

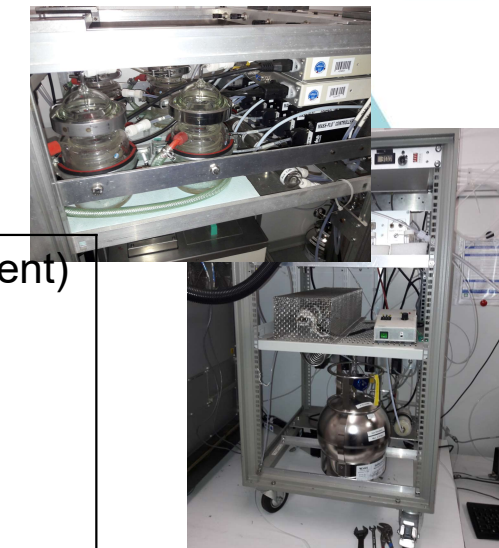
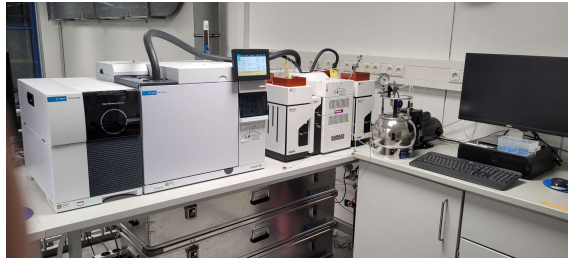


FZJV: Activity and implementations status

Andrea Marcillo, Katrin Seemeyer,
Peeyush Khare, Achim Grasse,
Roman Romany, Ralf Tillmann

Activity workshop 2024, Matera, Italy – November 7, 2024

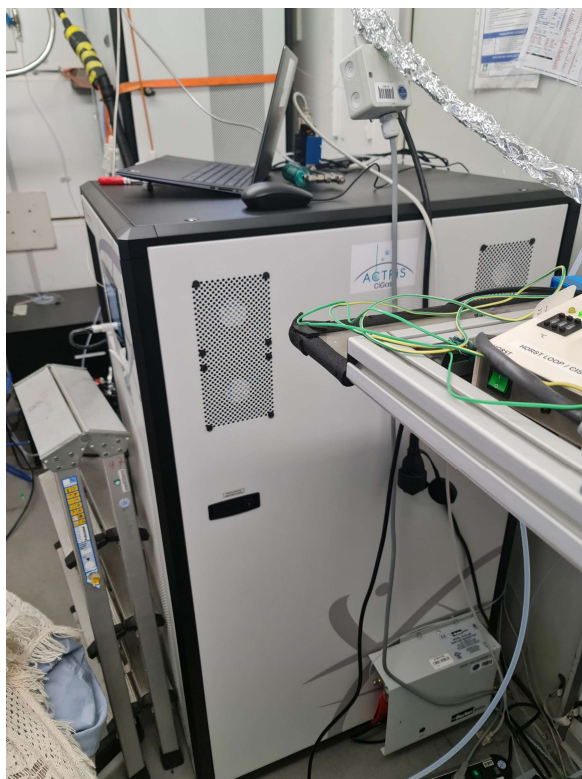
Activity/implementation status



- FUSION-PTR-TOF-MS 10K
- VOCUS
- PTR-TOF-MS 8000
- Charon
- TD-GC-FID/MS (Gerstel TDS-G; CIS)
- On-line TD-GC-FID/MS (Markes, Agilent)

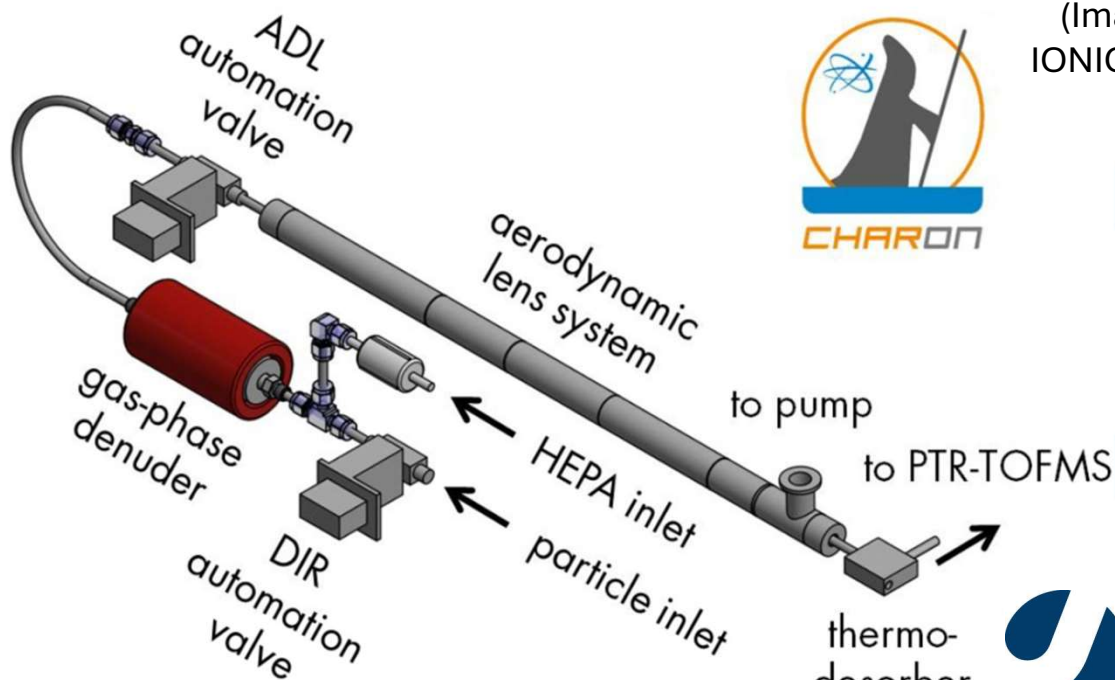
- Off-line TD-GC-FID/MS (Markes, Agilent)
- System for automated canister and sample tube analysis
- Round robins
- Liquid Calibration Unit
- Diffusion sources
- Certified laboratory standards (NPL)

FUSION-CHARON Mass Spectrometer



FUSION-CHARON

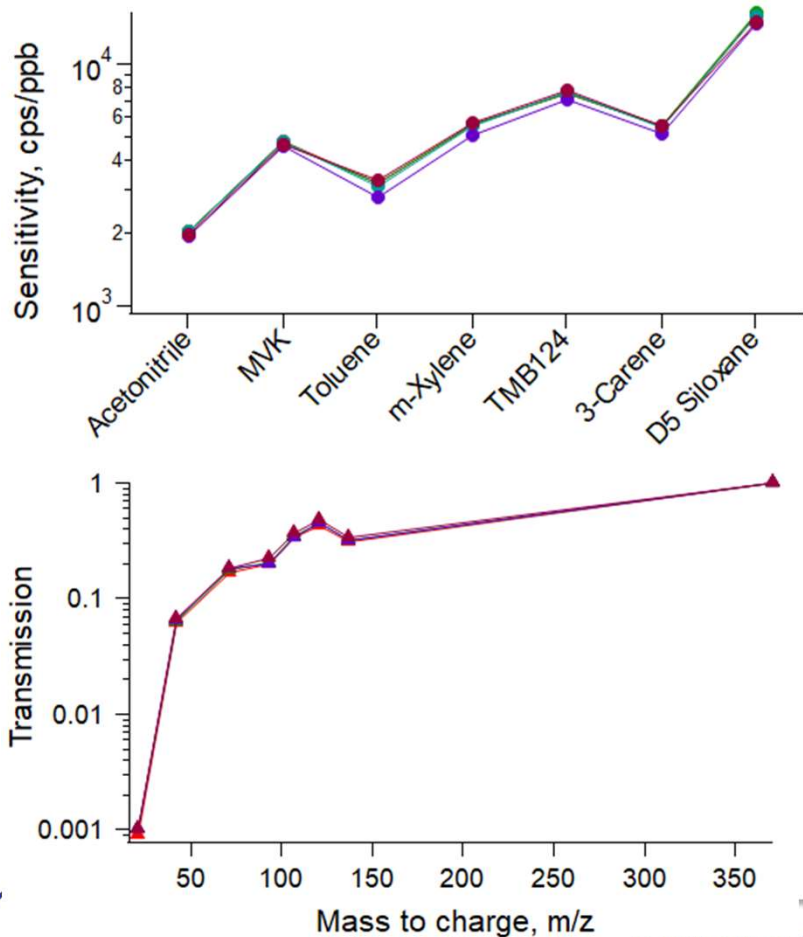
FUSION PTR-TOF 10k
Detection limit: < 0,2 pptv
Sensitivity: up to 80000 cps/ppbv
Mass resolution: > 10000



