

ACTRIS - CAMS2_21a

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



Atmosphere Monitoring

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7 November 2024, CiGas community meeting – ACTRIS Week 2024



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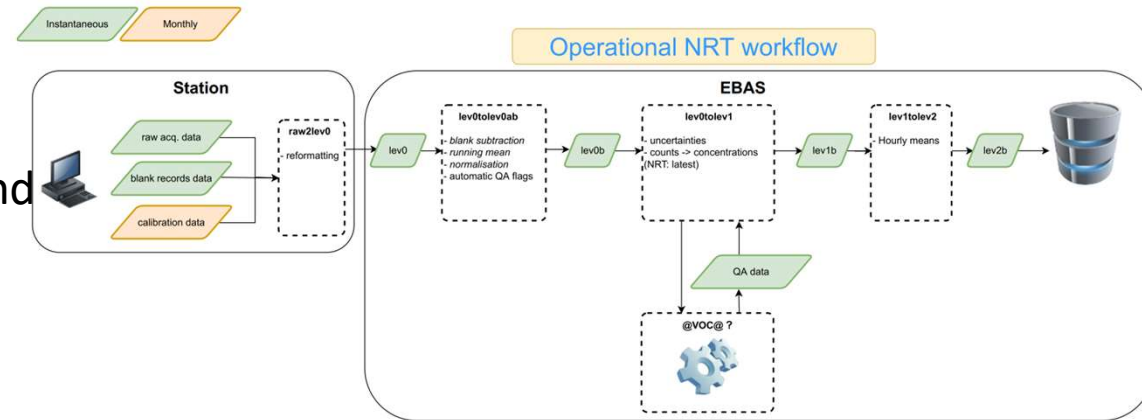


Developing procedures for high-quality VOC concentrations in NRT

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: Jungfraujoch (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



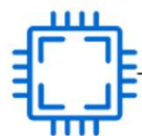
- Empa sites
 - Jungfrauoch: **code implemented, data flow running and tests on-going**
 - Beromunster: **planned**
- NRT scripts
 - NRT data upload from gcwerks: **code implemented**
 - QA on areas/rt: **code implemented**
 - Concentration calculations: **code implemented**
 - QA on concentrations: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



