

ACTRIS - CAMS2_21a

Near-Real-Time provision of aerosol and reactive species from ACTRIS and EMEP observation networks: WP2 update



Atmosphere Monitoring

8 April 2025



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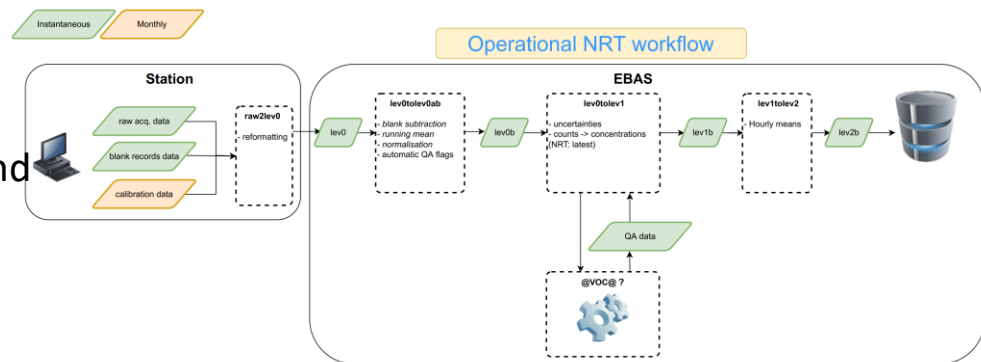


Developing procedures for high-quality VOC concentrations in NRT

VOCs of interest – testing phase: isoprene, benzene, toluene, acetaldehyde and acetone

Two main types of techniques TD-GC-FID-MS and PTR-MS

Pilot sites - 4 future ACTRIS NF: Jungfrauoch (Switzerland), Monte Cimone (Italy), Hyytiälä (Finland) and SIRTA (France) to be extended in a second step to additional NFs (Beromuenster (Switzerland) etc.)



Deliverables:

- To define the required specification for NRT data transmission of VOC data including automatic quality control, traceability & develop procedure and software for L0
- To perform real-scale testing of software at selected sites,
- To provide training to data operators for the implementation and application of NRT procedures,



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Near Real Time data delivery GC-MS-EMPA

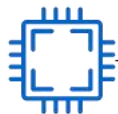


- Empa sites
 - Jungfraujoch: **code implemented, data flow running and tests on-going**
 - Beromunster: **in testing phase**
- NRT scripts
 - NRT data upload from gcwerks: **code implemented**
 - QA on areas/rt: **code implemented**
 - Concentration calculations: **code implemented**
 - QA on concentrations: **code implemented**

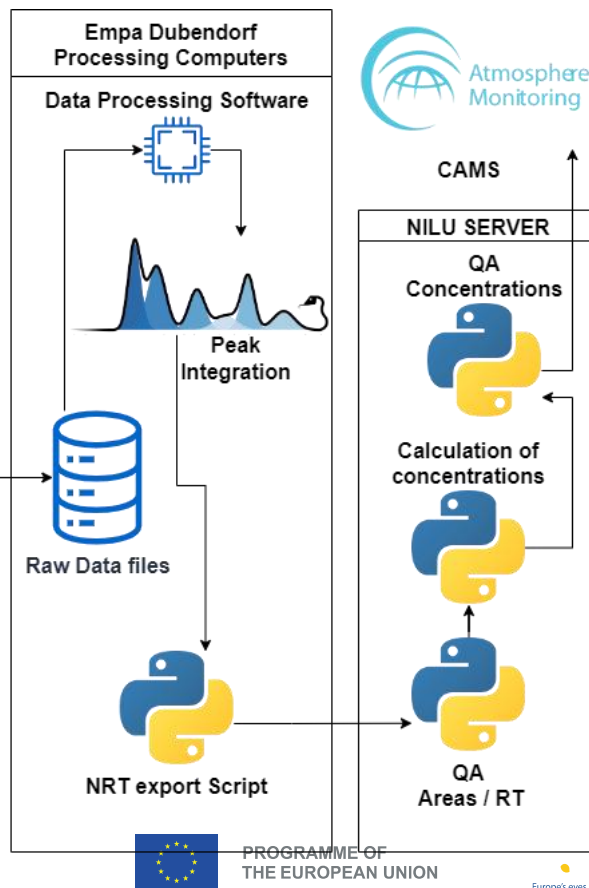


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Data flow for GC



Data acquisition
on sites



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P T R - Q u a d - M S N R T s t a t u s

