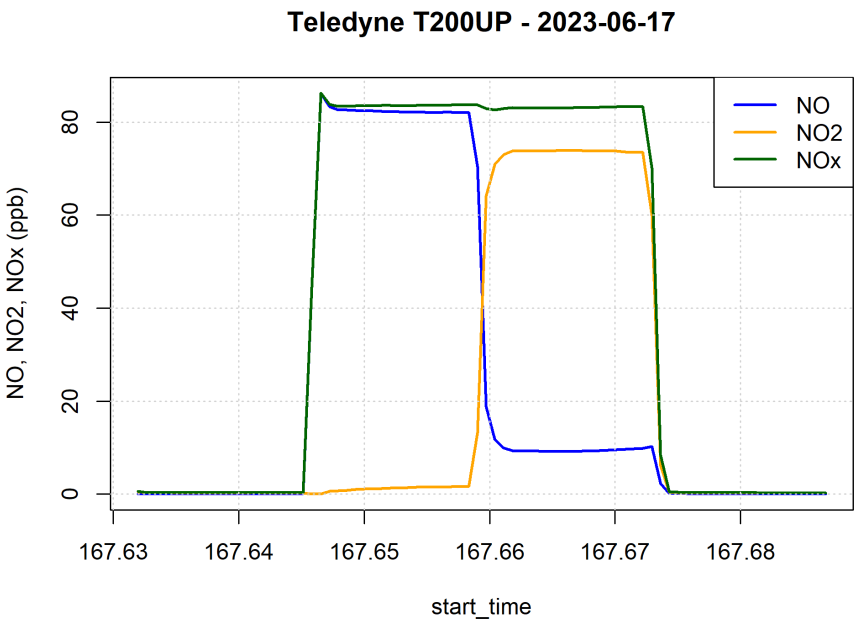
ZERO PHASE
Only synthetic air is added, it is for determining NO and NO_2 artifacts

NO SPAN PHASE
NO added from standard cylinder. The NO sensitivity is determined

GPT PHASE
NO_2 is produced from NO after O_3 is added, by GPT. In this phase, NO_2 is measured to determine the conversion efficiency (Sc)

Each calibration phase should last at least 15-20 min to allow the instrument to stabilize

Calibration by gas phase titration (GPT)



1) As a first step, we calculate the NO and NO_x calibration coefficients

$$NO_{COEF} = \frac{gas_conc_{SPAN}}{NO_{SPAN} - NO_{ZERO}}$$

$$NOx_{COEF} = \frac{gas_conc_{SPAN}}{NOx_{SPAN} - NOx_{ZERO}}$$

2) From these, we can get calibrated NO and NO_x values (NO_x is only temporarily calibrated, being now based only on NO)

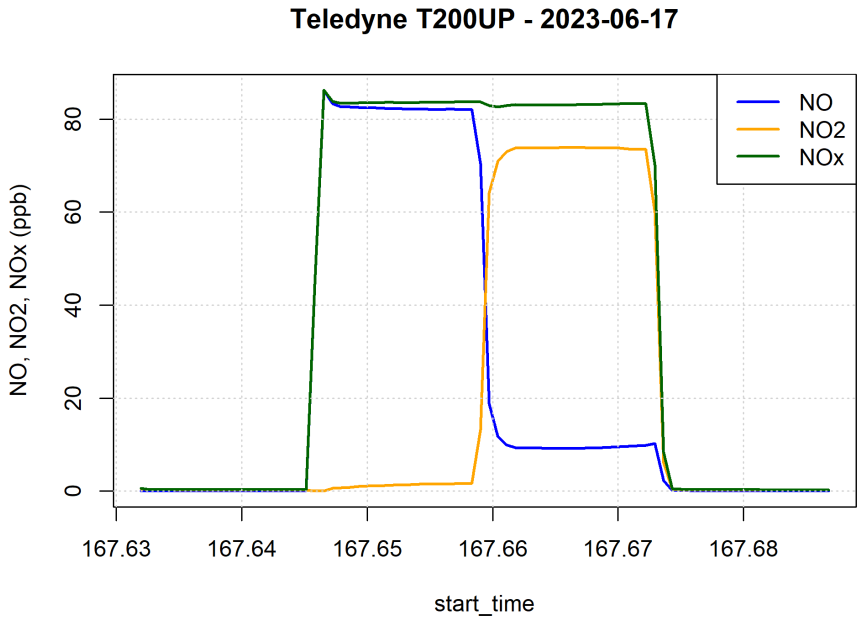
$$NO_{CALIB} = (NO \cdot NO_{COEF}) - NO_{ZERO}$$

$$NOx_{CALIB} = (NOx \cdot NOx_{COEF}) - NOx_{ZERO}$$

3) Then, we can derive the conversion efficiency (Sc)

$$Sc = \frac{NOx_{GPT} - NO_{2\,SPAN} - NO_{GPT}}{NO_{SPAN} - NO_{GPT}}$$

Calibration by gas phase titration (GPT)



4) Given the Sc, we can now compute NO_2 calibrated data, and the final NO_x calibrated value

$$NO_{2\,CALIB} = \frac{NOx_{CALIB} - NO_{CALIB}}{Sc}$$

$$NOx_{CALIB} = NO_{2\,CALIB} + NO_{CALIB}$$

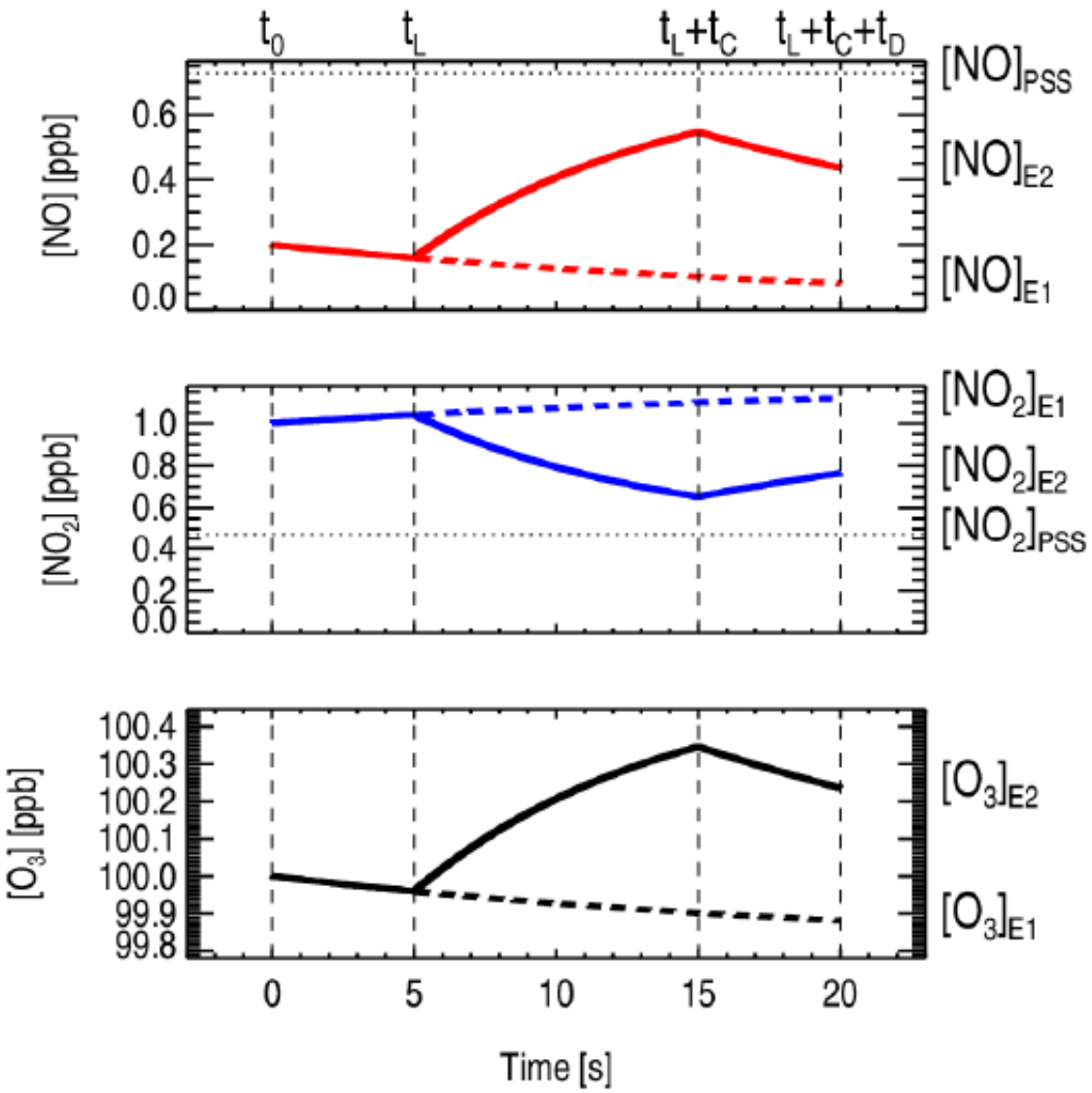
- Always check how calibration parameters (e.g., NO_{ZERO}, NO_{COEF}, ...) vary over time, to see that no drifts are present
- Do calibration results vary within acceptable limits?
- If NO_2 conversion efficiency falls below 40% or lamp intensity fluctuates excessively, check/change the lamps or the converter