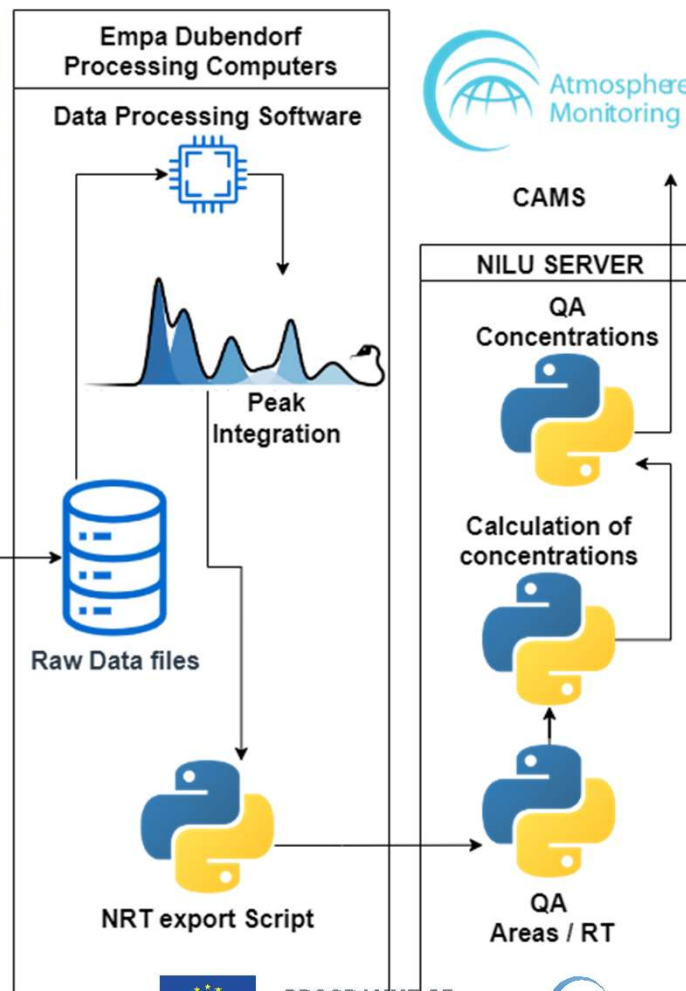


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Dataflow for GC



Data acquisition on sites



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PTRMS NRT status

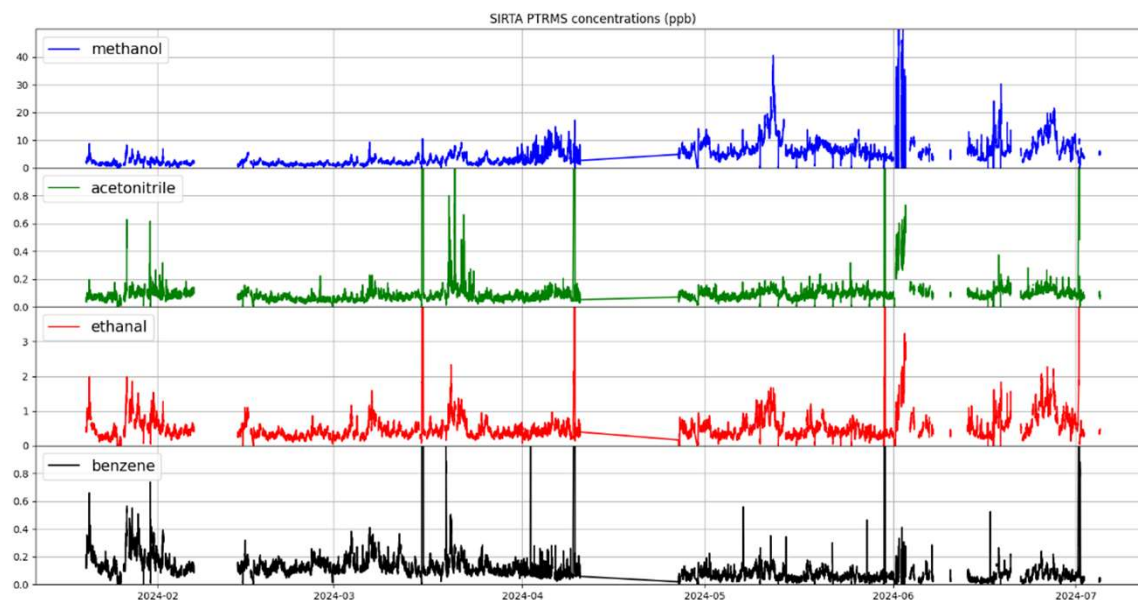
Code to process the PTR-MS data from cps to pmol/mol developed in Python and available on a git repository : https://gitlab.in2p3.fr/ipsi/sirta/ptr-ms/ptrms_lib

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



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P T R M S L e v e l 0

Source code for PTRMS level0 shared between contributors : https://www.icare.univ-lille.fr/depot/ACTRIS/CAMS/software/actris_ptrms_converter-v0.1.0.zip

