Forschungszentrum Jülich
in der Helmholtz-Gemeinschaft

EUROCHAMP
Networking Activity N1:
Raw Data Analysis, Data Inter-Comparison, and Quality Assurance

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N1 *outline*

- Quality assurance of data (**N1**)
  - Co-ordinated experiments:
  - Chamber characterisation
  - Simulation of standard scenarios at different chambers
  - Instrument intercomparison

- Exchange of experimental and model data (**N1, N2**)
  - Raw data format
  - Quality assurance of raw data

Schedule for activity N1

May 2009

8.N1.3 Outline implementation plan for the full duration of the activity N1 (including milestones [M] and deliverables [D])

PROJECT MILESTONES AND DELIVERABLES		*Year 1*				*Year 2*				*Year 3*				*Year 4*				*Year 5*			
		I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV
N1	*RAW DATA ANALYSIS, DATA INTER-COMPARISON AND QUALITY ASSURANCE*																				
	Definition of rules for quality-assured raw data analysis, report (D)																				
	Standard experiment in different chambers for data inter-comparison (D)																				
	Inter-comparison study of selected analytical devices, report (D)																				

Means of quality assurance in chamber research

- **Chamber characterisation (transfer of experiments)**
  - **Definition:**
    parameterization of chamber properties based on observations
  - SAPHIR: HONO source parameterization, applied to EUPHORE, PSI
- **Standard experiments (quality of chamber)**
  - **Definition:**
    repeated experiment under well defined conditions
  - long series in SAPHIR, EUPHORE, PSI, AIDA
- **Instrument intercomparison (quality of instrumentation)**
  - **Definition:**
    typical chamber experiment with different instruments measuring the same quantity
  - performed at SAPHIR, EUPHORE, PSI, AIDA, JRC, …
  - on: H2O, O3, HONO, OVOC, OH, HO2, HCHO, aerosol, NO3, N2O5

Rules for quality-assured raw data analysis

- **Well documented datasets:**
  - traceable (from measured quantity to *public* raw data)
  - accuracy (calibration)
  - precision (random noise, short term fluctutions..)

  → **basis for QA**
- **Chamber intercomparison**
  - purity of air supply
  - residence time of trace gases / aerosols (vs. tracers)
  - off gasing (HONO, HCHO, VOCs, …)
  - aerosol formation

  → **enables chamber selection for dedicated experiments**
- **Instrument intercomparison**
  - key measurements (radicals, VOCs, NOx, ...)
  - transfer standards / exchange of instruments
  - well documented and appropriate use of statistics

  → **helps chamber and field research**

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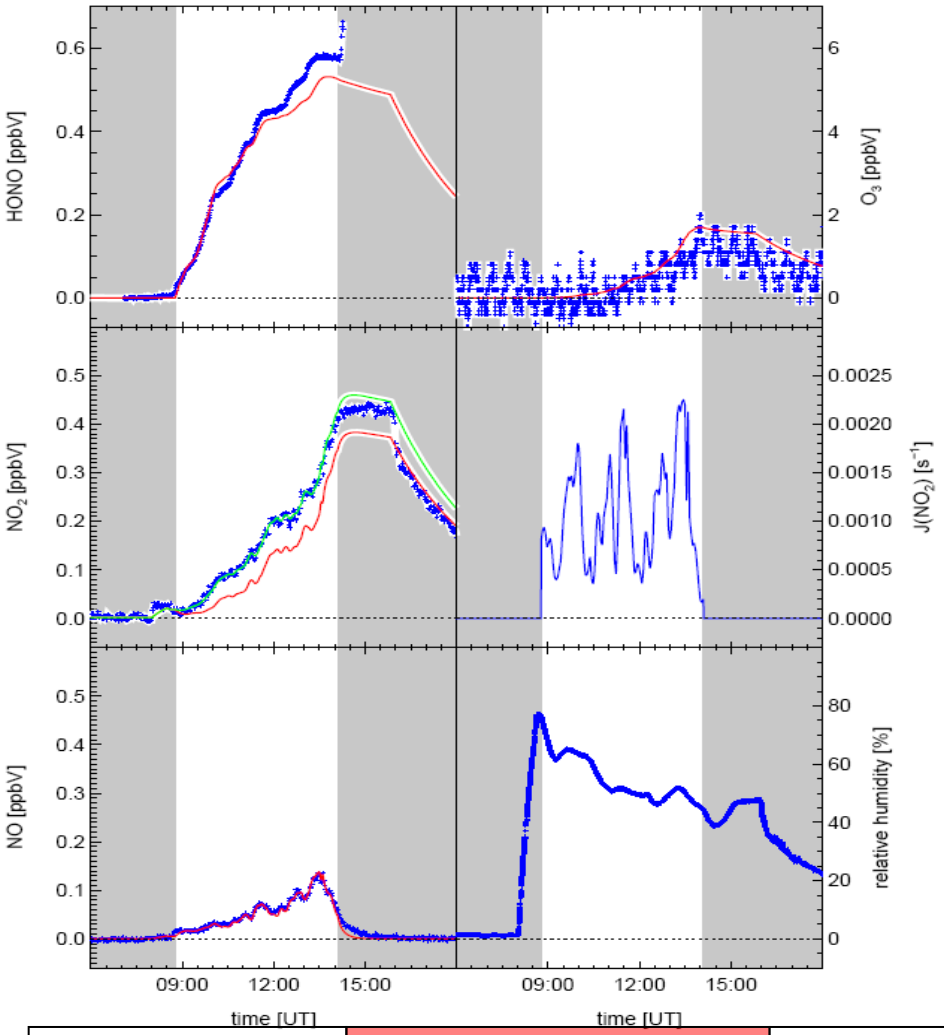
Table of Chambers within EUROCHAMP