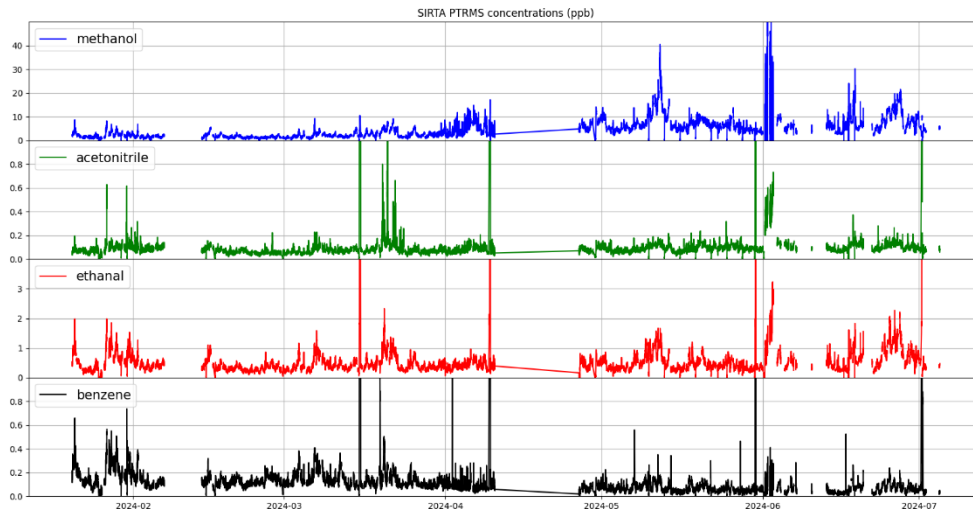
Code to process the PTR-MS data from cps to pmol/mol developed in Python and available on a git repository : https://gitlab.in2p3.fr/ipsl/sirta/ptr-ms/ptrms_lib

Received from SIRTa station:

- Concatenated zip file every hour.

Processing (blank correction, running mean, automatic QC):

- Every 3 hours.
- 1 output file per hour.
- blank saved for each file.



Continuous hourly outputs from 2023-12-13 to date



P T R M S L e v e l 0 - > 1 - > 2

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- Source code for PTRMS level0 shared between contributors :

https://gitlab.in2p3.fr/ipsl/sirta/ptr-ms/ptrms_lib

- Template for level0 with Sirta as a pilot site, with metadata, PTRMS vocabulary, flags,...published in EBAS and updated with more metadata: https://ebas-submit.nilu.no/templates/VOC/PTR-MS_lev0; To update the template with **VOCUS PTRMS** metadata; RT submission will use condensed raw data 1 min
- SOP PTRMS: Update with new masses
- Tool to convert PTRMS raw data to ACTRIS NASA Ames files developed and being tested at SIRTa's site. Code (installation, configuration, data transfer to the DC):
https://www.icare.univ-lille.fr/depot/ACTRIS/CAMS/software/actris_ptrms_converter-v0.1.0.zip
- Tools to convert PTRMS level 0 to level 1 and to level 2 developed and being tested at NILU for the SIRTa's measurements. Code : https://www.icare.univ-lille.fr/depot/ACTRIS/CAMS/software/actris_ptrms_concentration_converter-v0.0.0.zip

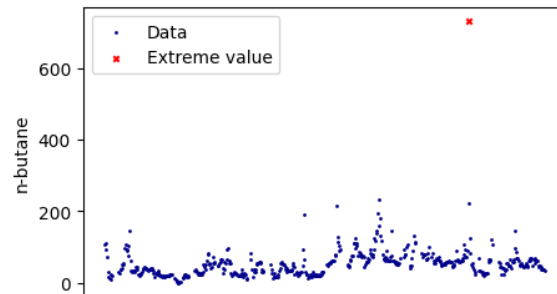
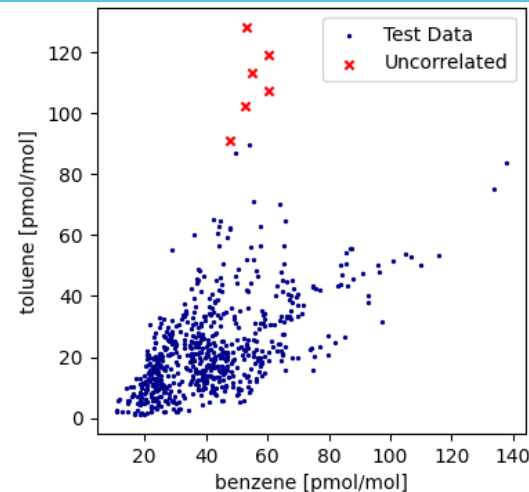