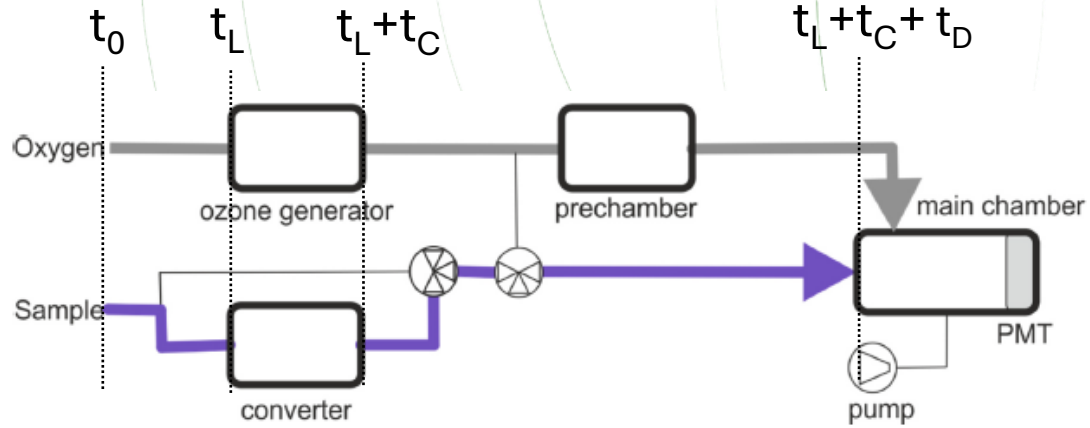
Calibration files

- One file for each calibration event (unless more than one calib on a specific day/calib spanning two days)
- 1-min time resolution
- Information about parameters during the calibration (e.g., *target_gas_conc*, *Oz_lamp_temp*, ...)
- Status and flags identify the different phases of the calibration

```
#date time daydec actual_gas_conc target_gas_conc Oz_lamp_temp actual_Gflow target_Gflow actual_Zflow target_Zflow actual_Tflow target_Tflow status flags
2025-05-13 11:07:00 132.463194 0.000 0.000 67.9 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:08:00 132.463889 0.000 0.000 67.8 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:09:00 132.464583 0.000 0.000 67.9 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:10:00 132.465278 0.000 0.000 67.9 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:11:00 132.465972 0.000 0.000 67.9 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:12:00 132.466667 0.000 0.000 67.9 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:13:00 132.467361 0.000 0.000 67.9 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:14:00 132.468056 0.000 0.000 67.8 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:15:00 132.468750 0.000 0.000 67.8 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:16:00 132.469444 0.000 0.000 67.8 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:17:00 132.470139 0.000 0.000 67.8 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:18:00 132.470833 0.000 0.000 67.9 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:19:00 132.471528 0.000 0.000 67.9 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:20:00 132.472222 0.000 0.000 67.9 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:21:00 132.472917 0.000 0.000 67.9 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:22:00 132.473611 0.000 0.000 67.8 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:23:00 132.474306 0.000 0.000 67.9 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:24:00 132.475000 0.000 0.000 67.9 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:25:00 132.475694 0.000 0.000 67.9 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:26:00 132.476389 0.000 0.000 67.9 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:27:00 132.477083 0.000 0.000 67.9 0.000 0.000 1997.487 2000.000 2005.486938 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:28:00 132.477778 0.000 0.000 67.9 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:29:00 132.478472 0.000 0.000 67.9 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:30:00 132.479167 0.000 0.000 67.8 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:31:00 132.479861 0.000 0.000 67.8 0.000 0.000 1998.791 2000.000 2006.791138 1992.000000 gas_B_span_0_ 0C002000
2025-05-13 11:32:00 132.480556 0.100 0.100 67.9 39.137 39.216 1958.334 1960.784 2005.470703 1952.000000 gas_B_span_1_ 0C00A000
2025-05-13 11:33:00 132.481250 0.100 0.100 67.8 39.164 39.216 1958.334 1960.784 2005.524902 1952.000000 gas_B_span_1_ 0C00A000
```

Chemistry in the inlet



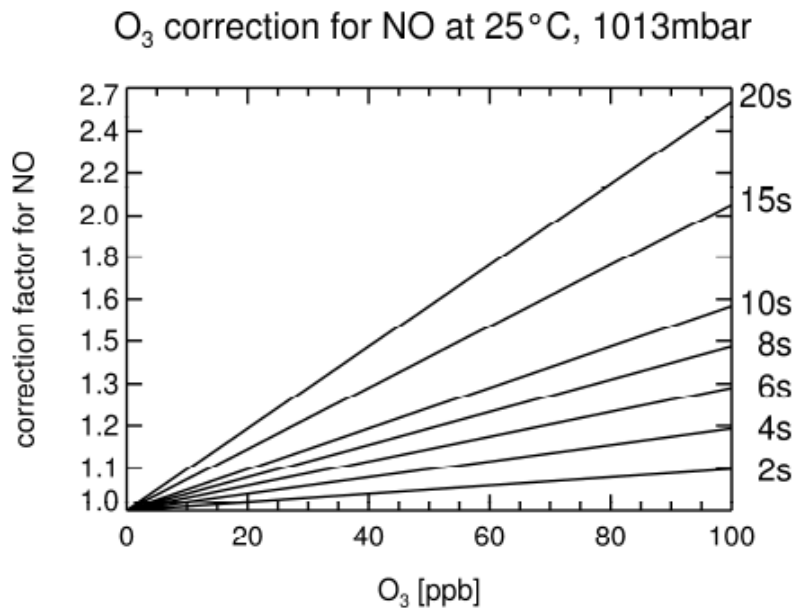


$$[NO]_0 = [NO]_{E1} \times e^{k_{O_3}L \times (t_L + t_B + t_D)}$$

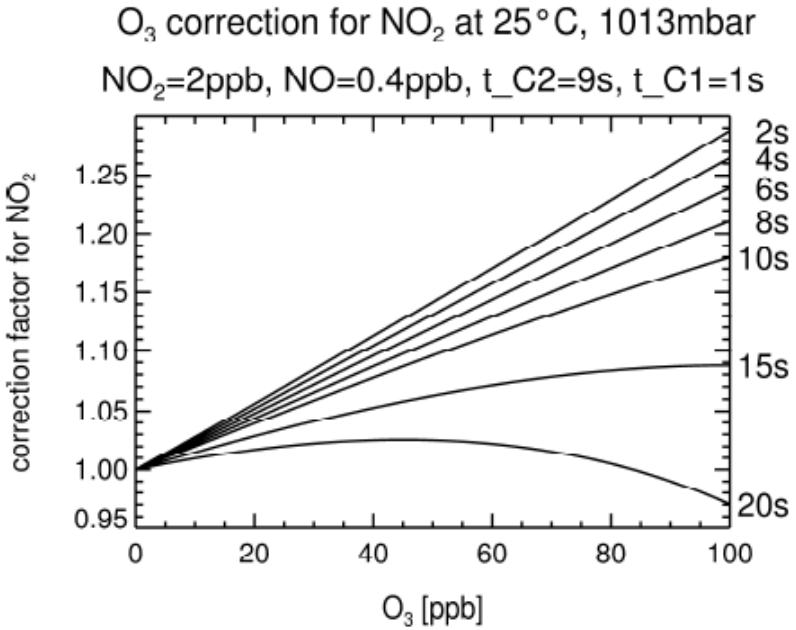
$$NO_2 \rightleftharpoons NO + O_3$$

- NO reacts with O_3 in the inlet manifold, in the photolytical converter and after passing the converter before the detection in the CLD
- O_3 is also produced in the converter, which can oxidize NO on its way to the detector