- available on the web: http://saphir.fz-juelich.de/eurochamp/

Institution	*Number*		1	1	1	1	2	2	
Institution	*Abreviation*		**BUW**	**BUW**	**BUW**	**BUW**	**JRC**	**JRC**	
Institution	*Name*		Bergische Universität Wuppertal	Bergische Universität Wuppertal	Bergische Universität Wuppertal	Bergische Universität Wuppertal	European Commission DG Joint Research Centre	European Commission DG Joint Research Centre	E
Institution	*Department*		Institut für Physikalische Chemie	Institut für Physikalische Chemie	Institut für Physikalische Chemie	Institut für Physikalische Chemie	Institute for Environment and Sustainability	Institute for Environment and Sustainability	
Institution	*Address*		Gaußstraße 20, D-42119 Wuppertal	Gaußstraße 20, D-42119 Wuppertal	Gaußstraße 20, D-42119 Wuppertal	Gaußstraße 20, D-42119 Wuppertal	Via E. Fermi 1, I-21020 Ispra (VA)	Via E. Fermi 1, I-21020 Ispra (VA)	V
Institution	*Phone*		+49-202-439-2515 / -3832	+49-202-439-2515 / -3832	+49-202-439-2515 / -3832	+49-202-439-2515 / -3832	+39-332-789076	+39-332-789076	
Institution	*Fax*		+49-202-439-2757	+49-202-439-2757	+49-202-439-2757	+49-202-439-2757	+39-332-785837	+39-332-785837	
Institution	*WWW*		http://www.physchem.uni-wuppertal.de/	http://www.physchem.uni-wuppertal.de/	http://www.physchem.uni-wuppertal.de/	http://www.physchem.uni-wuppertal.de/	http://www.jrc.cec.eu.int/	http://www.jrc.cec.eu.int/	h
PI	*Name*		Barnes	Barnes	Barnes	Barnes	Hjorth	Hjorth	Hj
PI	*First Name*		Ian	Ian	Ian	Ian	Jens	Jens	Je
PI	*email*		barnes@uni-wuppertal.de	barnes@uni-wuppertal.de	barnes@uni-wuppertal.de	barnes@uni-wuppertal.de	jens.hjorth@jrc.it	jens.hjorth@jrc.it	jen
Chamber	*Short Name*		**6M**	**3M**	**405**	**90**	**2000L**	**3000L**	
Chamber	*Long Name*		glass/quartz cylinder 2	glass/quartz cylinder 1	glass/quartz cylinder 3	glass/quartz cylinder 4	2000l Aerosol Reaction Chamber	Large Teflon Bag	
Chamber	*Type*		Indoor Photoreactor	Indoor Photoreactor	Indoor Photoreactor	Indoor Photoreactor	Indoor Chamber	Outdoor Photoreactor	
Chamber	**Shape**		**Cylinder**	**Cylinder**	**Cylinder with inner Cylinder**	**Cylinder with inner Cylinder**	**Cube**	**Bag**	
Chamber	**Volume**	m^3	**1.086**	**0.48**	**0.412**	**0.350**	**2**	**3 (variable)**	
Chamber	Surface	m^2	**9.41**	**4.56**	**3.85**	**4.45**	**9**	**variable**	
Chamber	Surface Volume Ratio	m^{-1}	**8.66**	**9.50**	**9.34**	**12.71**	**4.69**	**variable**	
Chamber	Length	m	6	3	1.5	1.5	1.25		
Chamber	Diameter	m	0.48	0.45	0.6	0.6			
Chamber	Length inner cylinder				1.5	1.5			
Chamber	Diameter inner cylinder				0.1	0.24			
Chamber	**Material**		**Quartz, Al end flanges**	**Duran Glass, Al end flanges**	**Duran Glass, Al end flanges**	**Duran / Quartz Glass, Al end flanges**	**FEP**	**FEP**	
Chamber	**Light Source**		**Lamps**	**Lamps**	**Lamps**	**Lamps**	**Lamps**	**Sunlight**	
Chamber	**Spectral Range Min**	**nm**	**254**	**320**	**254**	**254**	**300**		
Chamber	**Spectral Range Max**	**nm**	**480**	**480**	**480**	**480**	**600**		
Chamber	Lamps 1		**32 x 36W Philips TL/05 (Blacklights)**	**20 x 36W Philips TL/05 (Blacklights)**	**18 x 36W Philips TL/05 (Blacklights)**	**5 x 36W Philips TL/05 (Blacklights)**	**8 x Osram Ultra-Vitalux 300W**		**18**

SAPHIR experiment: HONO source identification

Rohrer et al., Atmos. Chem. Phys. 2005



- This experiment
  - Conditions:
    $J(O^1D) \approx 1\%$, $J(NO_2) \approx 30\%$ of outside values
    CO = 500 ppm
- 25 different experiments
  - HONO source