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Quality Assessment : GC and PTRMS

- X-Y correlations
 - Flag points outside of cloud
- Extreme values detection
 - Flag values outside of statistical range
- Retention time check (GC)
 - Ensure that the expected peak was integrated

=> Test with new PTRMS data: ongoing



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2023-04-22
2023-05-01
2023-05-08
2023-05-15
2023-05-22
2023-06-01
Date
ECMWF
eyes on Earth



W P 2 N e x t S t e p s

Atmo
Mon

- Continue bug-fixing the current NRT pipeline (for GC)
- Definition of a concept for PTRMS templates (Quad – ToF from Ionicon/VOCUS) to be implemented at additional sites: **ongoing VOCUS template definition**
- Processing software to be adapted to work with PTRMS level 0 file in EBAS NASA Ames:
 - ✓ level 0 creation and SIRTa implementation : **done**
 - ✓ lev0 processing to concentrations : **done**
 - ✓ link to NILU's server: **fixing bugs**
 - ✓ Conversion from level 0 to 1 and from 1 to 2 (with averaging tool for PTRMS): **fixing bugs**
- Additional pilot sites: for PTRMS (Hyytiälä – Finland); for GC (Beromünster)

CiGas-proposal for CAMS 21a-phase 2 project – WP2:

Developing procedures for quality-controlled VOC RT/NRT data provision

Deliverables and Milestones

Deliverables:				
#	Responsible	Nature	Title	Due
D21a.2.1.1 ✓	CiGas/EMPA	Report	Interim report on the further development of @VOC@ for NRT data checks	M12
D21a.2.1.2 ✓	CiGas/EMPA	Report	Procedure and software operational for L0 data preparation and submission	M24
D21a.2.2.1 ✓	CiGas/IMT	Report	Procedure and software operational for L0 data preparation and submission	M24
D21a.2.3.1	CiGas/EMPA	Report	Procedure and software operational for averaging and automatic online quality control, based on @VOC@.	M32
D2a1.2.4.1	CiGas/IMT	Report	Provision of 4 months of NRT Data for 5 VOCs at the pilot sites and assessment versus yearly validated dataset, upscaling potential of the NRT delivering system	M38

30/06/2025

31/12/2025

Milestones:				
#	Responsible	Title	Means of verification	Due
M21.2.1 ✓	CiGas/EMPA	Procedure and script development for L0 GC data submission	Short report	M18
M21.2.2 ✓	CiGas/IMT	Procedure and script development for L0 PTR-MS data submission	Short report	M18
M21a.2.3	CiGas/EMPA	NRT software development for averaging and automatic online quality control for both VOC instruments used in this project	Short report	M25
M21a.2.4	CiGas/IMT	Outcome of the real-scale testing	Short report	M36

31/10/2025

+ Deliverable D21a.4.2.2: Report on implementing RT data production for VOC and NMHC parameters by CiGas IMT: ✓

ACTRIS - CAMS2_21a WP3

Progress



Robert Wegener, Benjamin Winter

Research Center Jülich, FZJ

ACTRIS CiGas Topical Centre for Nitrogen Oxides

Markus Fiebig, Kjetil Tørseth,

Paul Eckhardt, Sverre Solberg

Stiftelsen NILU

ACTRIS Data Centre



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CAMS2_2a WP3

Deliverables:

- (CiGas and NILU): report comparing the data processing schemes of EMEP, ACTRIS and EEA data with existing datasets.
- (CiGas): report which demonstrates the extra value of the ACTRIS data processing scheme for NO_x using NO_x and NO_y datasets measured at the background site station of Hohenpeissenberg.
- (NILU): Demonstrate the capability of providing EMEP NO₂ and ozone data quality assured using statistical tests on a RRT schedule by selecting 1-2 stations with instrumentation, and assess the improvements as compared to data with less stringent quality assurance.