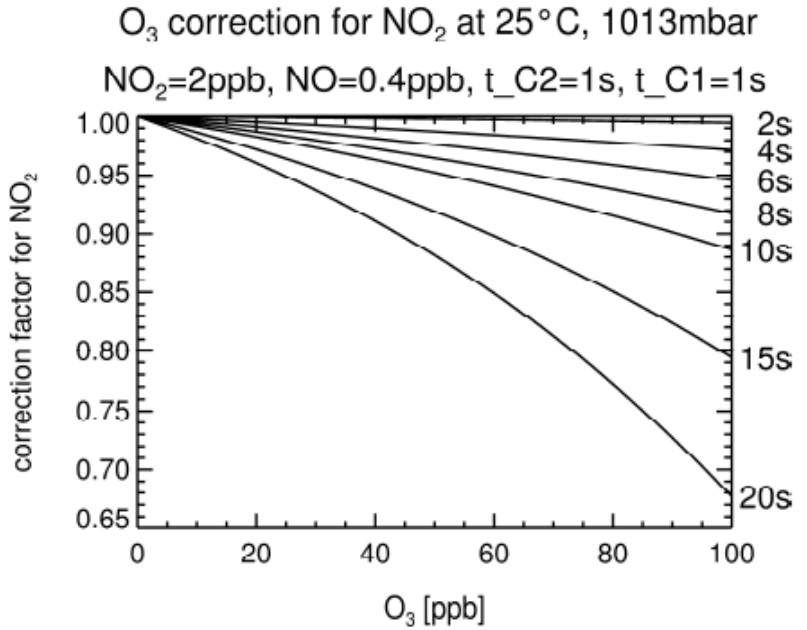
Chemistry in the inlet



Correction factor for NO at different residence time in sampling line



Correction factor for NO_2 at different residence time in sampling line



Correction factor for NO_2 at different residence time in sampling line

- Correction is necessary even with high sampling flows
- NO correction gets larger with larger O_3 concentration and longer residence time
- NO_2 correction gets larger/smaller with larger O_3 concentration (+−), longer inlet line (−), larger converter volume (+), larger NO concentration (−), better converter efficiency (-)

Inlet correction is needed for all NOx instruments, not only CLD

The humidity effect

$$NO + O_3 \rightarrow NO_2 + O_2$$
$$NO + O_3 \rightarrow NO_2^* + O_2$$
$$NO_2^* \rightarrow NO_2 + hv$$
$$NO_2^* + M \rightarrow NO_2 \quad , \mathrm{M} = \mathrm{N_2, O_2, H_2O, Ar}$$

$NO_2^* + N_2 \rightarrow NO_2$	$k(NO_2^* + N_2)$
$NO_2^* + O_2 \rightarrow NO_2$	$k(NO_2^* + N_2) * 1.115$
$NO_2^* + CO_2 \rightarrow NO_2$	$k(NO_2^* + N_2) * 2.05$
$NO_2^* + Ar \rightarrow NO_2$	$k(NO_2^* + N_2) * 0.5$
$NO_2^* + H_2O \rightarrow NO_2$	$k(NO_2^* + N_2) * 4.42$

Matthews et al. (1977)

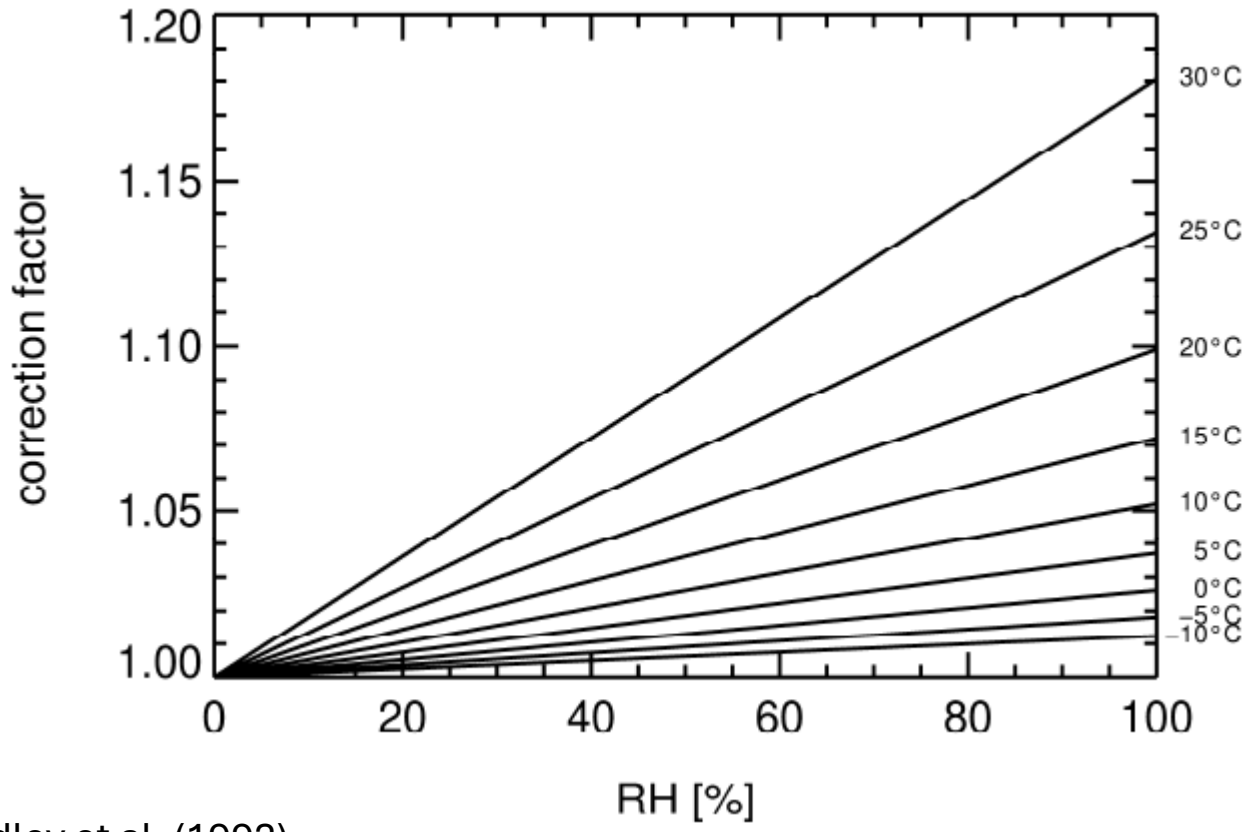
Factor for quenching in ambient air

21%	→	1.034
400 ppm	→	1.000
1%	→	0.995
1%	→	1.043

Consequences (for CLD instruments)

- No correction needed when frequent spiking of ambient air is performed
- 0-10% correction needed for calibrations using NO/N_2 diluted by synthetic air
- No water correction needed if the ambient air is dry or dried

The humidity effect



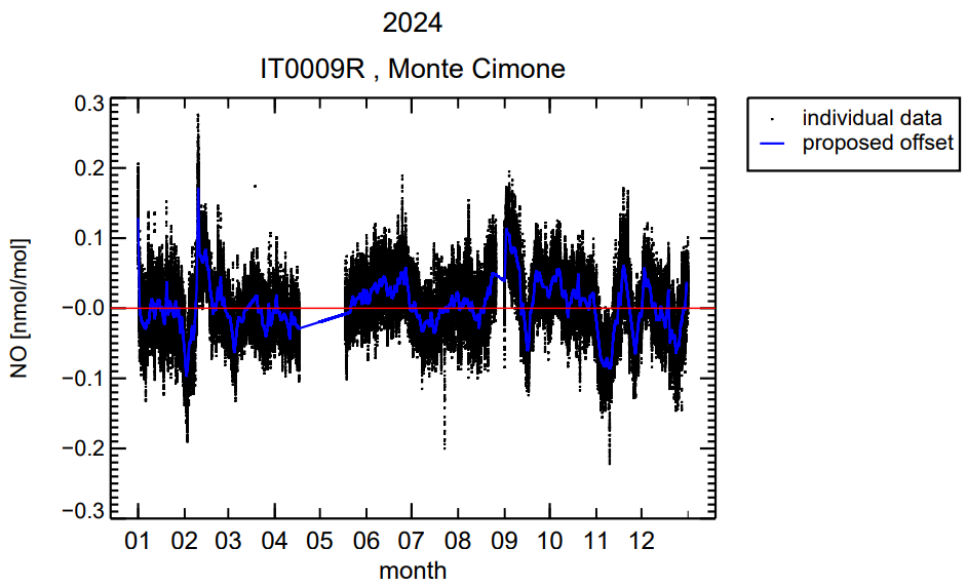
Ridley et al. (1992)