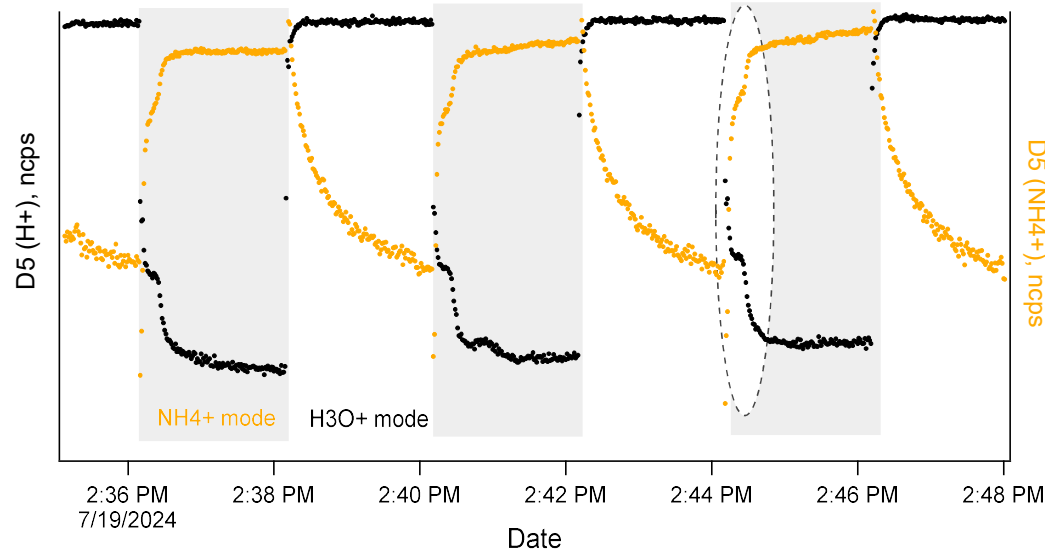
CHARON design
(Image credits:
IONICON Analytik)

FUSION-CHARON Instrument performance

Instrument stability (10 days)



Ion mode switching



Switching time < 1 min



Instrument data base development

Welcome to ACTRIS CiGas InstrumentDB

Repository of instruments for reactive trace gases in-situ measurements

Create Instrument Description

View Instrument Description



Presentation by
Roman Romany

OVOCs_PTR_CMN

PTRMS instrument description

Instrument name ? OVOCs_PTR_CMN
Facility name CMN-PV (#42)
PID —
Operator —
Status planned
Date of full operation Jan 1, 2025

Inlet System

Measurement height above ground ? 2 m
Measurement height above building ? 7 m
Distance from NOx inlet ? 0 m
Distance from condensables inlet ? —
Distance from ozone inlet ? 0 m
Distance from GC inlet ? —
Inlet tube material Other
Other tube material composed inlet: 1 m of Pyrex (main inlet for all the instruments) then PFA tube
Residence time ? 6 s
Inlet line heating? ✓
Inlet line heating temperature 20 °C
Filter material None
Oxidant removal None
Sample flow ? —

ACTRIS CiGas InstrumentDB

Search...



Instruments Actions Objects More Help

Instrument Description

• for action type: Instrument Description

Options Filters Search Multiple Objects...

ID	Name	Created Date	User	Last modified Date	User
94	OVOCs_PTR_CMN	Oct 16, 2024	Katrin Seemeyer (#4)	Oct 16, 2024	Katrin Seemeyer (#4)
93	OVOCs_PTR_SIRTA	Oct 14, 2024	Katrin Seemeyer (#4)	Oct 16, 2024	Katrin Seemeyer (#4)
92	OVOCs_PTR_HPBB	Oct 14, 2024	Katrin Seemeyer (#4)	Oct 16, 2024	Katrin Seemeyer (#4)
91	OVOCs_PTR_SMEAR_II	Oct 14, 2024	Katrin Seemeyer (#4)	Oct 15, 2024	Katrin Seemeyer (#4)
90	Condensables_API-TOF_2_SMEAR_II	Oct 7, 2024	Katrin Seemeyer (#4)	Oct 11, 2024	admin (#1)
89	Condensables_API-TOF_1_SMEAR_II	Oct 2, 2024	Katrin Seemeyer (#4)	Oct 11, 2024	admin (#1)
88	NMHCs_GC_offline_xx_NFName	Jul 23, 2024	admin (#1)	Jul 23, 2024	admin (#1)
87	NMHCs_GC_offline_under_construction_2_WAL	Jul 19, 2024	Katrin Seemeyer (#4)	Jul 19, 2024	Katrin Seemeyer (#4)
86	NMHCs_GC_offline_under_construction_1_WAL	Jul 19, 2024	Katrin Seemeyer (#4)	Jul 19, 2024	Katrin Seemeyer (#4)
85	NMHCs_GC_offline_under_construction_SMU	Jul 19, 2024	Katrin Seemeyer (#4)	Jul 19, 2024	Katrin Seemeyer (#4)