Milestones:

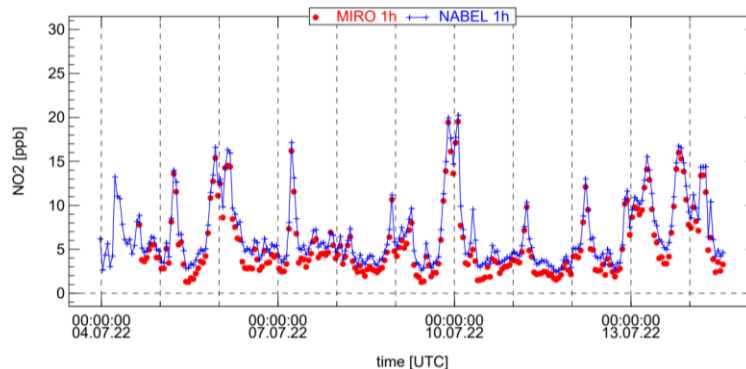
- M11: (CiGas and NILU): Description of NO_y and NO_x measurements at Hohenpeissenberg
- M11: Selection of **test sites** for demonstrating EMEP and ACTRIS NO_x ozone RT data delivery.



CiGas Audit in November
Inspect capacities for RRT Nox data delivery

Hohenpeissenberg,
Monte Cimone,
Košetice

NABEL-Station Zürich-Kaserne
Vergleich Stationsinstrumente – MIRO_0017/Picarro_LBDS2006



During the 2022 Campaign, the NABEL NO₂ data with Mo converter exceed the CiGas MIRO NO₂ data, when the values are low and the relative contribution of NO_y is high.



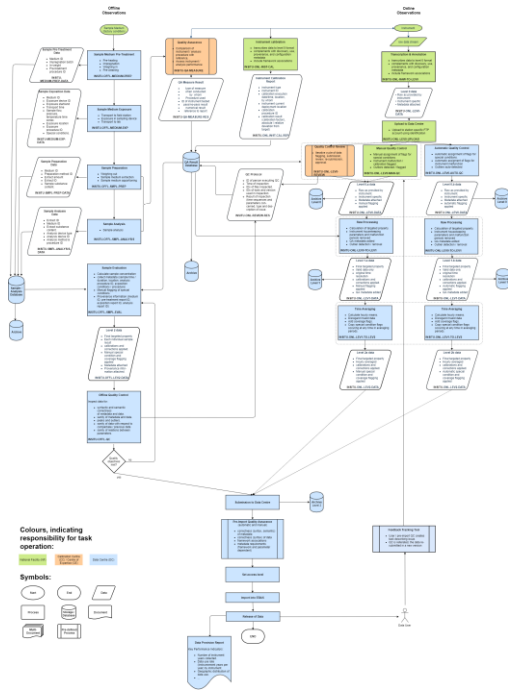
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NRT Data Submission- The NOx Perspective

Status



Defines responsibilities and Data levels:

Until 2022:

Stations submitted corrected level 0 or level 2 data or the TC corrected data

From 2023:

The Stations only submit uncorrected data. The TC does the corrections

NO2 data measured with Molybdenum converters cannot be accepted

Data Management Plan



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NRT Data Submission- The NOx Perspective

Status

NOx implementation of ACTRIS In Situ data levels:

Level 0a: data as provided by instrument, amount fraction and raw counts, flags applied.



Level 1a: calibrations applied, original time resolution, flags applied.



Level 2: hourly averages, offset correction applied, not sample line corrected.



Level 3: generated directly from level 1, offset correction applied, hourly averages, sample line corrected.



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NRT Data Submission- The NO_x Perspective

Status

Time from entry inlet line to entry of converter: 4.3 s

Duration of stay in converter or bypass line: 0.2 s

Duration of stay in converter: 2.5 s

Converter temperature: 308.15 K

converter_efficiency, %pressure, hPa, Location=inlet,

Matrix=instrumenttemperature, K, Location=inlet,

Matrix=instrument

NO_x Data Level 2

O₃ Data level 1 (calibrated)

Met Data level 0 (raw)