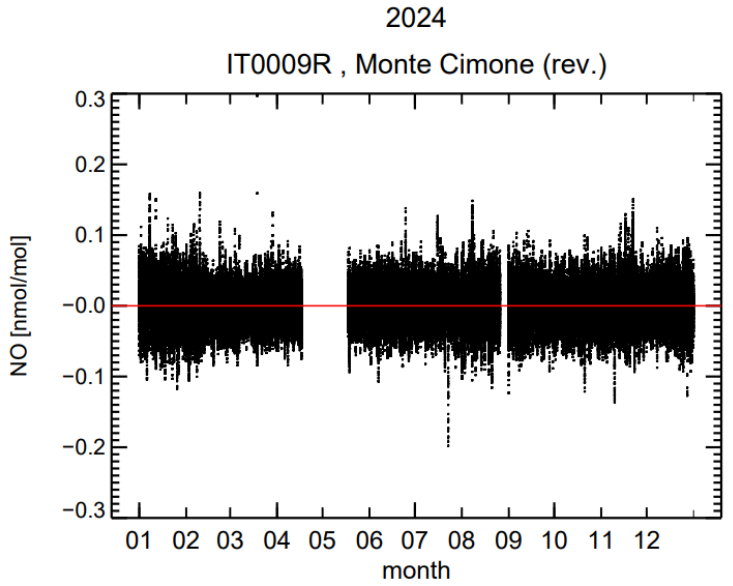
$$[NO_2]_{H20} = [NO_2]_M \times (1 + \alpha \times [H_2O])$$

$$\alpha = (4.3 \pm 0.3) \times 10^{-3} \times \frac{flow_{sample}}{flow_{sample} + flow_{ozone}}$$

Zero offset correction

- In remote environments where NO_x concentrations are low (<0.1 ppb) it is recommended to use the measured night-time NO signal as the **detector artefact** (Lee et al., 2009; Galbally et al., 2020)
- Ambient night-time NO concentrations are expected to equal zero due to reaction with ambient O_3
- To assess valid zero offset corrections, the following conditions must be met:
  - A level of O_3 > 20 ppb
  - Low ozone variability with a variation coefficient of < 0.1
  - No local sources of NO
  - Absence of sunlight
  - Steady meteorological conditions with wind speed < 2 m/s
  - Absence of high levels of VOCs





Corrections

Until 2022

Stations submitted corrected level 0 or level 2 data, or the Topical Centre (TC) corrected data

From 2023

ozone, humidity and zero offset corrections will be directly applied by the TC, so stations must submit NO_x level 0 and level 1 data. Hourly level 2 and level 3 data will be produced by the TC

NO_x guidelines

https://ebas-submit.nilu.no/SOPs

GAW has prepared new measurement guidelines

Draft November, 26th, 2021

GLOBAL ATMOSPHERE WATCH

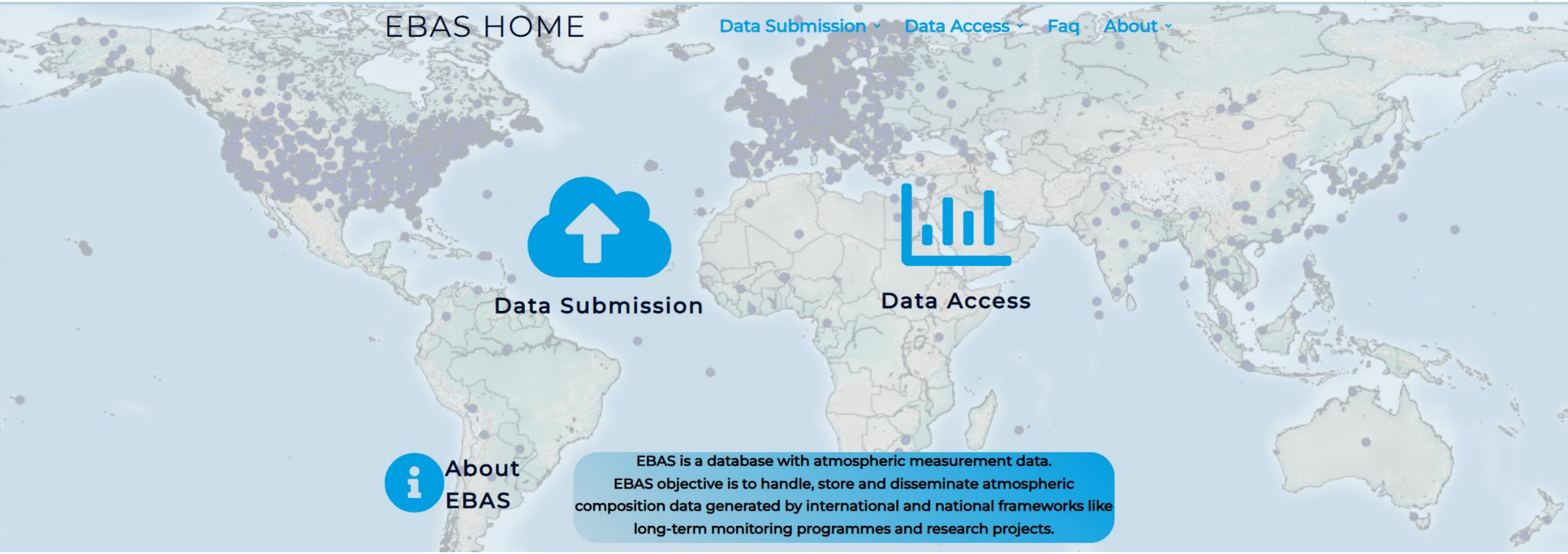
Guidelines for continuous measurement of nitrogen oxide (NO) and nitrogen dioxide (NO_2) in the troposphere

Authors (in alphabetical order)

Paul Brewer, Ian Galbally, Dagmar Kubistin, Chris Reed, Martin Steinbacher, Dave Worton, Robert Wegener

NO_x data submission

- **World Data Centre for Reactive Gases (WDCRG)**
- Database hosted by **NILU**: https://ebas.nilu.no/