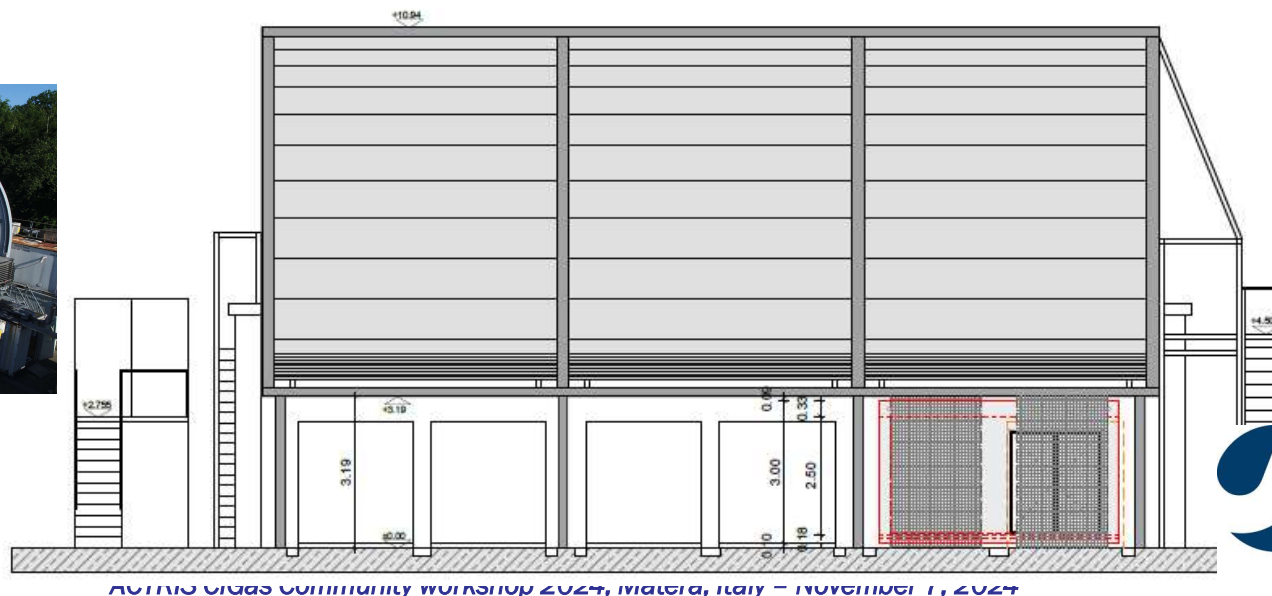
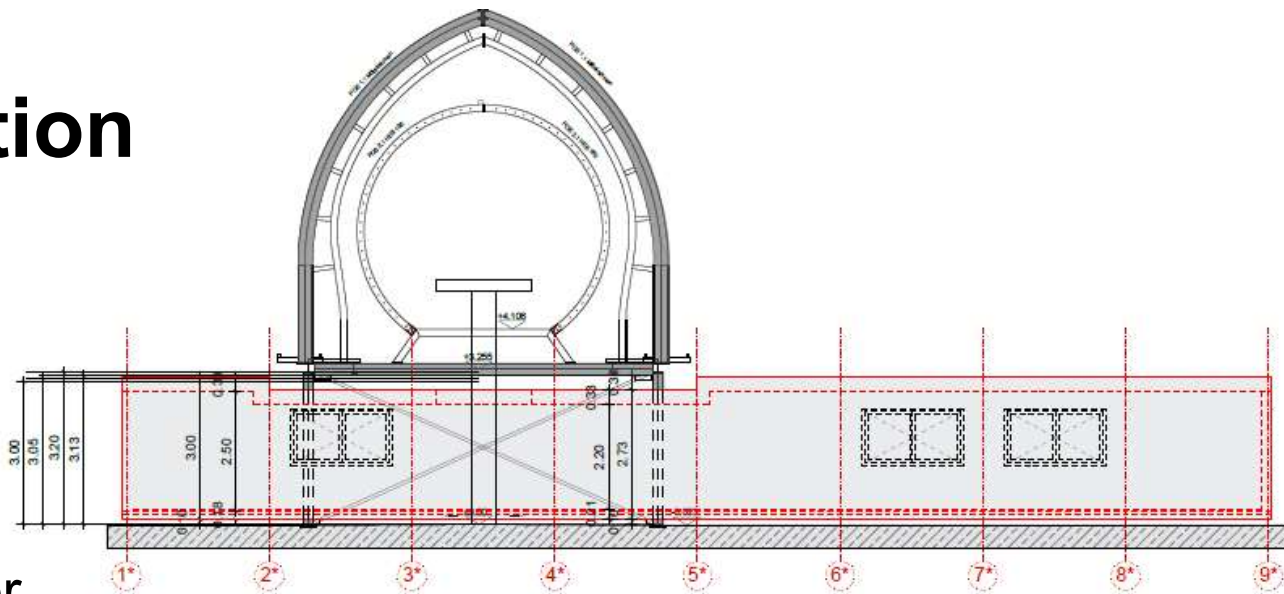
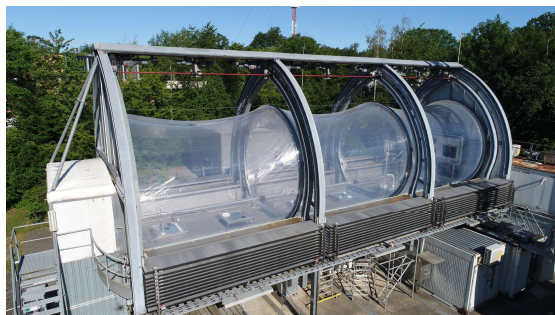
rkshop 2024, Matera, Italy – November 7, 2024



JÜLICH
Forschungszentrum
Shaping Change

Implementation outlook

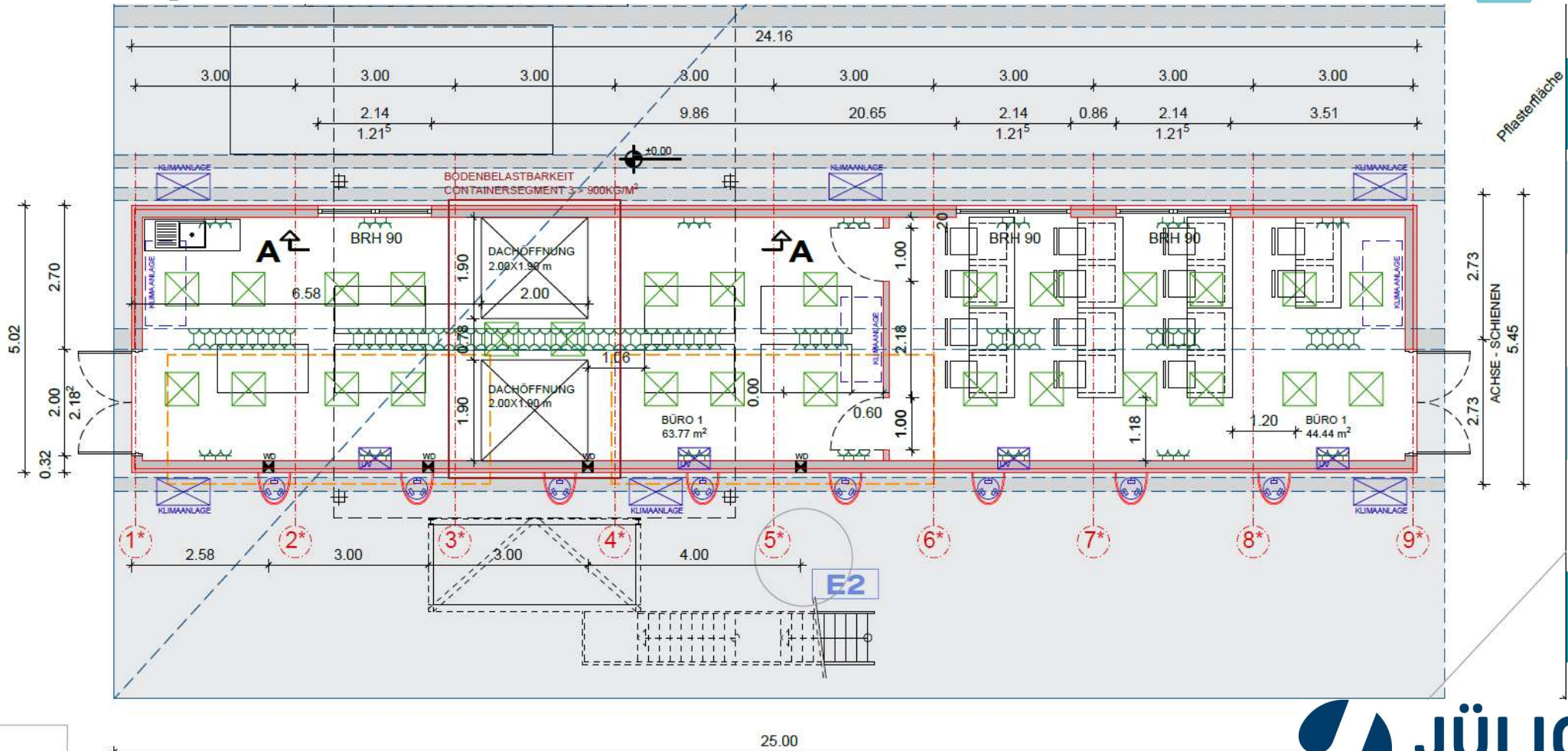
Training & inter-comparison facility at the Atmospheric Simulation Chamber SAPHIR