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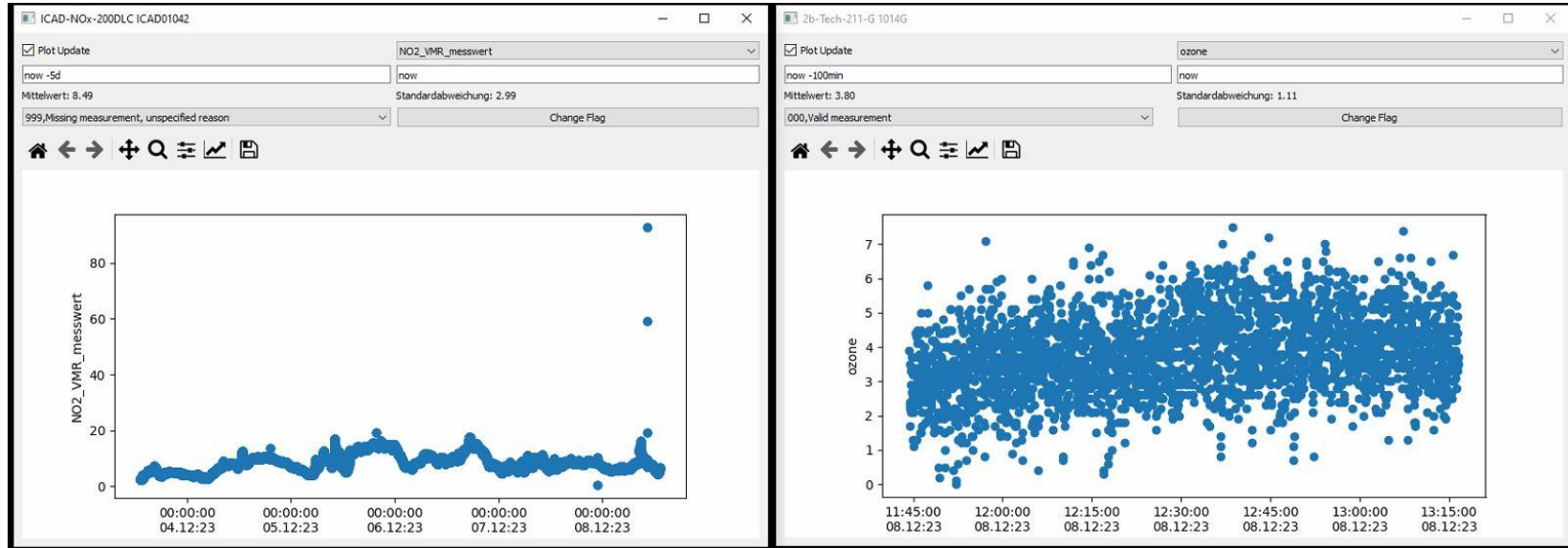
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NRT Data Submission- The NOx Perspective

The Status (CAMS2-21a WP3)



done in NRT ?



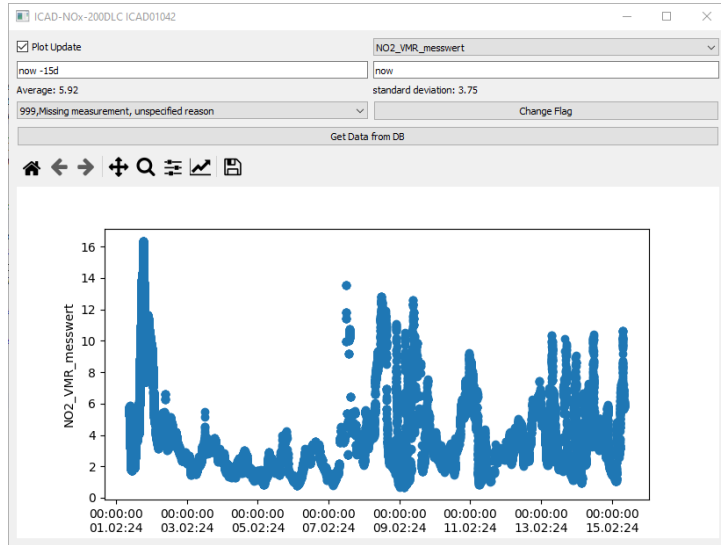
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The Status (CAMS2-21a WP3)

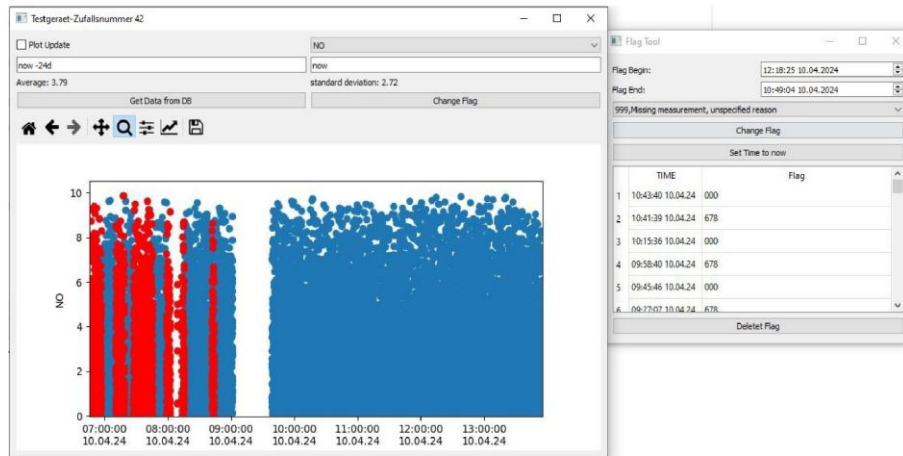


Tested with
NOx monitors
Ozone monitors
GHG monitors



NRT Data Submission- The NOx Perspective

Where do we go from here ?