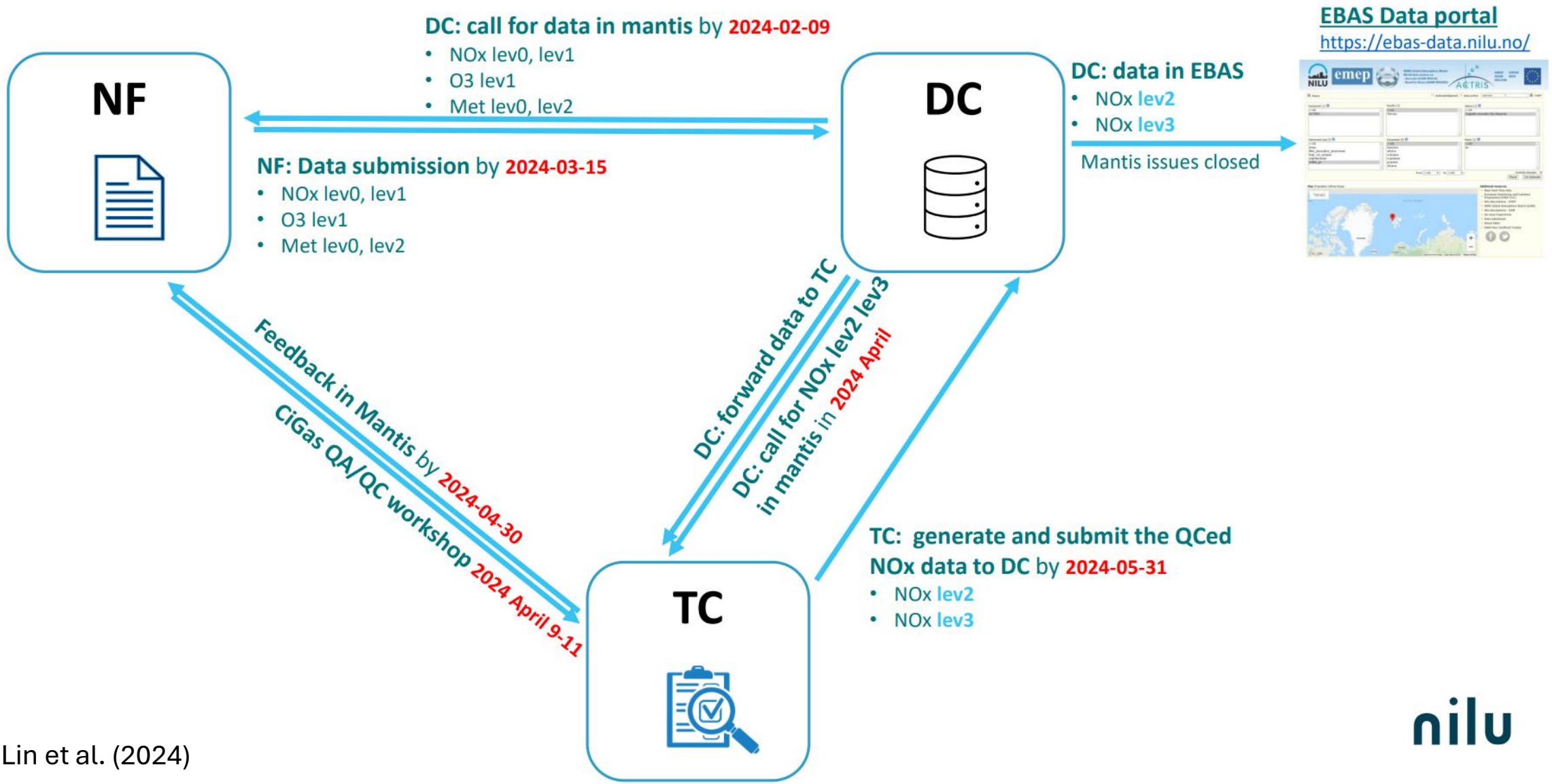


Data levels

- Data format is EBAS NASA Ames 1001 (ASCII text)
- Data levels to be submitted:
  - **Level 0**: data as provided by instrument, amount fraction and raw counts (when available), flags applied
  - **Level 1**: calibrations applied, original time resolution, flags applied
- Data produced by the Topical Centre (TC), from 2023:
  - **Level 2**: hourly averages, offset correction applied, not sample line corrected
  - **Level 3**: hourly averages, offset correction applied, sample line corrected
- To perform corrections, the TC also requires ozone (lev1) and meteo (lev0, lev2) data, if available

```
Humidity/temperature control: None
Humidity/temperature control description: Passive, inlet air heated from atmospheric to converter temperature
Detection limit expl.:        Determined by instrument counting statistics
Measurement uncertainty expl.: Includes statistical uncertainty of individual sample and calibration uncertainty
Zero/negative values code:    Zero/negative possible
Zero/negative values:         Zero and neg. values may appear due to statistical variations at very low concentrations
QA1 measure ID:               ACTRIS NOx s-b-s 2012
QA1 date:                     20121116000000
QA1 document URL:             "http://fp7.actris.eu/Portals/97/deliverables/PU/WP4_D4.6_M24_final_v2.pdf"
QA2 measure ID:               ACTRIS NO round robin 2012
QA2 date:                     20121201000000
QA2 document URL:             "http://fp7.actris.eu/Portals/97/deliverables/PU/WP4_D4.4_M24.pdf"
Originator:                   Fiebig, Markus, Markus.Fiebig@nilu.no, Norwegian Institute for Air Research, NILU, Atmosphere and Climate Department, Instituttveien 18,, 2007, Kjeller, Norway, ORCID=0000-0002-3380-3470
Originator:                   Someone, Else, Someone@somewhere.no, Some nice Institute, WOW, Super interesting division, Street 18,, X-9999, Paradise, Noway
Submitter:                    Fiebig, Markus, Markus.Fiebig@nilu.no, Norwegian Institute for Air Research, NILU, Atmosphere and Climate Department, Instituttveien 18,, 2007, Kjeller, Norway, ORCID=0000-0002-3380-3470
Acknowledgement:              Request acknowledgement details from data originator
Comment:
starttime    endtime  p_inlet    p_det  T_inlet    T_det cal  zero  NO#  NOc# NO_sens cvt_eff      numflag      NO   NO_ac   NO_pr  NO_dl   numflag_NO      NO2  NO2_ac  NO2_pr NO2_dl  numflag_NO2
0.000000   0.000694  839.400  921.400  299.700  290.210   0     0   258  5200   1.283  45.351  0.000000000  0.041  0.0010  0.0003  0.001  0.000000000   0.753  0.0020  0.0010  0.010  0.000000000
0.000694   0.001385  839.766  921.787  299.750  291.232   0     0   310  4780   1.283  45.351  0.000000000  0.046  0.0014  0.0003  0.001  0.000000000   0.735  0.0024  0.0012  0.012  0.000000000
0.001385   0.002083  839.821  921.833  299.761  291.987   0     1    21     3   1.283  45.351  0.686000000  0.001  0.0010  0.0003  0.001  0.686000000   0.002  0.0005  0.0013  0.012  0.686000000
0.002083   0.002778  839.801  921.788  299.886  292.232   0     2     9     1   1.283  45.351  0.686000000  0.002  0.0010  0.0003  0.001  0.686000000   0.001  0.0004  0.0010  0.015  0.686000000
0.002778   0.003472  839.633  921.654  300.021  292.012   1     0   644    21   1.283  45.351  0.687000000  0.120  0.0015  0.0005  0.001  0.687000000   0.012  0.0004  0.0011  0.012  0.687000000
0.003472   0.004167  839.601  921.522  299.988  291.987   3     0   654    12   1.283  45.351  0.687000000  0.120  0.0015  0.0004  0.001  0.687000000   0.022  0.0005  0.0011  0.011  0.687000000
0.004167   0.004861  839.601  921.522  299.988  291.987   4     0     4   653   1.283  45.351  0.687000000  0.000  0.0005  0.0001  0.001  0.687000000   0.123  0.0015  0.0011  0.011  0.687000000
0.004861   0.005556  839.801  921.788  421.122  291.232   0     0  7342 96379   1.283  45.351  0.699000000 73.832  3.2349  9.7289  8.234  0.699000000  83.234 32.2724 62.1346  7.234  0.699000000
0.005556   0.006251 9999.999 9999.999 9999.999 9999.999  99    99  9999 99999  99.999 999.999  0.999000000 99.999 99.9999 99.9999 99.999  0.999000000  99.999 99.9999 99.9999 99.999  0.999000000
```

Workflow



Lin et al. (2024)

level 0

https://ebas-submit.nilu.no/templates/NOx/lev0

Acknowledgement: Request acknowledgement details from data originator
Comment:

starttime	endtime	p_inlet	p_det	T_inlet	T_det	cal	zero	NO#	NOc#	NO_sens	cvt_eff	numflag	NO	NO_ac	NO_pr	NO_dl	numflag_NO	NO2	NO2_ac	NO2_pr	NO2_dl	numflag_NO2
0.000000	0.000694	839.400	921.400	299.700	290.210	0	0	258	5200	1.283	45.351	0.000000000	0.041	0.0010	0.0003	0.001	0.000000000	0.753	0.0020	0.0010	0.010	0.000000000
0.000694	0.001385	839.766	921.787	299.750	291.232	0	0	310	4780	1.283	45.351	0.000000000	0.046	0.0014	0.0003	0.001	0.000000000	0.735	0.0024	0.0012	0.012	0.000000000
0.001385	0.002083	839.821	921.833	299.761	291.987	0	1	21	3	1.283	45.351	0.686000000	0.001	0.0010	0.0003	0.001	0.686000000	0.002	0.0005	0.0013	0.012	0.686000000
0.002083	0.002778	839.801	921.788	299.886	292.232	0	2	9	1	1.283	45.351	0.686000000	0.002	0.0010	0.0003	0.001	0.686000000	0.001	0.0004	0.0010	0.015	0.686000000
0.002778	0.003472	839.633	921.654	300.021	292.012	1	0	644	21	1.283	45.351	0.687000000	0.120	0.0015	0.0005	0.001	0.687000000	0.012	0.0004	0.0011	0.012	0.687000000
0.003472	0.004167	839.601	921.522	299.988	291.987	3	0	654	12	1.283	45.351	0.687000000	0.120	0.0015	0.0004	0.001	0.687000000	0.022	0.0005	0.0011	0.011	0.687000000
0.004167	0.004861	839.601	921.522	299.988	291.987	4	0	4	653	1.283	45.351	0.687000000	0.000	0.0005	0.0001	0.001	0.687000000	0.123	0.0015	0.0011	0.011	0.687000000
0.004861	0.005556	839.801	921.788	421.122	291.232	0	0	7342	96379	1.283	45.351	0.699000000	73.832	3.2349	9.7289	8.234	0.699000000	83.234	32.2724	62.1346	7.234	0.699000000
0.005556	0.006251	9999.999	9999.999	9999.999	9999.999	99	99	9999	99999	99.999	999.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000

starttime Start time of each sample, as floating value (offset in days from the reference date). Jan 1st is expressed as 0
Example: 2024-01-01 10:00:00 = 0 + 10/24 = 0.416667

endtime End time of each sample, same format as starttime

p_inlet
p_det
T_inlet
T_det Temperatures and pressures measured in the inlet and in the detector