ACTRIS CiGas community workshop 2024, Matera, Italy - November 1, 2024



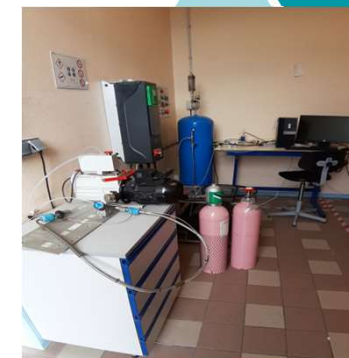
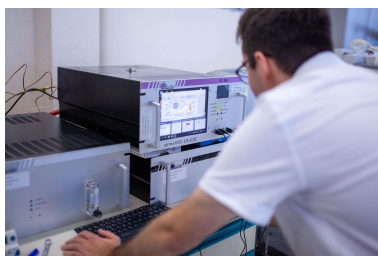
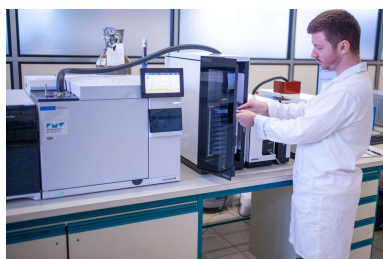
Implementation outlook



CiGas – IMT Nord Europe - Implementation Status 2024 – OVOCs activities, contribution to NMHC and NOx – Instrumentation update



IMT Nord Europe
École Mines-Télécom
IMT-Université de Lille



Available:

- PTR VOCUS 2R (AIM, nitrate inlets)
- PTR-QiToF-MS Ionicon
- PTR-ToF-MS KORE
- Aerodyne TILDAS formaldehyde analyzer
- DNPH samplers/HPLC-UV
- Many TD-GC FID/FID; TD-GC-FID/MS (offline & online) for NMHC, OVOC, Terpenes

- Liquid Calibration Unit; Gas Calibration Unit
- Permeation system
- Target gas cylinder filling system
- Multi-gas generation systems & intercomparison platform

+ Certified laboratory standards (NPL, NIST, upcoming VSL)

CiGas – IMT Nord Europe: PTRMS update



Measurement Guideline for VOC Analysis by PTR-MS

Authors: S. Dusanter, R. Holzinger, F. Klein, T. Salameh, M. Jamar

Reviewers: ...

Summary: This SOP provides information that enables proper operation of PTR-MS in the field and addresses quality assurance parameters needed to produce high-quality data sets that meet the ACTRIS standard.

The SOP contains the following topics:

1. General introduction	1
2. Principle of the PTR-MS technique	3
3. Quality Assurance	7
a. Blank measurements	7
b. Calibration	7
c. Figures of merit	9
4. Field operation	12
a. Sampling	12
b. Frequency of blanks and calibrations	13
c. Operating conditions	13
5. Data extraction: Retrieval of ambient VMR from mass spectra	14
6. References	17
Annex 1: Non-exhaustive list of compounds detected at specific m/Q values	18
Annex 2: NPL gas standard	19
Annex 3: Evaluation of primary ion purity and distribution	21
Annex 4: Examples of humidity-dependent sensitivities	22

VOC by PTR-MS: existing^{1st} draft; New version to be published *end of 2024*

General content:

- ❑ Instrument set-up (sampling lines, instruments)
- ❑ Calibration
- ❑ QA/QC, uncertainties estimation
- ❑ Data management

- PTRMS vocabulary developed with DC
- PTRMS template level0 NRT for CAMS, for Ionicon (Quad) => new versions for ToF and VOCUS under development: https://ebas-submit.nilu.no/templates/VOC/PTR-MS_lev0
- Calibration standard SI-traceable from NPL (Worton et al. 2023), *1 year stability*

To come: organization of a hands-on training on PTRMS

CiGas – IMT Nord Europe: Round-robin participation & ammonia intercomparison organisation

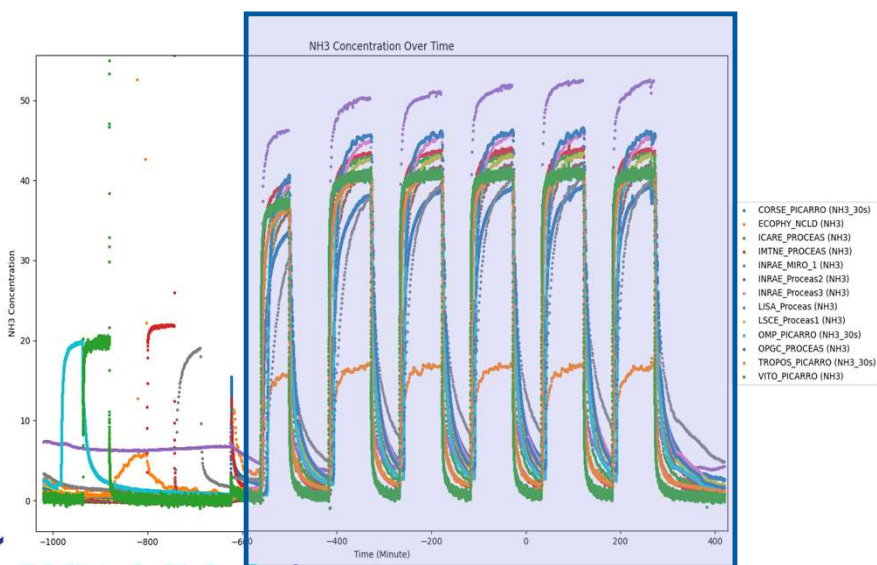


Participation to a Round-Robin 2024 – stability check: evaluation of 3 target gases with 3 GC (NMHC, OVOC, terpenes)

Ammonia intercomparison from 4 to 10 June 2024



- Instrumentation :**
- 2 MIRO (INRAE)
 - 6 PROCEAS (INRAE, LSCE, LISA, OPGC, IMT NE)
 - 4 PICARRO (TROPOS, Qualit'air Corse, OMP, VITO)



Gaz	Gaz de dilution	Paliers nominaux couverts (ppb)
NH ₃ - Portable	Air (sec)	20
NH ₃	Air (sec)	0 - 10 - 20 - 30 - 50
NH ₃	Air (Humide <65%)	0 - 10 - 20 - 30 - 50
NH ₃	Air (sec)	0 (Critère LoD < 100ppt)
NH ₃	Air (sec)	0 – 40 (5 cycles)
Air ambient « dopé » NH ₃	-	Suivant conditions ambiantes + 20

Répétabilité humide

ACTRIS CiGas Community workshop 2024, Matera, Italy – November 7, 2024



CiGas – IMT Nord Europe: Training

- HAAR Training School, - Greece, for PhD students
- ATMO-ACCESS RIURBANS training for public authorities on VOCs
- ATMO ACCESS virtual training : course on trace gases



<https://www.youtube.com/playlist?list=PLt9H9knj6cga9JZVubvvoNwFL-0-Cfifc>



YouTube IT

Rechercher

Se connecter

ATMO ACCESS - RI-URBANS Webinar on ...
de ATMO-ACCESS
Playlist • 4 vidéos • 32 vues