    $S(HONO) = a \times J(NO_2)$

    $\times (1 + (RH/11.8\%)^2)$

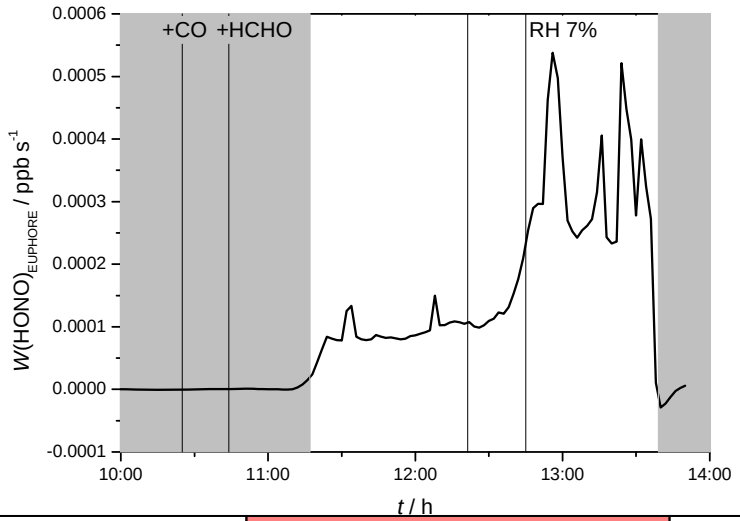
    $\times \exp(-3950K / T)$

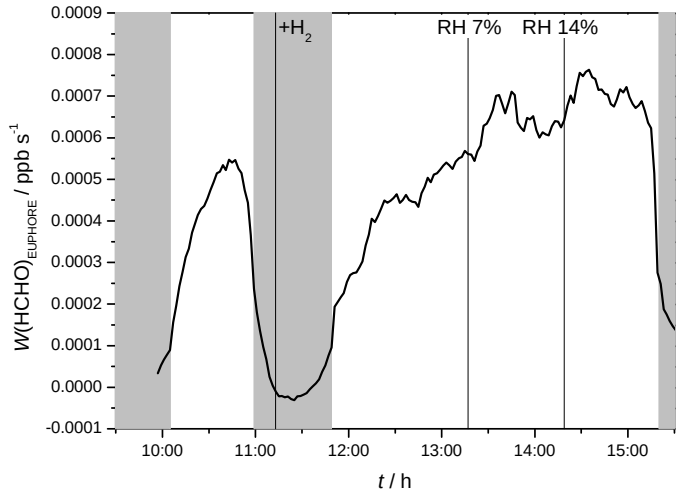
Chamber radical sources in EUPHORE

Zádor et al., J. Atmos. Chem., 2005

- Collaboration of CEAM and LEEDS
- 3 zero NOx experiments, coupled with rate of production analysis and local and global uncertainty analysis
- Production of HCHO and HONO related to wall processes. Rates:

$$W(HONO) = j_{NO2} \times (a + b \times RH^{1/2})$$
$$W(HCHO) = j_{NO2} \times c$$