cal This number indicates the calibration standard ID. Calibration measurements shall be flagged with **flag 687**
Example: 1 corresponds to the 1° standard used in the year, e.g. "Status calibration standard: 1, Manufacturer: NPL, Batch: D109110"

zero It indicates how the zero is performed during calibrations. Zero measurements shall be flagged with **flag 686**
Example: 0 = N/A, 1 = internal zero, 2 = external zero

level 0

https://ebas-submit.nilu.no/templates/NOx/lev0

Acknowledgement: Request acknowledgement details from data originator
Comment:

starttime	endtime	p_inlet	p_det	T_inlet	T_det	cal	zero	NO#	NOc#	NO_sens	cvt_eff	numflag	NO	NO_ac	NO_pr	NO_dl	numflag_NO	NO2	NO2_ac	NO2_pr	NO2_dl	numflag_NO2
0.000000	0.000694	839.400	921.400	299.700	290.210	0	0	258	5200	1.283	45.351	0.000000000	0.041	0.0010	0.0003	0.001	0.000000000	0.753	0.0020	0.0010	0.010	0.000000000
0.000694	0.001385	839.766	921.787	299.750	291.232	0	0	310	4780	1.283	45.351	0.000000000	0.046	0.0014	0.0003	0.001	0.000000000	0.735	0.0024	0.0012	0.012	0.000000000
0.001385	0.002083	839.821	921.833	299.761	291.987	0	1	21	3	1.283	45.351	0.686000000	0.001	0.0010	0.0003	0.001	0.686000000	0.002	0.0005	0.0013	0.012	0.686000000
0.002083	0.002778	839.801	921.788	299.886	292.232	0	2	9	1	1.283	45.351	0.686000000	0.002	0.0010	0.0003	0.001	0.686000000	0.001	0.0004	0.0010	0.015	0.686000000
0.002778	0.003472	839.633	921.654	300.021	292.012	1	0	644	21	1.283	45.351	0.687000000	0.120	0.0015	0.0005	0.001	0.687000000	0.012	0.0004	0.0011	0.012	0.687000000
0.003472	0.004167	839.601	921.522	299.988	291.987	3	0	654	12	1.283	45.351	0.687000000	0.120	0.0015	0.0004	0.001	0.687000000	0.022	0.0005	0.0011	0.011	0.687000000
0.004167	0.004861	839.601	921.522	299.988	291.987	4	0	4	653	1.283	45.351	0.687000000	0.000	0.0005	0.0001	0.001	0.687000000	0.123	0.0015	0.0011	0.011	0.687000000
0.004861	0.005556	839.801	921.788	421.122	291.232	0	0	7342	96379	1.283	45.351	0.699000000	73.832	3.2349	9.7289	8.234	0.699000000	83.234	32.2724	62.1346	7.234	0.699000000
0.005556	0.006251	9999.999	9999.999	9999.999	9999.999	99	99	9999	99999	99.999	999.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000

NO# NO counts provided by the instrument [cps]; not provided by our T200UP

NOc# NO converter counts provided by the instrument [cps]; not provided by our T200UP

NO_sens NO sensitivity [(pmol/mol)/cps]; not provided by our T200UP

cvt_eff Converter efficiency [%]; this parameter is calculated during the calibrations, and can be interpolated between the different calibrations (up to the instrument PI)

NO NO concentration [nmol/mol or ppb] as derived from the instrument
NO_ac NO expanded uncertainty 2 sigma
NO_pr NO precision
NO_dl NO detection limit, that can be calculated from the zero during calibrations
Important: If NO_ac, NO_pr, NO_dl are constant throughout the year, they can be added in the header and the corresponding column can be deleted

NO2 As for NO, there are corresponding columns for NO_2

level 0

https://ebas-submit.nilu.no/templates/NOx/lev0

Acknowledgement: Request acknowledgement details from data originator
Comment:

starttime	endtime	p_inlet	p_det	T_inlet	T_det	cal	zero	NO#	NOc#	NO_sens	cvt_eff	numflag	NO	NO_ac	NO_pr	NO_dl	numflag_NO	NO2	NO2_ac	NO2_pr	NO2_dl	numflag_NO2
0.000000	0.000694	839.400	921.400	299.700	290.210	0	0	258	5200	1.283	45.351	0.000000000	0.041	0.0010	0.0003	0.001	0.000000000	0.753	0.0020	0.0010	0.010	0.000000000
0.000694	0.001385	839.766	921.787	299.750	291.232	0	0	310	4780	1.283	45.351	0.000000000	0.046	0.0014	0.0003	0.001	0.000000000	0.735	0.0024	0.0012	0.012	0.000000000
0.001385	0.002083	839.821	921.833	299.761	291.987	0	1	21	3	1.283	45.351	0.686000000	0.001	0.0010	0.0003	0.001	0.686000000	0.002	0.0005	0.0013	0.012	0.686000000
0.002083	0.002778	839.801	921.788	299.886	292.232	0	2	9	1	1.283	45.351	0.686000000	0.002	0.0010	0.0003	0.001	0.686000000	0.001	0.0004	0.0010	0.015	0.686000000
0.002778	0.003472	839.633	921.654	300.021	292.012	1	0	644	21	1.283	45.351	0.687000000	0.120	0.0015	0.0005	0.001	0.687000000	0.012	0.0004	0.0011	0.012	0.687000000
0.003472	0.004167	839.601	921.522	299.988	291.987	3	0	654	12	1.283	45.351	0.687000000	0.120	0.0015	0.0004	0.001	0.687000000	0.022	0.0005	0.0011	0.011	0.687000000
0.004167	0.004861	839.601	921.522	299.988	291.987	4	0	4	653	1.283	45.351	0.687000000	0.000	0.0005	0.0001	0.001	0.687000000	0.123	0.0015	0.0011	0.011	0.687000000
0.004861	0.005556	839.801	921.788	421.122	291.232	0	0	7342	96379	1.283	45.351	0.699000000	73.832	3.2349	9.7289	8.234	0.699000000	83.234	32.2724	62.1346	7.234	0.699000000
0.005556	0.006251	9999.999	9999.999	9999.999	9999.999	99	99	9999	99999	99.999	999.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000

numflag Flags for each record/variable. The final numflag can be a combination of 3-digits flags.

Flag	Description
000	Valid data, no flag
111	Irregular data checked and accepted by data originator. Valid measurement
147	Below theoretical detection limit or formal Q/A limit, but a value has been measured and reported and is considered valid
559	Unspecified contamination or local influence, but considered valid
686	Invalid due to zero check. Used for Level 0.
687	Invalid due to span check. Used for Level 0.
699	Mechanical problem, unspecified reason.
999	Missing measurement, unspecified reason.

level 1

https://ebas-submit.nilu.no/templates/NOx/lev1

Comment:

starttime	endtime	p_inlet	T_inlet	numflag	NO	NO_ac	NO_pr	NO_dl	numflag_NO	NO2	NO2_ac	NO2_pr	NO2_dl	numflag_NO2	NOx	NOx_ac	NOx_pr	NOx_dl	numflag_NOx
0.000000	0.000694	839.400	299.700	0.000000000	0.041	0.0010	0.0003	0.001	0.000000000	0.753	0.0020	0.0010	0.010	0.000000000	0.794	0.0029	0.0013	0.010	0.000000000
0.000694	0.001385	839.766	299.750	0.000000000	0.046	0.0014	0.0003	0.001	0.000000000	0.753	0.0024	0.0012	0.012	0.000000000	0.796	0.0036	0.0015	0.012	0.000000000
0.001385	0.002083	839.821	299.761	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.002083	0.002778	839.801	299.886	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.002778	0.003472	839.633	300.021	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.003472	0.004167	839.601	299.988	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.004167	0.004861	839.801	339.122	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.004861	0.005556	839.801	339.122	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.005556	0.006251	9999.999	9999.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000

starttime Start time of each sample, as floating value (offset in days from the reference date). Jan 1st is expressed as 0
Example: 2024-01-01 10:00:00 = 0 + 10/24 = 0.416667

endtime End time of each sample, same format as starttime

p_inlet
T_inlet Temperature and pressure measured in the inlet

NO Calibrated NO concentration [nmol/mol or ppb]
NO_ac NO expanded uncertainty 2 sigma
NO_pr NO precision
NO_dl NO detection limit, that can be calculated from the zero during calibrations
Important: If NO_ac, NO_pr, NO_dl are constant throughout the year, they can be added in the header and the corresponding column can be deleted