Tout lire

Video Title	Duration	Views	Time
Webinar ATMO-ACCESS & RI-URBANS / VOCs, PM and BC / Part 4: OP service tools	12:14	13 vues	il y a 13 jours
Webinar ATMO-ACCESS & RI-URBANS / VOCs, PM and BC / Part 3: Determination of BC mass concentration	23:56	14 vues	il y a 13 jours
Webinar ATMO-ACCESS & RI-URBANS / VOCs, PM and BC / Part 2: Guidance and monitoring for PM	36:52	11 vues	il y a 13 jours
Webinar ATMO-ACCESS & RI-URBANS / VOCs, PM and BC / Part 1: VOCs: guidance, monitoring, added value	36:29	23 vues	il y a 13 jours

ACTRIS CiGas Community workshop 2024, Matera, Italy – November 7, 2024

CiGas – IMT Nord Europe: Projects update



IMT Nord Europe
École Mines-Télécom

2 Service
Tools
published



Compounds Service
Tool

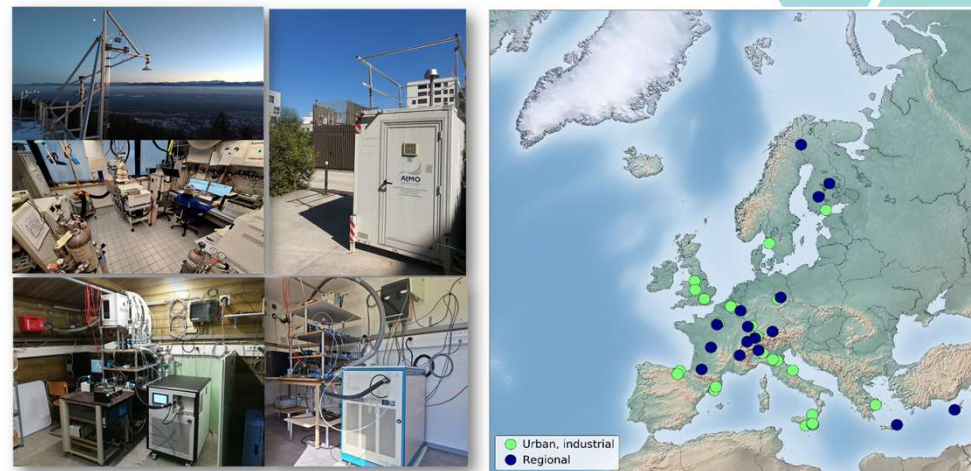
“EUROVOC: EUROpe-wide intensive campaign on Volatile Organic Compounds” co-coordination
2nd pan European intensive measurement period (IMP) on VOCs
organized by the TFMM-EMEP/ACTRIS/RIURBANS

“Member States may use the method which it considers suitable for the objective sought and methods that are being standardised by the European Committee for Standardization (CEN) shall be used once available.”

Table of Contents

1. ABOUT THIS DOCUMENT	1
2. DEFINITION OF VOC	1
COMPLEXITY OF THE POOL OF AMBIENT VOCs	1
3. MEASUREMENT METHODS AND QUALITY CONTROL OF VOC	2
3.1 REFERENCE METHODS	6
3.2 OTHER EXISTING RELEVANT GUIDANCE	7
3.2.1 NMHC online measurements	8
3.2.1.1 Sampling	8
3.2.1.2 Analysis	8
3.2.1.3 Reference materials	8
3.2.2 VOC online measurements using PTR-MS	8
3.2.2.1 Sampling	11
3.2.2.2 Analysis	11
3.2.3 NMHC offline measurements	11
3.2.3.1 Sampling	11
3.2.4 OVOC offline measurements	11
3.2.4.1 Sampling	11
3.2.5 Instrument performance evaluation	11
4. PAN-EUROPEAN OVERVIEW	11
5. RECOMMENDATIONS	15
6. REFERENCES	18

- No European reference methods available for VOCs (ongoing work: 6 TS) within CEN/TC 264 WG13;
- 5 existing norms only for benzene measurement CEN/TC 264 WG12
- Guidelines ACTRIS, EMEP, GAW



45 urban and rural sites across Europe (ACTRIS NF, EMEP, GAW, Local Air Quality Monitoring Networks, ACTRIS/ICOS sites)

Period: 1 month - September 2024

Collaboration with instrument manufacturers

+ VOC Source apportionment Service Tool

orkshop 20.

Data QA/QC, modeling, PhD at IMT starting October 2025

1781 start of weather (systematic) observations at the Meteorological Observatory Hohenpeissenberg (MOHp)

Since 1952 Observatory of the German Meteorological Service (Deutscher Wetterdienst)

Since 1994 WMO GAW site

ACTRIS (2011): **NF and TC** unit

65km SW of Munich, Southern Germany

47°48' N
11°01' O
985 m NN



CiGas-DWD Implementation Status

Anja Claude (VOC-PI), Robert Holla (NOx-PI), Annika Kuss (ACTRIS-D scientist), Florian Hochenauer, Max Prostedter, Marita Hofmann, Katja Michl, Erasmus Tensing, Elisabeth Eckert (ACTRIS-D), Dagmar Kubistin

ACTRIS Week Matera, Italy, November 5-7th, 2024



This project receives funding from the European Union's Horizon 2020 research and innovation programme under grant agreements No 654109 and 739530

Tasks of CiGas-DWD in-situ

DWD-CiGas is supporting the following activities *in the field of NMHCs, bVOC and NOx*

- measurement guidelines development and updates (Activity 4)
- working standard and target gas calibration (Activity 5)
- the support and organisation of intercomparisons (Activity 5)
- Links with associated communities (Activity 2)

And provides expertise and feedback in

- the data QA/QC process and preparation of data workshops
- Consultancy (Activity 3)
- labelling process (Activity 6)
- training sessions (Activity 3): GAW-TEC courses
- Tests of new instrumentation and calibration methods with respect to long-term monitoring (Activity 7)



Implementation at CiGas-DWD

Tests of **target gases**

- ...fresh-filled cylinders (VOCs) : new Luxfer, „old“ NPL cylinders spiked with high-concentrated NMHCs (NPL mixture) and diluted with N₂ or AIR
- ...comercial cylinders (NO_x): 50ppb cylinders (tolerance ~ 5%)



Guidelines for the use of target gases

Improving the guest manifold (for small scale *intercomparisons*) with housekeeping sensors

Assessment of **NO_x calibration gases and methods** / transfer standards:
+ determination of NO_y contamination of NO/NO₂ target and calibration gases
+ implementing a permeation system for the NO_x and NO_y calibration