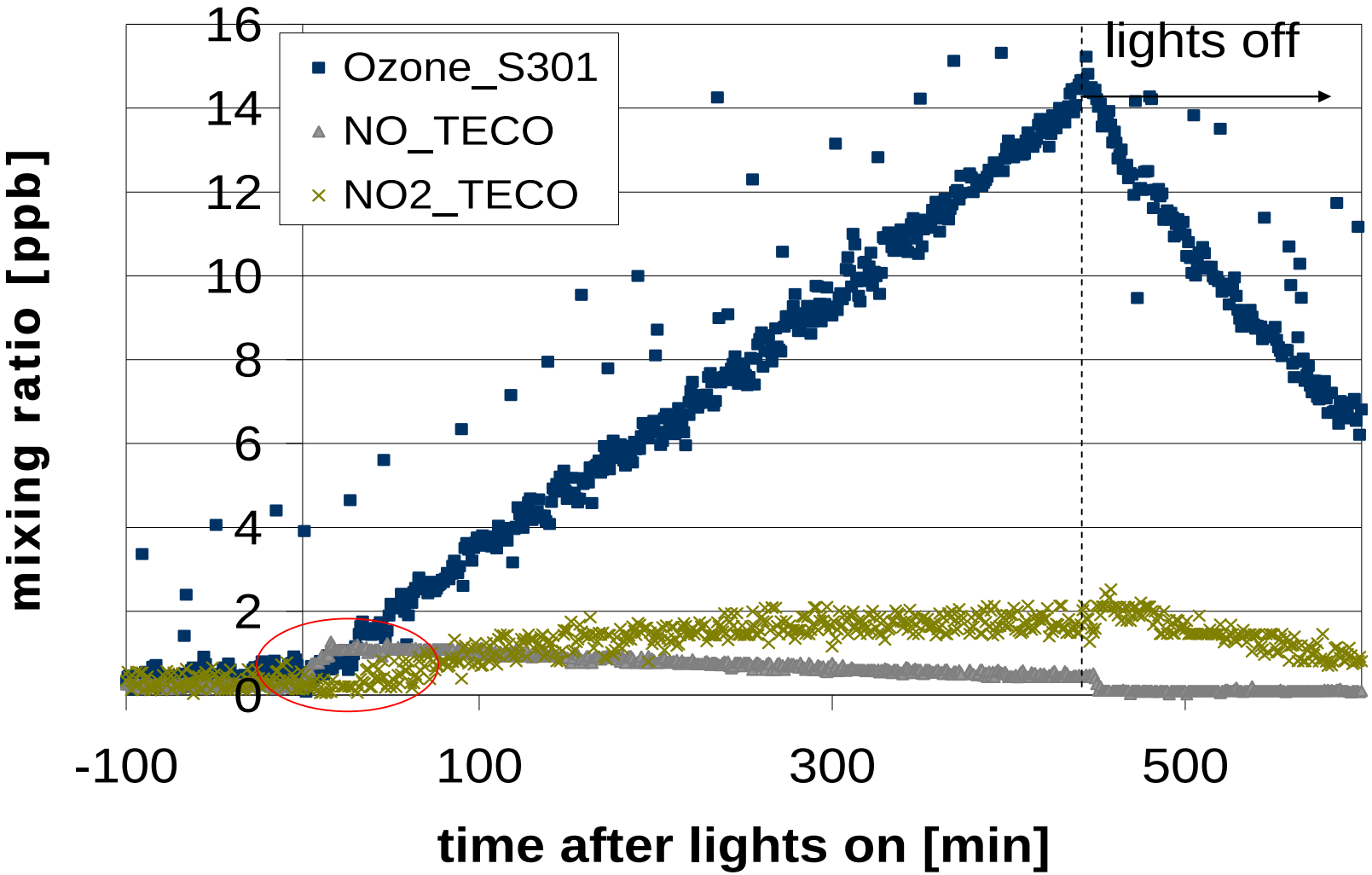
Intercomparison of chamber experiments

- Development of scenarios → intercomparison of chamber results → standard scenarios
- Definition of the required parameters:
  - physical data (temperature, pressure, humidity, ..)
  - chamber parameter (gas fluxes, ...)
  - measurement errors: precision and accuracy