NO2 As for NO, there are corresponding columns for calibrated NO_2

NOx As for NO, there are corresponding columns for calibrated NO_x, where $NO_x = NO + NO_2$

level 1

https://ebas-submit.nilu.no/templates/NOx/lev1

Comment:

starttime	endtime	p_inlet	T_inlet	numflag	NO	NO_ac	NO_pr	NO_dl	numflag_NO	NO2	NO2_ac	NO2_pr	NO2_dl	numflag_NO2	NOx	NOx_ac	NOx_pr	NOx_dl	numflag_NOx
0.000000	0.000694	839.400	299.700	0.000000000	0.041	0.0010	0.0003	0.001	0.000000000	0.753	0.0020	0.0010	0.010	0.000000000	0.794	0.0029	0.0013	0.010	0.000000000
0.000694	0.001385	839.766	299.750	0.000000000	0.046	0.0014	0.0003	0.001	0.000000000	0.753	0.0024	0.0012	0.012	0.000000000	0.796	0.0036	0.0015	0.012	0.000000000
0.001385	0.002083	839.821	299.761	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.002083	0.002778	839.801	299.886	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.002778	0.003472	839.633	300.021	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.003472	0.004167	839.601	299.988	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.004167	0.004861	839.801	339.122	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.004861	0.005556	839.801	339.122	0.000000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000
0.005556	0.006251	9999.999	9999.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	99.999	99.9999	99.9999	99.999	0.999000000	999.999	99.9999	99.9999	99.999	0.999000000

numflag Flags for each record/variable. The final numflag can be a combination of 3-digits flags.

Flag	Description
000	Valid data, no flag
111	Irregular data checked and accepted by data originator. Valid measurement
147	Below theoretical detection limit or formal Q/A limit, but a value has been measured and reported and is considered valid
559	Unspecified contamination or local influence, but considered valid
999	Missing measurement, unspecified reason.

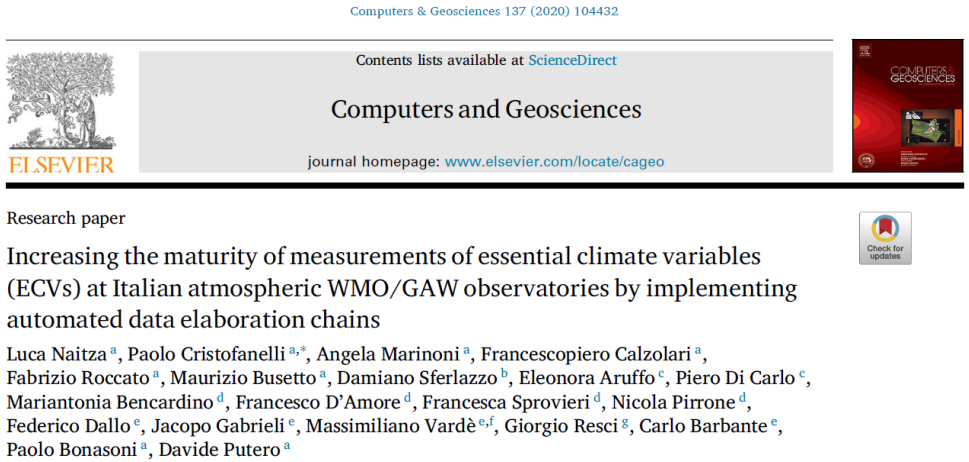
- all invalid flags in lev0 must become 999 in lev1
- all measurements corresponding to the 999 flag must be substituted by the corresponding null_value (e.g., **99.999**) in lev1

Automatic procedures at CNR-ISAC

At CNR-ISAC we have been developing a set of **automatic and standardized procedures** for the data management and preparation, starting from the raw files for each instrument. These were first produced in R (Naitza et al., 2020), and now revised and upgraded using Python

The workflow is the following:

- Raw data are collected and stored on a common server
- Corrections, calibrations, etc. are automatically applied for each measurement
- Inlet measurements are directly integrated as ancillary parameters
- Interactive (plotly) graphical products are produced
- EBAS files are automatically generated, for different levels



Computers & Geosciences 137 (2020) 104432

Contents lists available at ScienceDirect

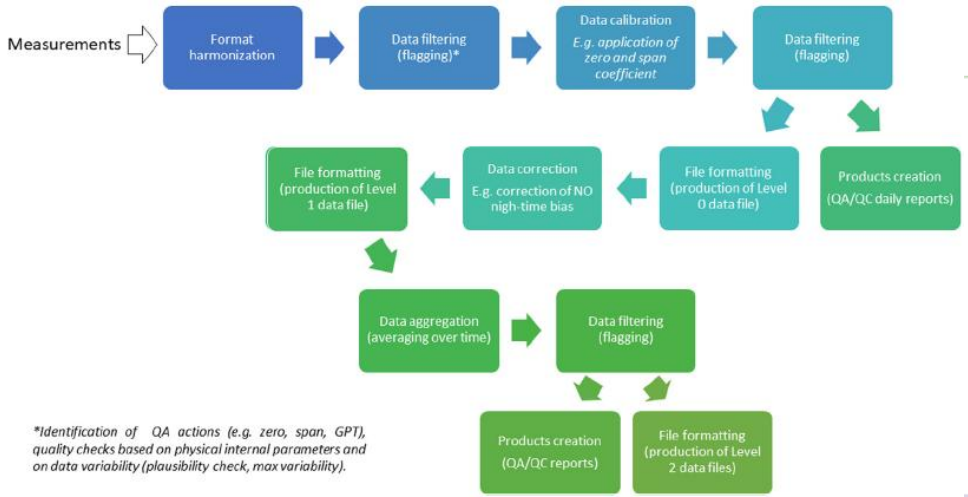
Computers and Geosciences

journal homepage: www.elsevier.com/locate/cageo

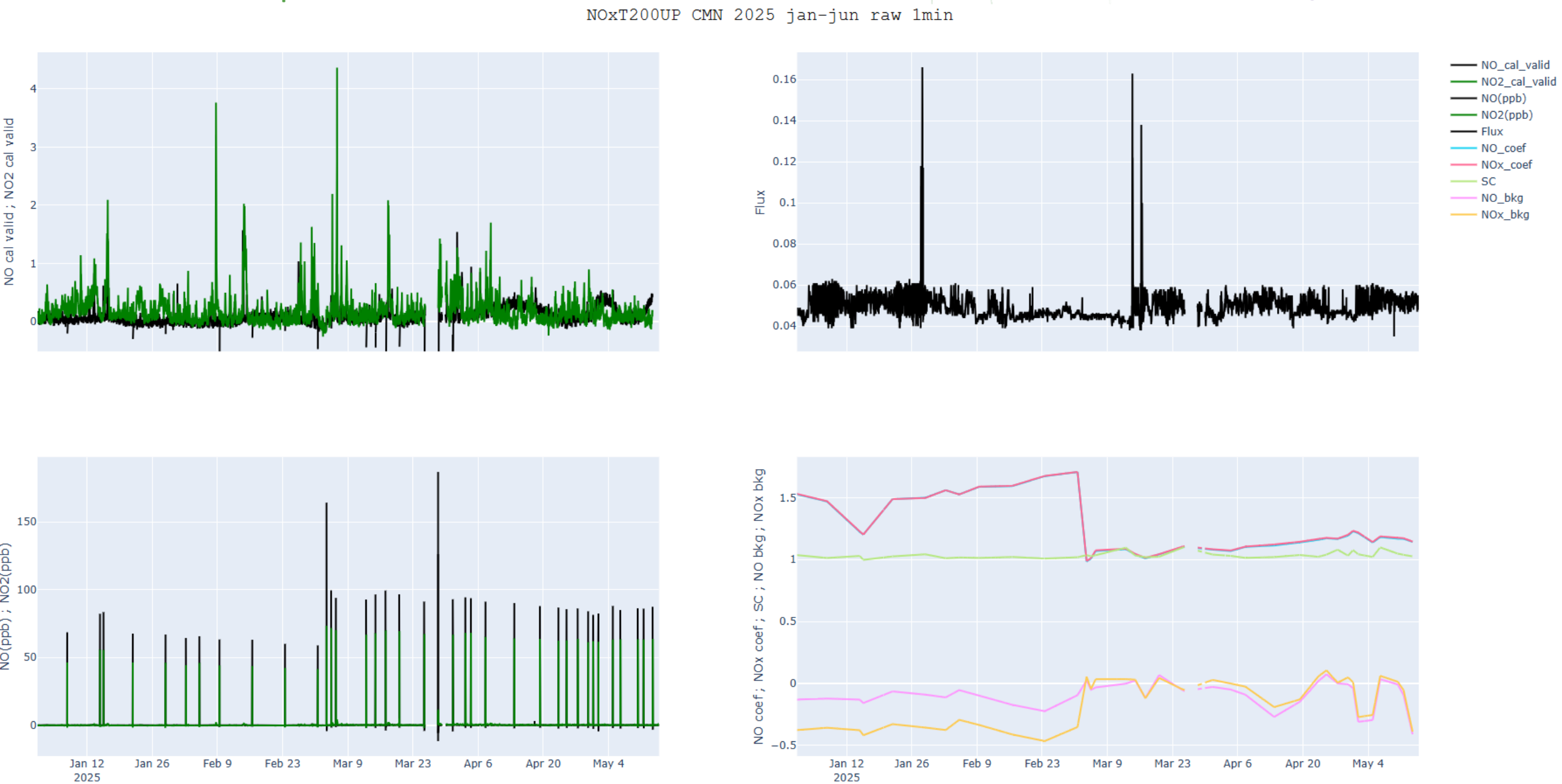
Research paper

Increasing the maturity of measurements of essential climate variables (ECVs) at Italian atmospheric WMO/GAW observatories by implementing automated data elaboration chains