Python – based Software
Programmed by Benjamin Winter (FZJ)
GUI
Data flagging is possible (automatic / manual)
Data can be sent to Data centre
β-Version tested at Hohenpeissenberg



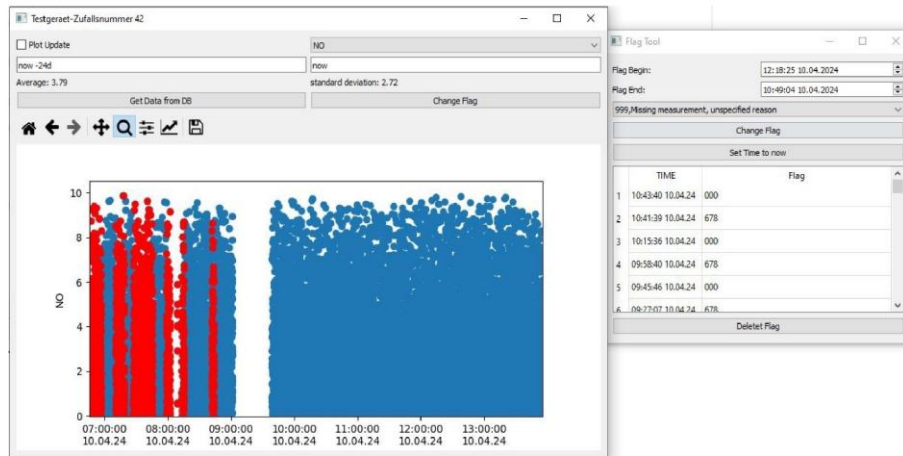
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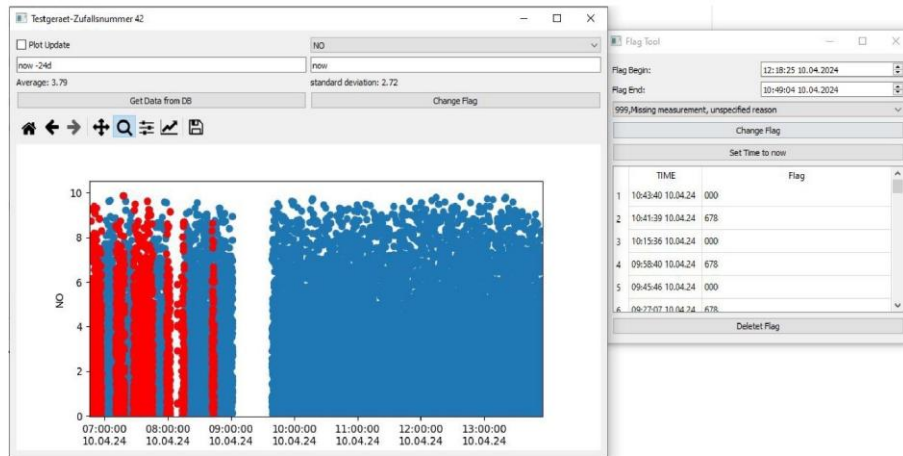
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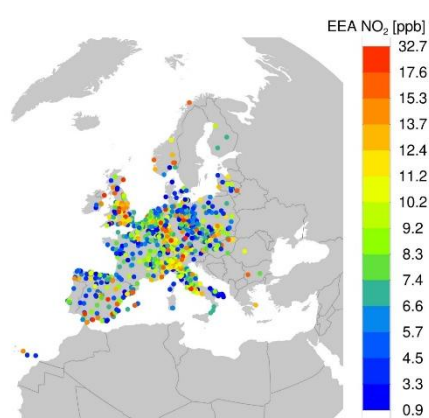