+ hosted **test** labelling audit



Assessment of NO_x calibration gases and methods / transfer standards

+ implementing a permeation system for the NO_x and NO_y calibration

+ determination of NO_y contamination of NO/NO₂ target and calibration gases

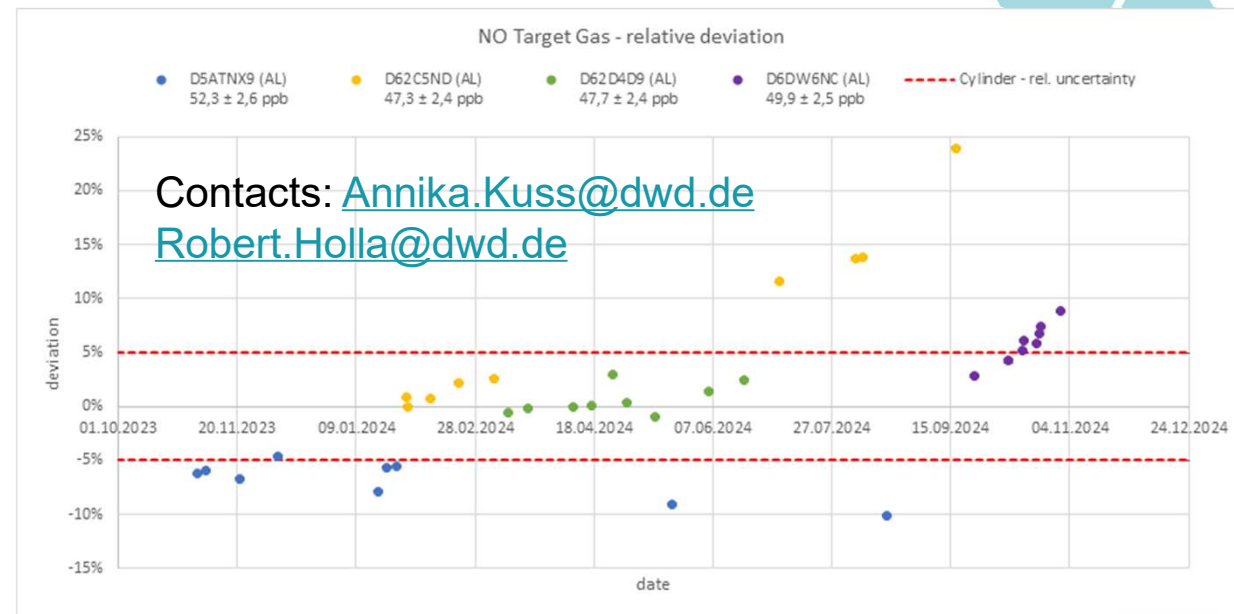
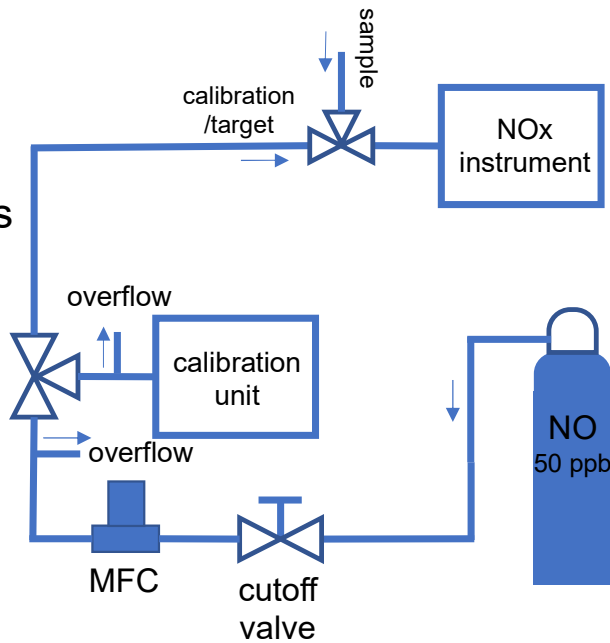
Contacts: Annika.Kuss@dwd.de
Robert.Holla@dwd.de



Implementation at CiGas-DWD – NOx target gases

Commercially available NO ~50ppb cylinders (tolerance ~ 5%) have been acquired and are currently running in our lab

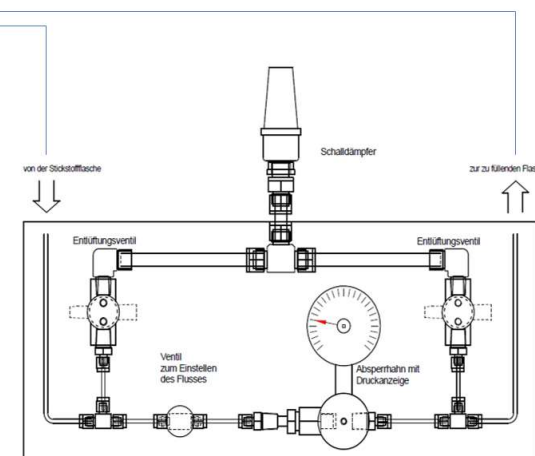
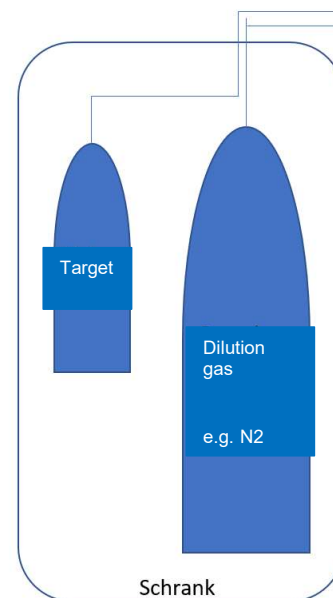
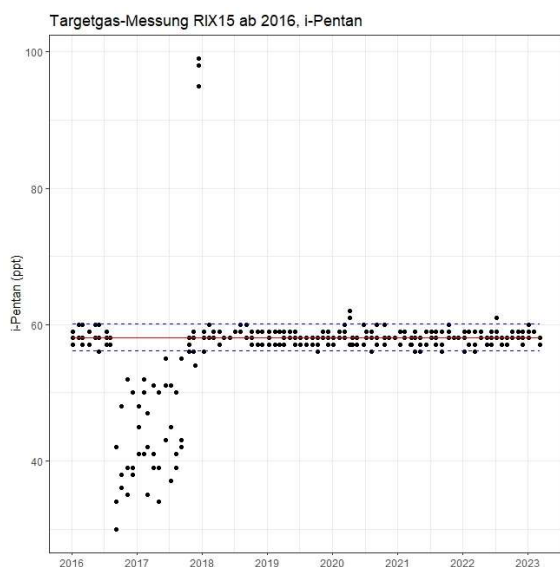
flow chart for target gas measurements



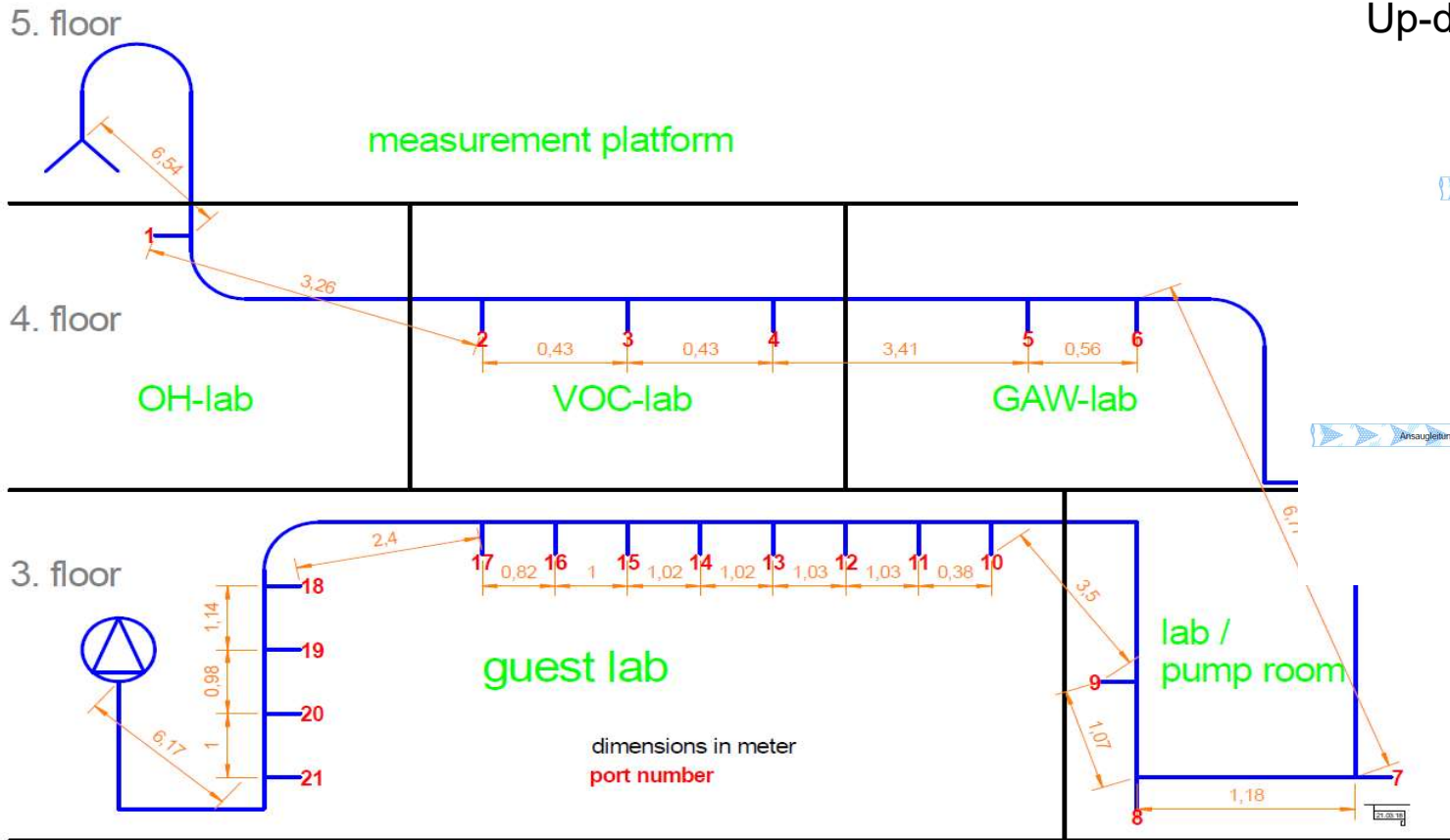
issues: high consumption, equilibration period long, accuracy of commercial cylinders,.... testing continues!