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

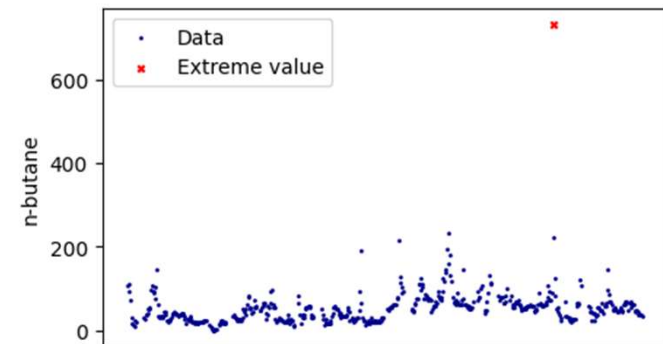
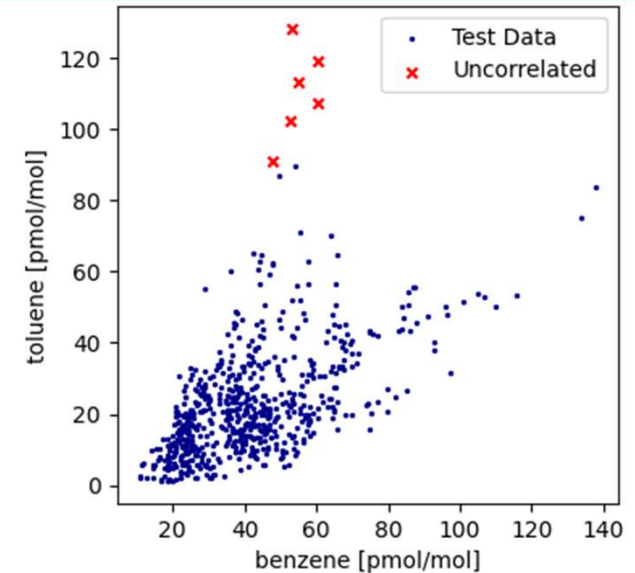
Update of the template with **VOCUS PTRMS** metadata; RT submission will use condensed raw data 1 min resolution (when there are fluxes measured at high time resolution); update of the vocabulary with new mass group numbers



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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



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2023-04-22
2023-05-01
2023-05-08
2023-05-15
2023-05-22
2023-06-01
opernicus
Data bys on Earth

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

- Continue bug-fixing the current NRT pipeline (for GC)
- Define a concept for PTRMS templates (Quad – ToF from Ionicon/VOCUS) to be implemented at additional sites: **ongoing**
- 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: **done**
- For GC and for PTRMS: Procedure and software operational for L0 data preparation and submission
- Additional pilot sites: for PTRMS (Hyytiälä – Finland); for GC (Beromunster)



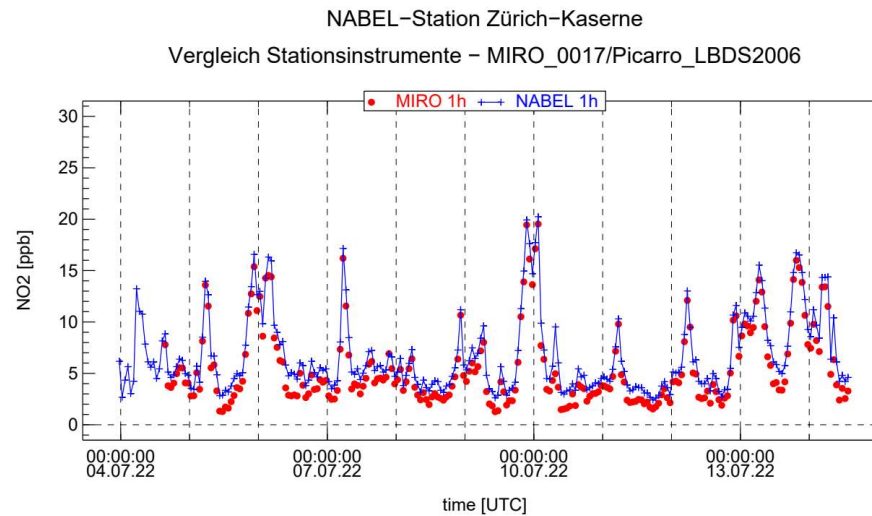
CAMS2_2a WP3

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. ✓



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.