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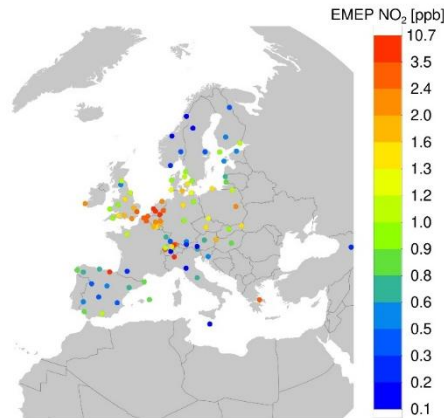
CAMS2_2a WP3: NO_x Data availability




Overview of NO_x data availability and quality measures from EEA, EMEP and ACTRIS routes of delivery (M14)



EEA Network 1006 sites



EMEP Network 97 sites



EMEP COPERNICUS ROUTE

Copernicus Atmosphere Monitoring Service

D21a.3.1.1

Overview of NO_x data availability and quality measures from EEA, EMEP and ACTRIS routes of delivery

Issued by: CiGas (FZJ) / Robert Weeener



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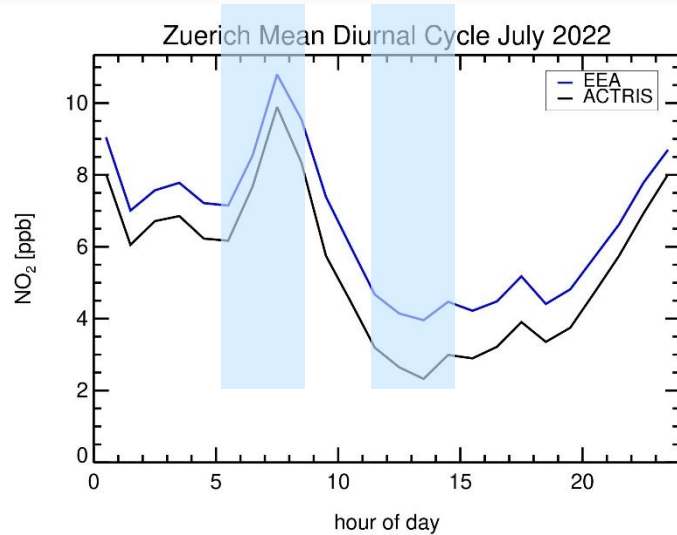
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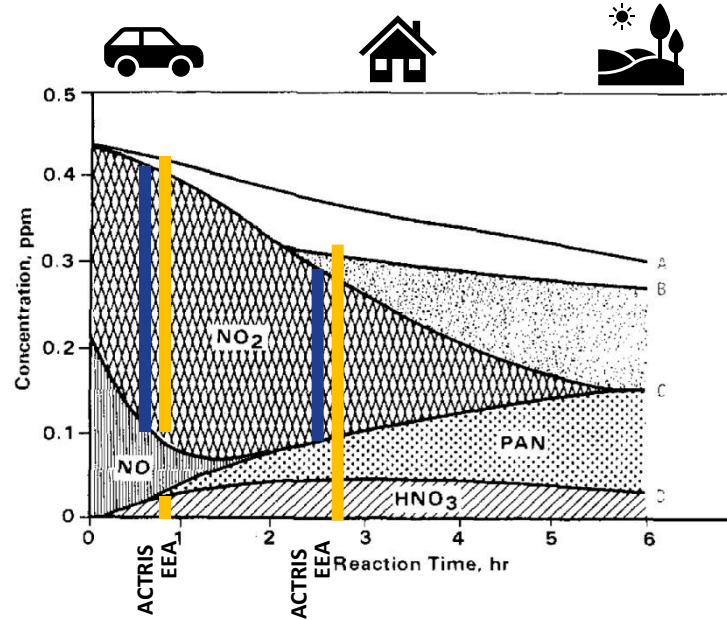


CAMS2_2a WP3: Comparison of NOy and NOx Data

Comparison of NOy and NOx data measured at the background site Hohenpeissenberg (M26)



Data from NABEL / EMPA Stefan Reimann



Spicer, C. W. (1983). "Smog chamber studies of nitrogen oxide (NOx) transformation rate and nitrate precursor relationships." *Environmental Science & Technology* **17**(2): 112-120.