Test of cylinders spiked with high-concentrated NMHCs (NPL mixture) and diluted with N₂ or AIR

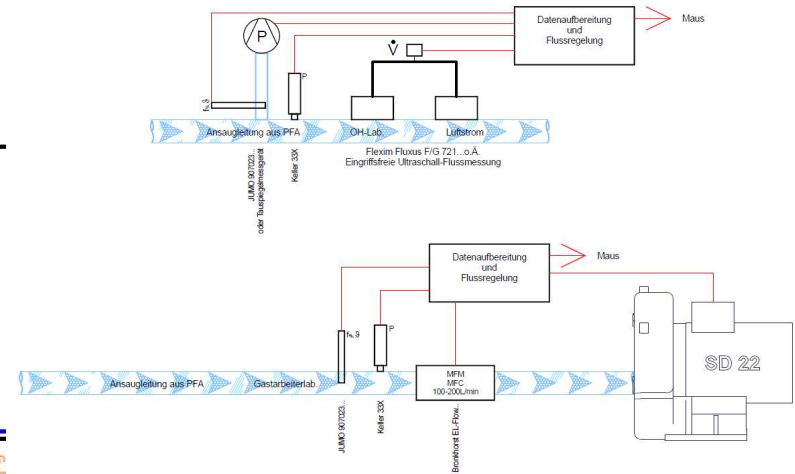
→ long-term stability, initial losses



Interested in a working standard or target gas **for NMHCs?**
Contact us via SAMU or Email: anja.claude@dwd.de



Up-date of housekeeping sensors

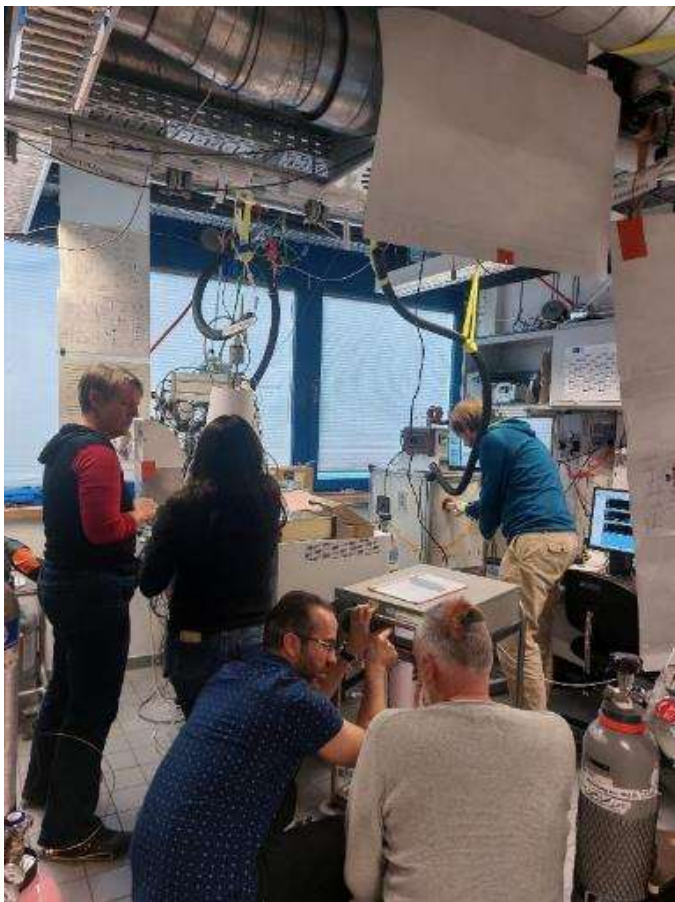


29.06.18

PFA 1/4" manifold



Implementation Status at CiGas-DWD –
Hosting the CiGas test audit in November 2023



Deutscher Wetterdienst
Wetter und Klima aus einer Hand



Thank you !
<http://www.dwd.de/mohp>

Contact:

robert.holla@dwd.de (NO_x) TC unit deputy
anja.claude@dwd.de (VOCs) TC unit head



FONA
Forschung für Nachhaltigkeit



ACTRIS Week Matera, Italy, November 5-7th, 2024



This project receives funding from the European Union's Horizon 2020 research and innovation programme under grant agreements No 654109 and 739530

The logo for ACTRIS features the word "ACTRIS" in a white, sans-serif font. The letter 'C' is replaced by a white circle. A white vertical line extends upwards from the top of the 'C' circle, and a white arc curves over the top of the text. To the right of the vertical line, there are three white circles of increasing size, arranged in a diagonal pattern.

ACTRIS

CiGas-UHEL – condensable vapours &
direct aerosol precursors

Activity / implementation update 2024

Silja Häme, Nina Sarnela, University of Helsinki, Finland

CiGas-UHEL, University of Helsinki, Finland

Condensing vapours and direct aerosol precursors such as sulfuric acid and Highly Oxygenated Molecules (HOM; e.g. $C_{10}H_{14}O_9$)

Centre for Reactive Trace Gases in Situ Measurements (CiGas)						
	CiGas-FZJV	CiGas-FZJN	CiGas-IMT	CiGas-UHEL	CiGas-DWD	CiGas-EMPA
Management & coordination	TC lead	Unit lead	Unit lead	Unit lead	Unit lead	Unit lead
Link with associated communities	Expert groups and networks					
Training & consultancy						
Measurement & data procedures & tools	NMHCs OVOCs	NO _x	OVOCs	Condensable	NMHCs NO _x	NMHCs OVOCs
Measurement & data quality monitoring						
NF labelling & evaluation	Evaluation and audits					
New scientific & technological developments	Methodology, technical and scientific developments for reactive trace gases in-situ variables and measurement techniques					

Target compounds: condensable vapours
 Instruments: *chemical ionization mass spectrometers (CIMS)*
 Status: Implementation ongoing / full operation of the unit is expected in 2026

Reactive Trace Gases In Situ National Facility Technical requirements

- Measurements of condensable vapours are not required to fulfill the ACTRIS reactive trace gases in-situ minimum requirements.
- *BUT for the optimum reactive trace gases in-situ setup:*
 - Measurements of direct aerosol precursors should be performed (e.g., by online techniques, such as CI-API-TOF MS, *chemical ionization atmospheric pressure interface time-of-flight mass spectrometer*) when the station also performs aerosol and gas-to-particle conversion studies.