- Standard scenarios allow to keep track of the conditions of an existing chamber (intercomparison of today's chamber with the same chamber N years ago)
- There is no standard scenario for all chambers but there might be experiments which can be carried out in 2 or 3 chamber under *the same* (similar) conditions.

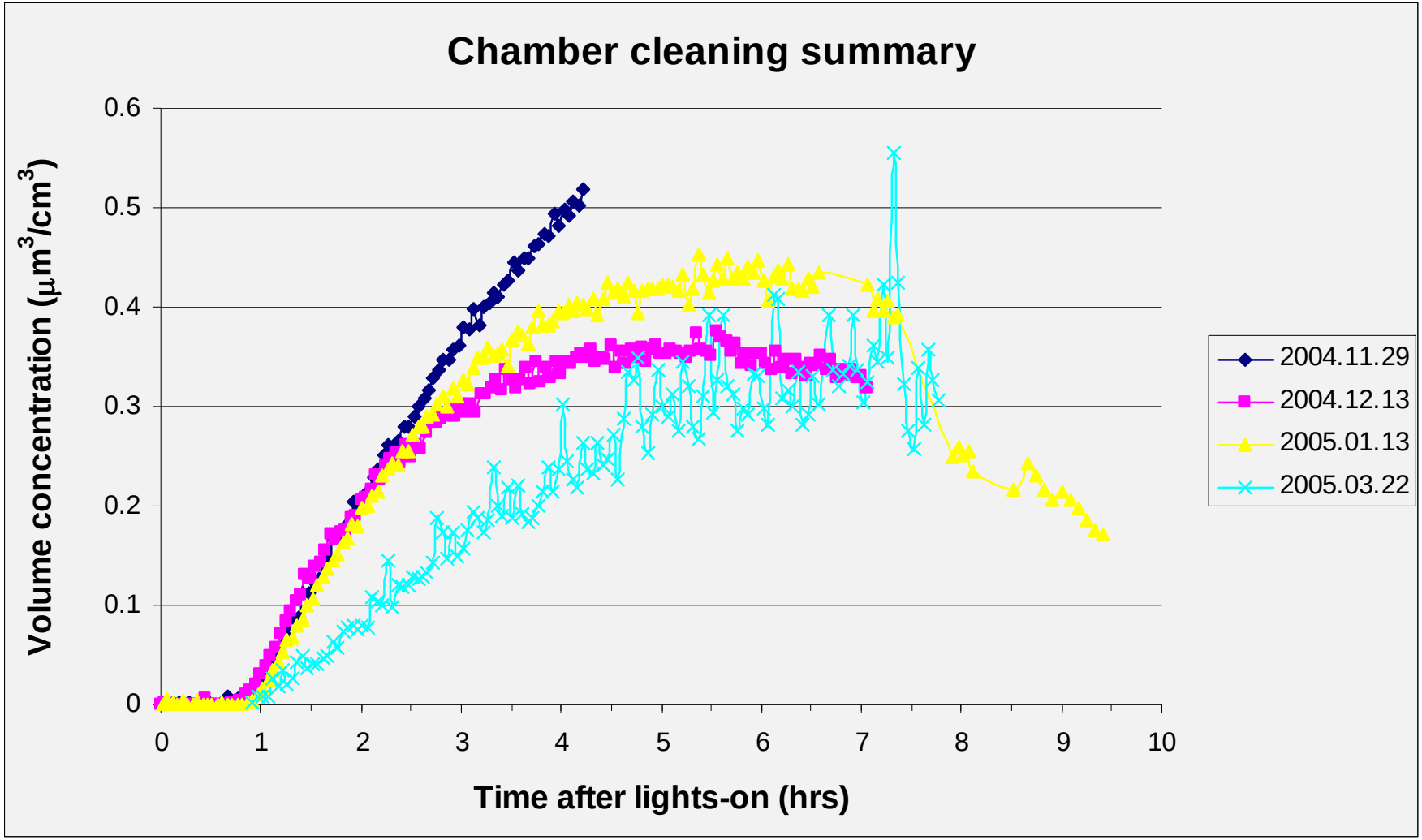
QA through standard or reference experiments