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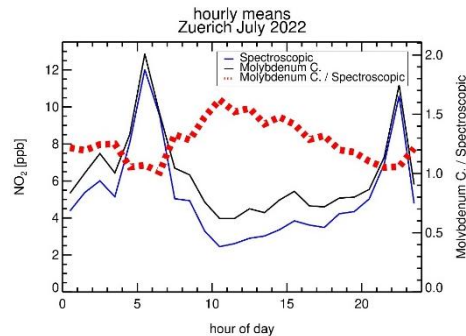
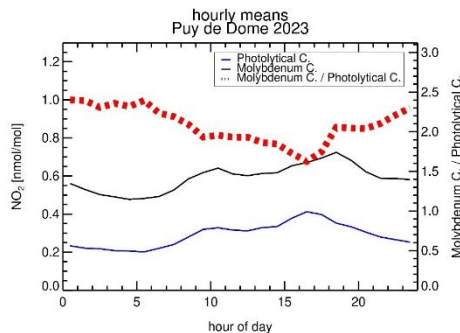
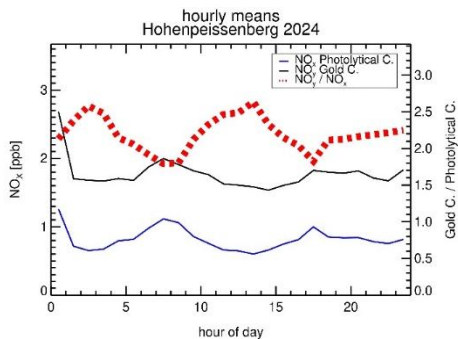
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CAMS2_2a WP3: Comparison of NOy and NOx Data



Comparison of NOy and NOx data measured at the background site Hohenpeissenberg (M26)



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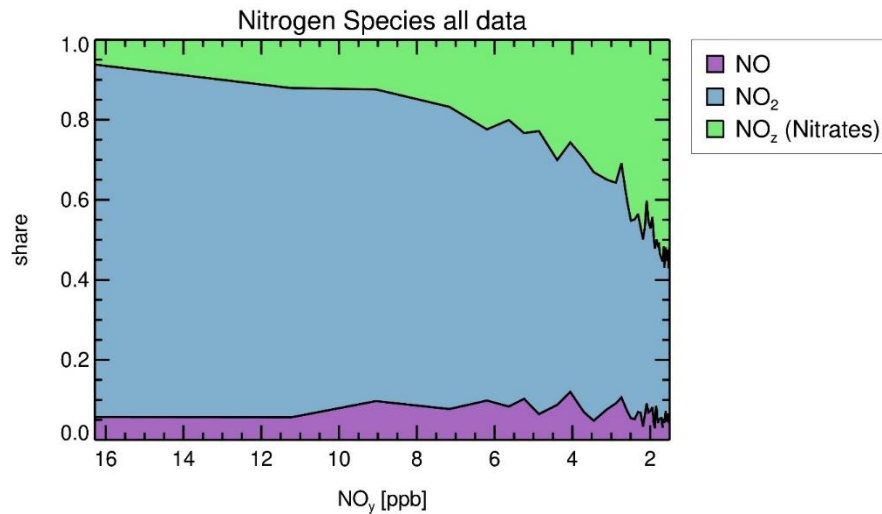
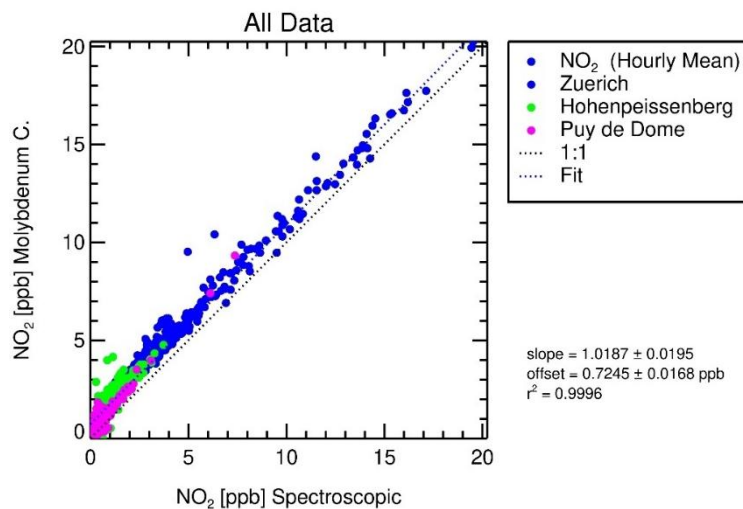
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CAMS2_2a WP3: Comparison of NO_y and NO_x Data



Comparison of NO_y and NO_x data measured at the background site Hohenpeissenberg (M26)



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