Measurement guidelines supporting quantitative measurements of aerosol precursor vapours are under development!

CiGas-UHEL Personnel



*Unit Head, Staff Scientist,
Dr. Silja Häme
(silja.hame@helsinki.fi)*



*High-resolution mass spectrometry expert,
Staff Scientist
Dr. Nina Sarnela
(nina.sarnela@helsinki.fi)*



*Deputy Unit Head, Professor
Dr. Tuukka Petäjä
(tuukka.petäjä@helsinki.fi)*

Our Unit's e-mail: actris-api@helsinki.fi



CiGas-UHEL – Main activities



- ❖ **Activity 1. Management and coordination:** contribution to the management of CiGas
- ❖ **Activity 2. Links with associated communities:** close collaboration with e.g., instrument manufacturers and Finnish Centre of Excellence VILMA (Virtual laboratory for molecular level atmospheric transformations) collaboration towards more quantitative data on condensable vapors
- ❖ **Activity 3. Training and consultancy:** consultation for condensable vapor measurements; training activities as part of CiGas-UHEL intercomparison workshops, ACTRIS courses etc.
- ❖ **Activity 4. Measurement and data procedures and tools:** provision of measurement guidelines (expected to be ready 2025/2026); data format and submission related work in collaboration with ACTRIS DC
- ❖ **Activity 5. Measurement and data quality monitoring:** s-b-s intercomparison workshops for chemical ionization mass spectrometers; individual instrument calibrations for nitrate-CIMS (at the moment: sulfuric acid calibrations, in the future also calibrations for certain HOMs); data review (starting in 2026/2027)
- ❖ **Activity 6. NF labelling and evaluation:** reviewing the labelling applications for condensables, official audits can be made when the CIMS measurement guidelines exist.



- ❖ **Activity 7. New scientific and technological developments:** improving sulfuric acid calibration method and practices; development of transmission calibration improving the quantification of other condensables such

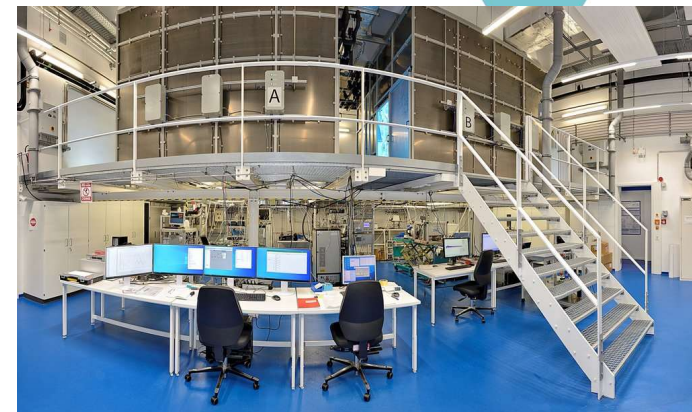
CiGas-UHEL intercomparison workshops

TROPOS Atmospheric Chemistry
Department – Chamber (ACD-C)

1st Intercomparison workshop for chemical ionization mass spectrometers to measure condensable vapors (chamber)

- **Timing:** February 27th – March 10th, 2023
- **Place:** TROPOS, Leipzig, Germany
- 10 instruments joined

University of Helsinki (CiGas-UHEL) in collaboration with OrGanic Tracers and Aerosol Constituents - Calibration Centre (OGTAC-CC, CAIS-ECAC)



2nd Intercomparison workshop for chemical ionization mass spectrometers to measure condensable vapors (field)

- **Timing:** July 29th – August 11th, 2024
- **Place:** SMEAR II station, Hyytiälä, Finland
- 6 instruments joined

3rd Intercomparison workshop for chemical ionization mass spectrometers to measure condensable vapors in 2026 (tbd)

More in Nina Sarnela's talk today!



SMEAR II, s-b-s intercomparison measurement area

Upcoming 2nd Karsa & ACTRIS CiGas-UHEL workshop

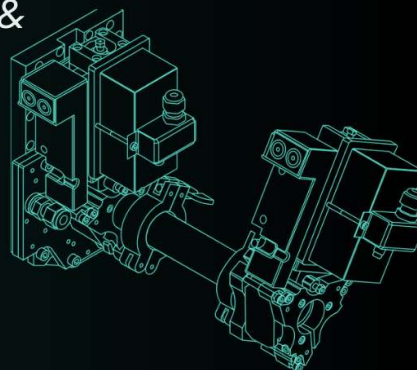
Workshop vol. 2

MION & ORBITRAP™ IN ATMOSPHERIC SCIENCES

Opportunities to discover existing applications & discuss best practices with current users!

29 November 2024

Helsinki & online



Registration link will be sent to ACTRIS community

MION (Multi-scheme chemical IONization inlet)

Orbitrap (new high-res mass spectrometer to measure condensable vapours & VOCs)



CiGas-FZJN

Robert Wegener, Max Gerrit Adam

ACTRIS Week 2024, Nov. 7th 2024

FZJN Implementation status

Challenges

NO

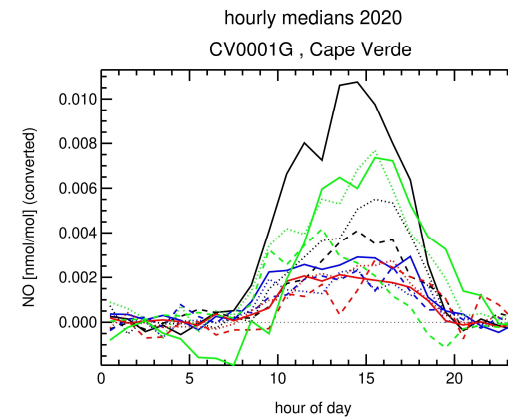
- Traceable gas standard available from CCL
- NO level extremely low at some ACTRIS sites
- Sensitive CL reference instrument

NO₂

- No traceable gas standard available
- Spectroscopic mobile NO₂ instrument as transfer reference instrument

Interferences

- Must be characterized on site
- Ozone and humidity measurement needed



FZJN Implementation status

Personnel recruitment complete

Purchase

NO

Sensitive CL reference instrument

- **To be delivered Dec. 2024**

NO₂

Spectroscopic mobile NO₂ instrument
as transfer reference instrument

- **Delivered**

Interferences

Ozone and humidity measurement needed

- **Delivered**

Measurements and laboratory

- Calibration Lab for NO set up
- Calibration Lab for NO₂ set up
- Mobile NO/NO₂ instrument set up

- **NO measurements operational**
- **NO₂ measurements and mobile measurement unit operational**



Activities

- **Analysis of ozone precursor data within TOAR**
- **Developing procedures for RRT data submission for NO_x Data**
- **Further analysis and eventual publication of intercomparison campaign JUNOx23**
 - **advancing measurement guidelines**

TOAR
tropospheric
ozone
assessment
report
Phase II



Activities

- **First On-Site-Audit at Hohenpeissenberg**
 - Next audit at Jungfrauoch (~3500m asl), Switzerland
- **Training and consultancy**
 - Two community workshops in 2024
 - topic suggestions/questions welcome for 2025