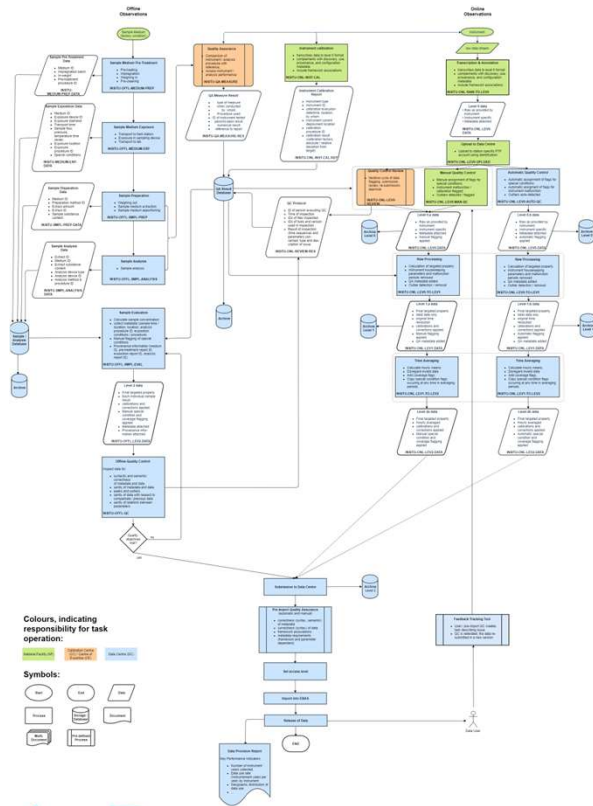
CiGas Audit in November
Inspect capacities for RRT Nox data delivery

Hohenpeissenberg,
Monte Cimone,
Košetice



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



NRT Data Submission- The NOx Perspective

Status

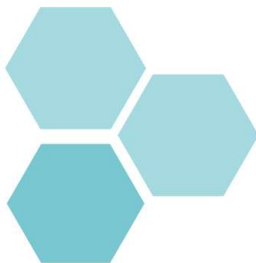
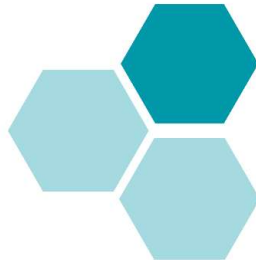
NOx implementation of ACTRIS In Situ data levels:

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.



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

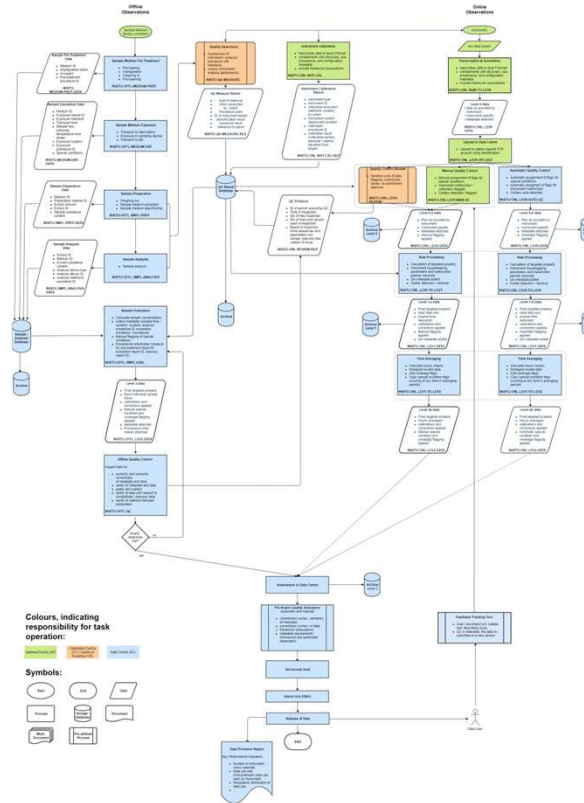
O₃ Data level 1 (calibrated)

Met Data level 0 (raw)