Luca Naitza [a], Paolo Cristofanelli [a,*], Angela Marinoni [a], Francescopiero Calzolari [a], Fabrizio Roccato [a], Maurizio Busetto [a], Damiano Sferlazzo [b], Eleonora Aruffo [c], Piero Di Carlo [c], Mariantonia Bencardino [d], Francesco D'Amore [d], Francesca Sprovieri [d], Nicola Pirrone [d], Federico Dallo [e], Jacopo Gabrieli [e], Massimiliano Vardè [e,f], Giorgio Resci [g], Carlo Barbante [e], Paolo Bonasoni [a], Davide Putero [a]



Automatic procedures at CNR-ISAC



Automatic procedures at CNR-ISAC

There are **several advantages** for the PI of each variable (a lot of time can be saved!)

- Access the plots and check whether everything is fine
- Directly edit the metadata (by editing the different fields) required by the EBAS files
- Insert information about calibration coefficients (e.g., for O_3), or manual corrections to be applied to data (for specific periods), or assign manual flags to the measurements
- Run the procedures on demand and automatically

start_date	start_time	end_date	end_time	new_flag	variable
2025-03-04	09:30:00	2025-03-04	11:32:00	699	NO(ppb)
2025-03-04	09:30:00	2025-03-04	11:32:00	699	NO2(ppb)
2025-03-28	09:00:00	2025-03-28	10:24:00	699	NO(ppb)
2025-03-28	09:00:00	2025-03-28	10:24:00	699	NO2(ppb)

Manual flags (can be applied to all variables)

start_date	end_date	standard	number
2021-01-01	2021-12-31	"Status calibration standard: 1, Manufacturer: Unknown, Batch: Unknown"	1
2022-01-01	2022-12-31	"Status calibration standard: 1, Manufacturer: Unknown, Batch: Unknown"	1
2023-01-01	2023-12-31	"Status calibration standard: 1, Manufacturer: NPL, Batch: 2243R"	1
2024-01-01	2024-02-13	"Status calibration standard: 1, Manufacturer: NPL, Batch: 2243R"	1
2024-02-14	2024-07-17	"Status calibration standard: 2, Manufacturer: MESSER, Batch: 53591848"	2
2024-07-18	2024-12-31	"Status calibration standard: 3, Manufacturer: NPL, Batch: D109110"	3
2025-01-01	2025-12-31	"Status calibration standard: 1, Manufacturer: NPL, Batch: D109110"	1

Information on calibration standards (NO_x)

date_start	time_start	date_end	time_end	slope	offset
2022-01-01	00:00	2022-01-01	00:01	1	0
2022-04-12	10:16	2022-04-13	08:14	1.00387	0.330034
2022-07-06	20:07	2022-07-07	20:01	1.013825	0.448273
2022-10-04	11:10	2022-10-06	19:44	0.999387	0.425932
2023-02-09	20:33	2023-02-13	04:46	1.012745	0.286634
2023-05-08	08:20	2023-05-09	22:24	1.0137415	1.047491
2023-07-12	19:59	2023-07-28	00:22	1.0183794	0.8445554
2023-08-30	09:36	2023-08-30	16:30	1	0
2023-12-14	11:09	2023-12-18	23:43	1	0
2024-03-13	09:30	2024-03-19	04:42	1.003997	0.8309722
2024-05-17	09:13	2024-05-20	07:34	1.002979	0.7728407
2024-08-07	12:51	2024-08-08	10:43	1.003696	0.780166
2024-11-20	09:36	2024-11-26	08:27	1.007327	0.777547
2025-02-27	08:55	2025-02-28	13:16	1.001404	0.775677
2025-05-14	11:56	2025-05-15	06:56	1.006475	0.799019
2025-12-31	23:58	2025-12-31	23:59	1	0

Calibration coefficients (O_3), that will be linearly interpolated among calibrations

Automatic procedures at CNR-ISAC

There are **several advantages** for the PI of each variable (a lot of time can be saved!)

- Access the plots and check whether everything is fine
- Directly edit the metadata (by editing the different fields) required by the EBAS files
- Insert information about calibration coefficients (e.g., for O_3), or manual corrections to be applied to data (for specific periods), or assign manual flags to the measurements
- Run the procedures on demand and automatically

If interested, you can contact:

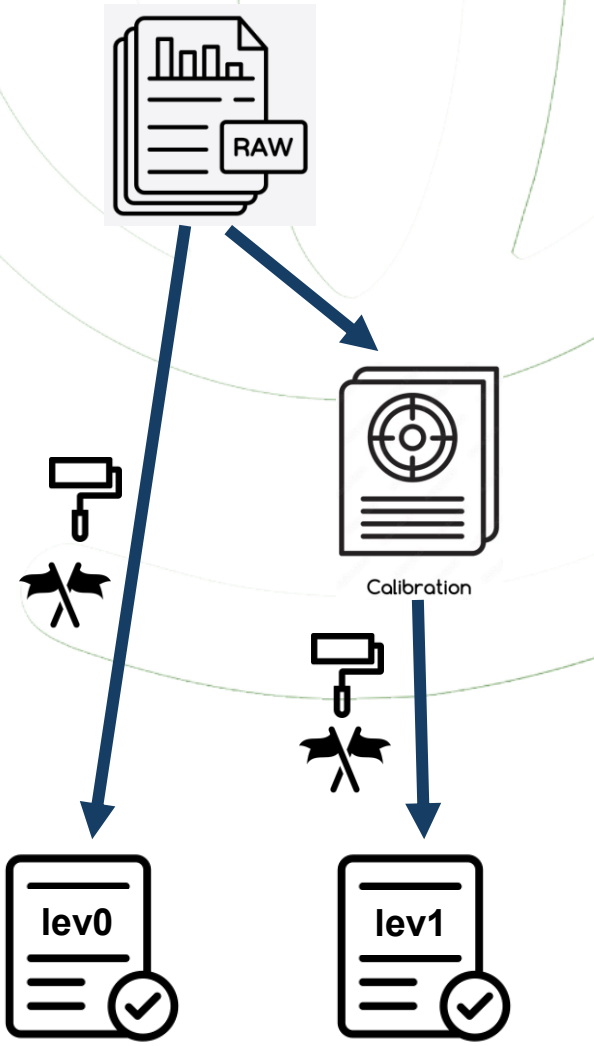
Maurizio Busetto m.busetto@isac.cnr.it
Davide Putero d.putero@isac.cnr.it

Assignment

- Download:
  - Daily raw data files (one month in total, March 2024)
  - Calibration raw data files (4 calibration events)

- Prepare the EBAS lev0 file:
  - Create the starttime and endtime in the right format
  - Prepare (format/create) the columns needed for the lev0 file
  - Assign the flags to each data record
  - Generate the lev0 file in the requested format

- Prepare the EBAS lev1 file:
  - Retrieve calibration data and calculate the calibration parameters
  - Linearly interpolate the calibration parameters and merge with the dataframe
  - Create NO, NO_2 and NO_x calibrated data
  - Assign the flags to each data record
  - Generate the lev1 file in the requested format



THANKS!

IR0000032 – ITINERIS, Italian Integrated Environmental Research Infrastructures System
(D.D. n. 130/2022 - CUP B53C22002150006) Funded by EU - Next Generation EU PNRR-Mission 4 “Education and Research” - Component 2: “From research to business” - Investment 3.1: “Fund for the realisation of an integrated system of research and innovation infrastructures”

Finanziato dall'Unione europea NextGenerationEU
Ministero dell'Università e della Ricerca
Italiadomani