- ***"empty chamber" (+ light)***
  - HONO / NO formation
    FZJ, CEAM, PSI
  - HCHO formation
    FZJ, CEAM
  - particle formation
    PSI , FZK
- ***"well defined mixtures"***
  - ozone vs. tracer lifetime
  - NOx budget
  - ozonolysis of ethene as source of formaldehyde
  - tri-methyl-benzene + NOx + light
  - aerosol lifetime …

Ozone and NOx formation in the PSI chamber

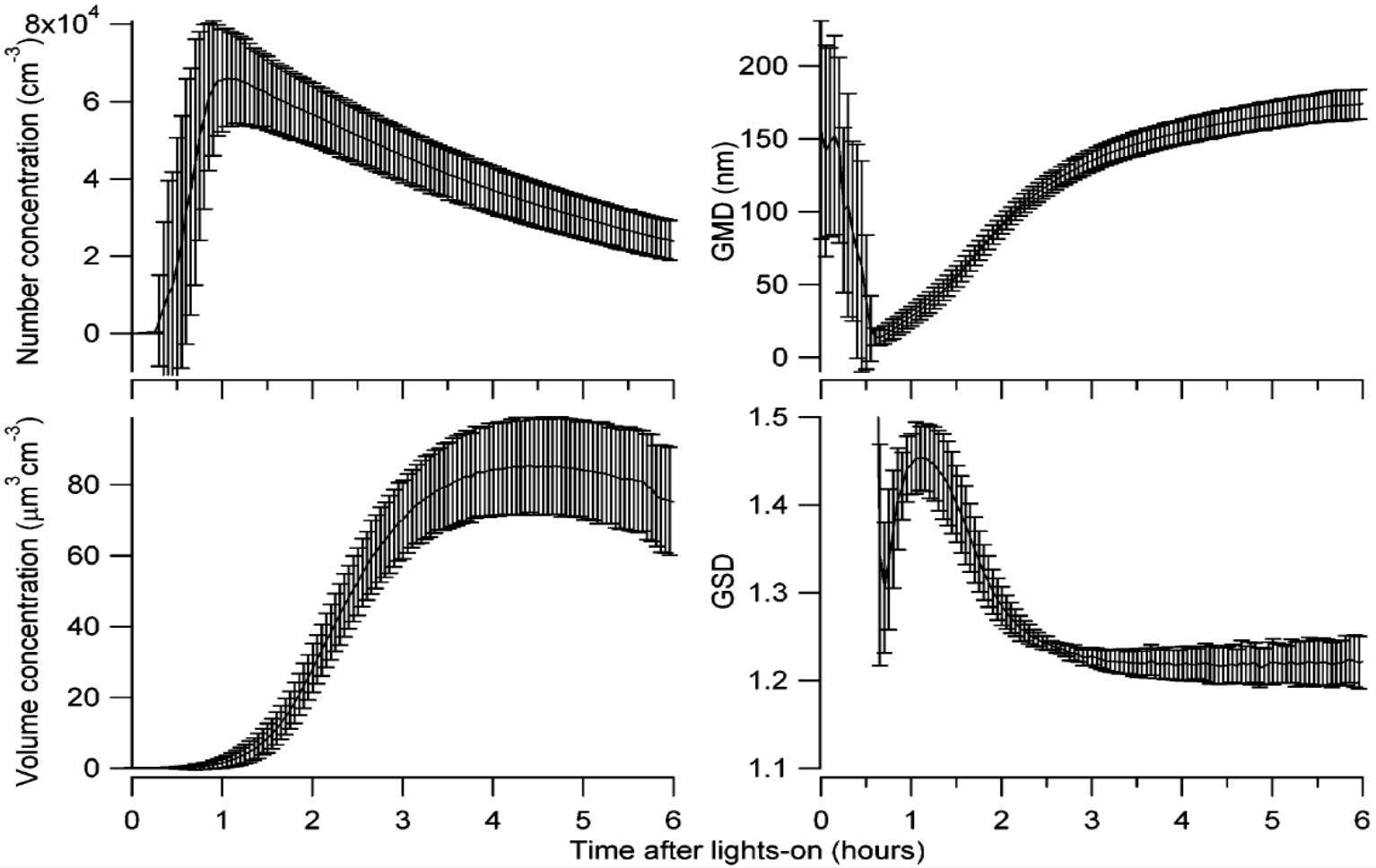


Aerosol formation in the flushed PSI chamber

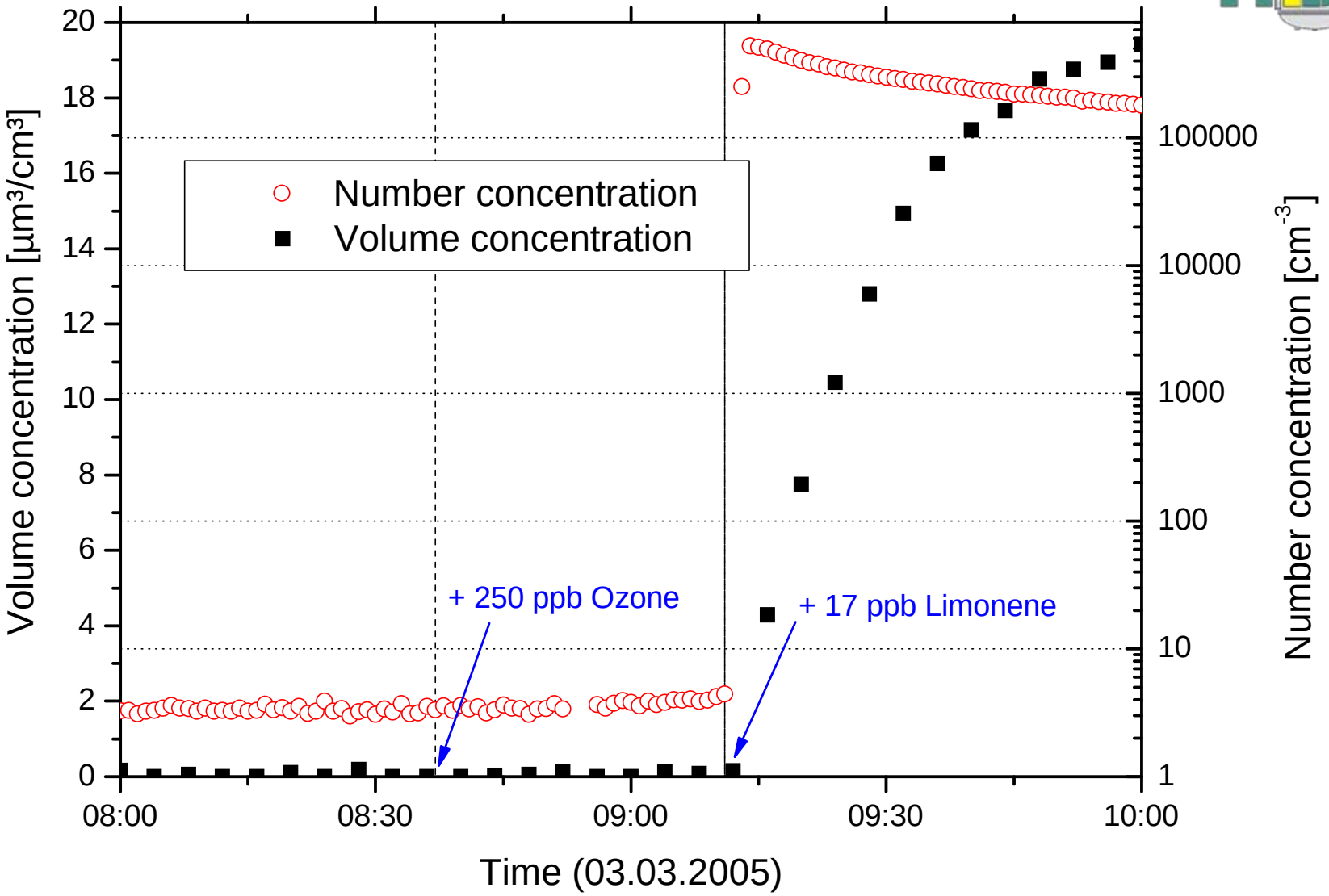


PSI chamber 14 standard experiments on aerosol formation

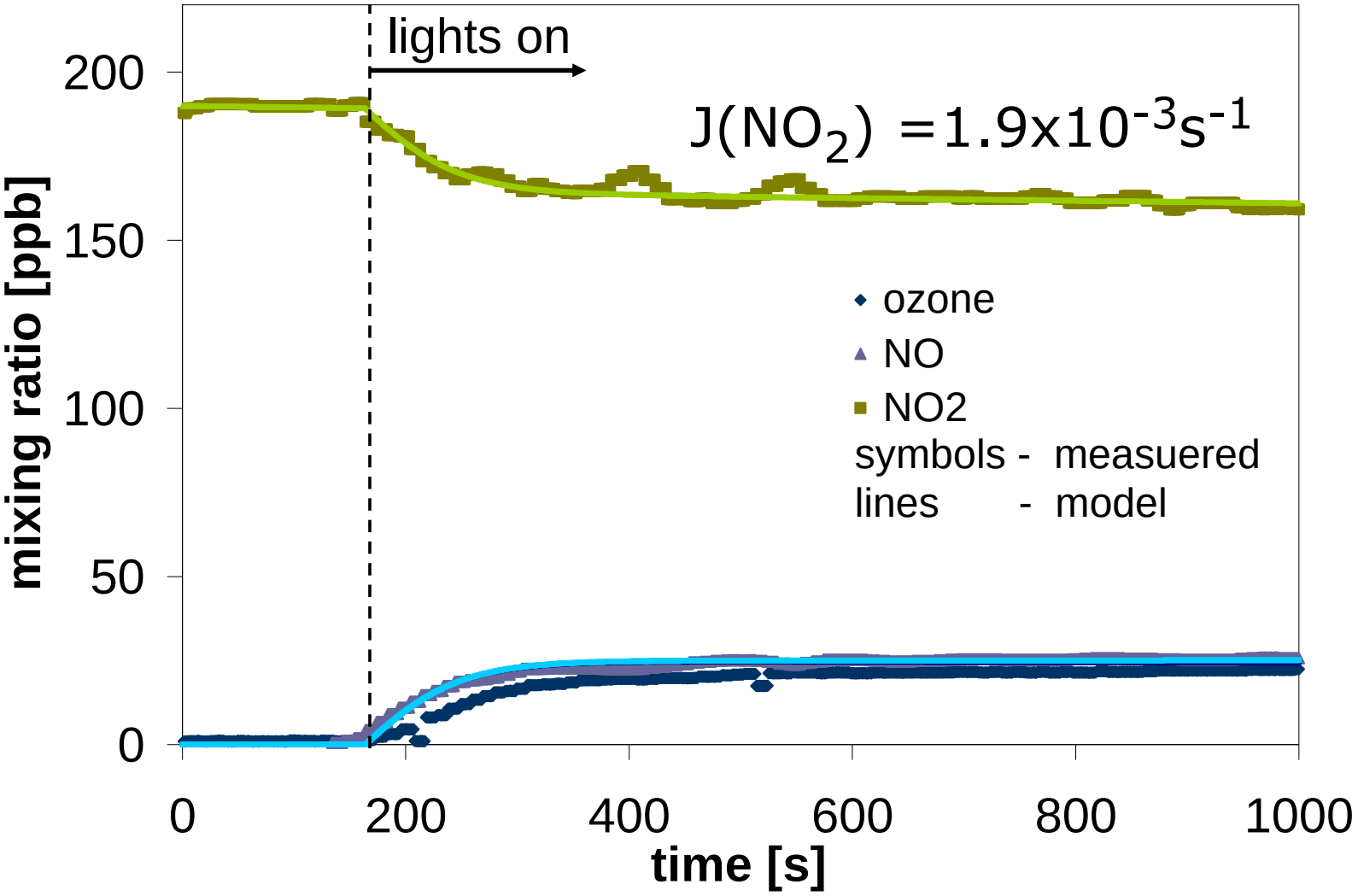
Paulsen et al., Environ. Sci. Technol. 39, doi:10.1021/es0489137, 2005