NRT Data Submission- The NOx Perspective

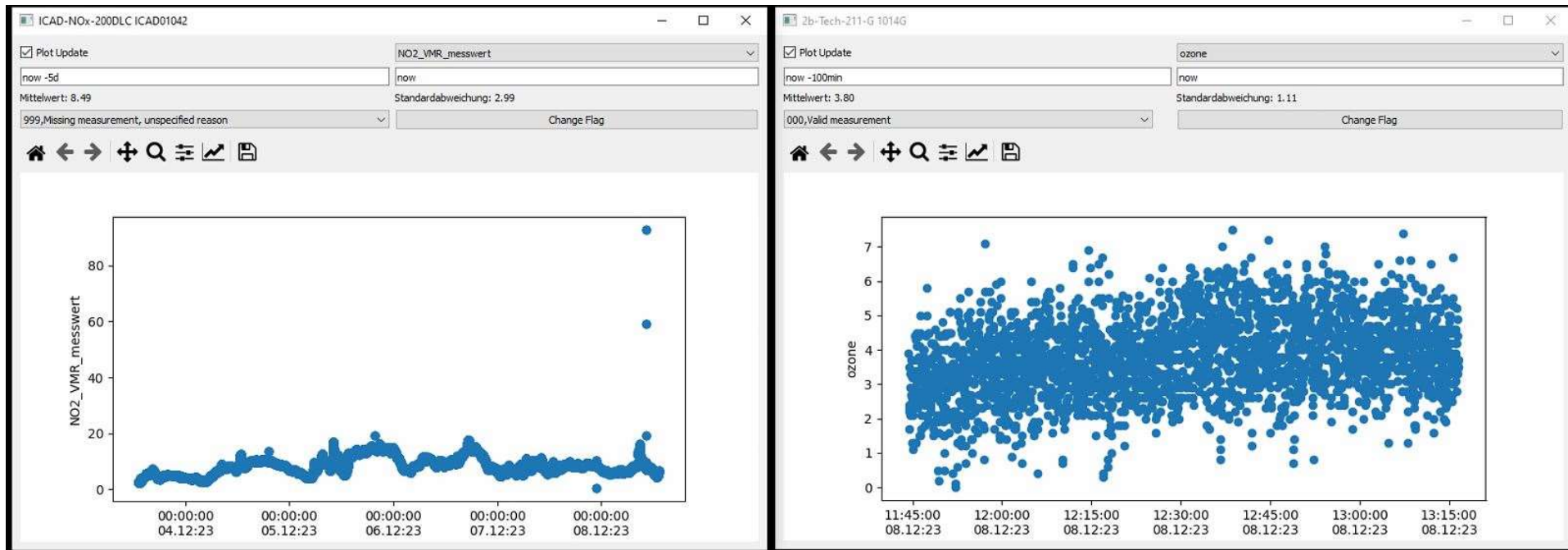
The Vision



Can this be done in NRT ?

NRT Data Submission- The NOx Perspective

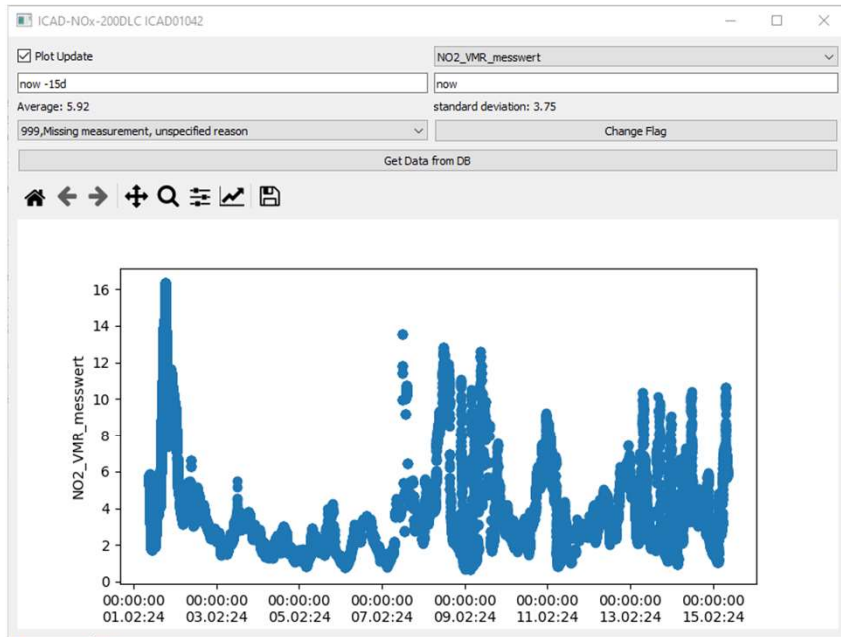
The Status (CAM52-21a WP3)



done in NRT ?

NRT Data Submission- The NOx Perspective

The Status (CAMS2-21a WP3)

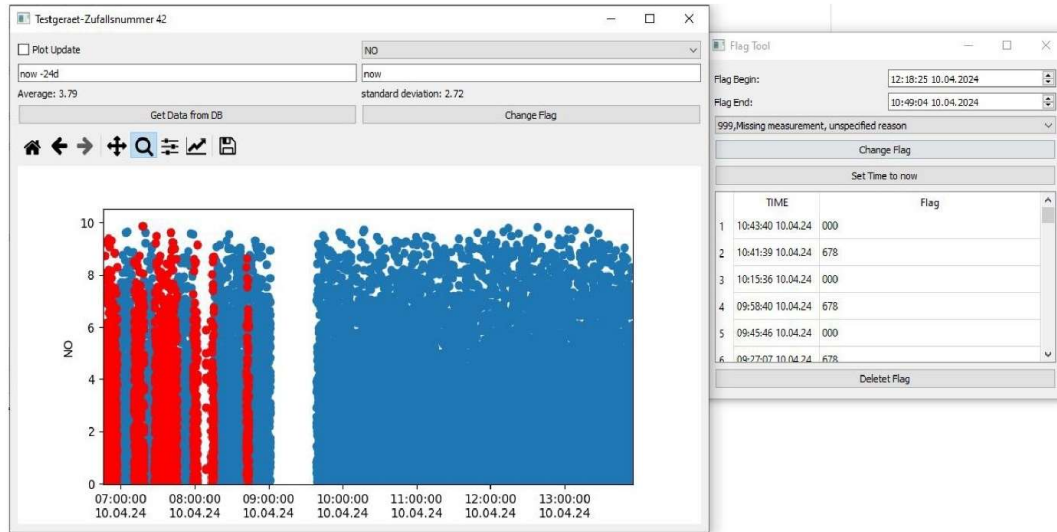


Tested with
NOx monitors
Ozone monitors
GHG monitors



NRT Data Submission- The NOx Perspective

Where do we go from here ?

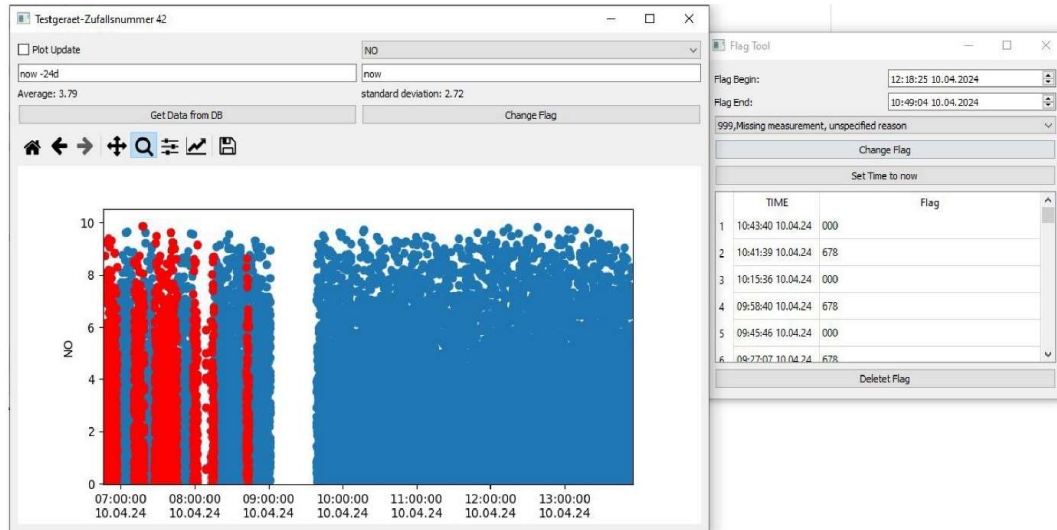


Python – based Software
Programmed by Benjamin Winter (FZJ)
GUI
Data flagging is possible (automatic / manual)
Data can be sent to Data centre
β-Version tested at Hohenpeissenberg

NRT Data Submission- The NOx Perspective

The status

Connection to instrument database
Connection to calibration database



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