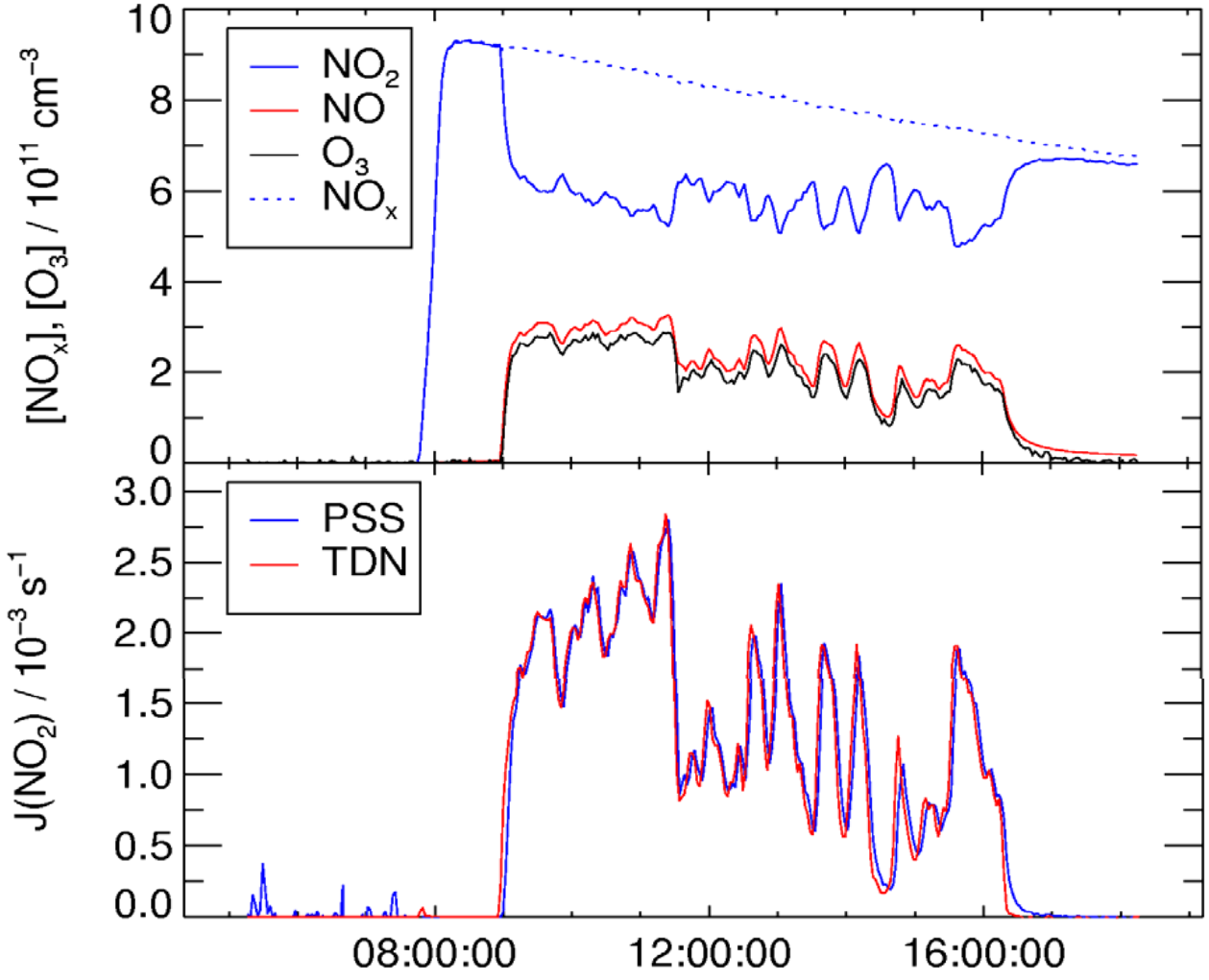
Aerosol formation in the AIDA chamber



NO_2 Photolysis in PSI chamber



NO_2 Photolysis in SAPHIR chamber



Intercomparison of instruments

- Guidelines for meaningful instrument intercomparisons in chamber experiments
- Documentation of the conditions of the chamber, the instruments, and the supporting parameters
- Definition of the measurement errors:
  seperate precision (i.e. noise) and accuracy (calibration) in order to enable meaningful statistical tests
- Instrument intercomparison activities (field and chamber)
- Co-ordination of EUROCHAMP activities with ACCENT activities.

Instrument Intercomparison Achievements 1

- **Aerosol (informal):** 8 instruments
  5 different methods measuring absorbing/coated aerosol particles
  in AIDA in 2003 (EUROCHAMP Partner 3&9: FZJ, FZK)
- **Hydroxyl radical (informal):** 2 instruments (DOAS, LIF)
  in SAPHIR in 2003 (EUROCHAMP Partner 3: FZJ)
  publication JAC
- **HONO (informal):** (DOAS vs. LOPAP, LOPAP vs. PTR-MS) experiments
  in SAPHIR in 2003 and 2004 (EUROCHAMP Partner 3: FZJ)
- **Ozone (formal):** Within the CCQM gas working group
  yielding excellent agreement
  at BIPM, Paris in 2004 EUROCHAMP Partner 11: SP)
- **Hygrometer (informal):** 3 different instruments
  in SAPHIR (ambient T, 2004) & in AIDA(-70°C, 2005)
  (EUROCHAMP Partners 3&9:FZJ, FZK)
- **HCHO (informal):** (2 DOAS and 1 Hantzsch) experiments
  in SAPHIR in 2004 and 2005 (EUROCHAMP Partner 3: FZJ)
  publication ACP
- **HCHO (informal):** (DOAS, HPLC, FTIR, and Hantzsch)
  in EUPHORE in 2005 (EUROCHAMP Partner 2: CEAM)

Instrument Intercomparison Achievements 2

- **Oxygenated Volatile Organic Compounds (OVOCs) (formal):**
  18 different instruments from 12 institutions
  results presented by a ACCENT/EUROCHAMP co-sponsored workshop (N3)
  in SAPHIR in Jan 2005 (EUROCHAMP Partners 2&3: CEAM, FZJ)
  publication ACP (2x), JGR (1x)
- **OH and HO_2 radical (formal),** HOxCOMP: 4 LIF, DOAS, CIMS, ESR instruments
  in SAPHIR in Jul 2005 (EUROCHAMP Partners 3&10: FZJ, LEEDS)
  publication submitted to ACPD
- **Aerosol mass spectrometer (informal),** CHAOS:
  6 new or newly modified instruments
  (AMS , ATOF-MS (single particle), LDI-MS, PTR-MS, IC-MS)
  from 4 different groups, partly published,
  in PSI Chamber in Oct/Nov 2005 (EUROCHAMP Partner 8: PSI)
- **Single Particle Analysis (informal):**
  Single Particle Analysis and Sizing System (JRC) vs.
  the commercial ATOFMS (TSI Inc.) particle mass spectrometer
  Teflon bag (JRC) in Dec 2005 (EUROCHAMP Partner 2: JRC)
- **Ice Particles (informal):**
  10 instruments from 5 groups,
  in AIDA in Mar 2007 (EUROCHAMP Partner 9: FZK)

Instrument Intercomparison Achievements 3

- **NO_3 and N_2O_5 (informal)**, NO_3-N_2O_5-COMP
  Workshop held Nov 2006
  (EUROCHAMP Partners 1&3&6&11: BUW, FZJ, UCC, SP)
  measurements took place in SAPHIR in Jun 2007
  (EUROCHAMP Partners 1&3&6&11: BUW, FZJ, UCC)
  2 publications ACP, 3 in preparation
- **Water Vapour (formal)** , AquaVIT
  Workshop in Jun 2007
  measurements in AIDA in Oct 2007
  (EUROCHAMP Partners 3&9: FZJ, FZK)
  whiite paper

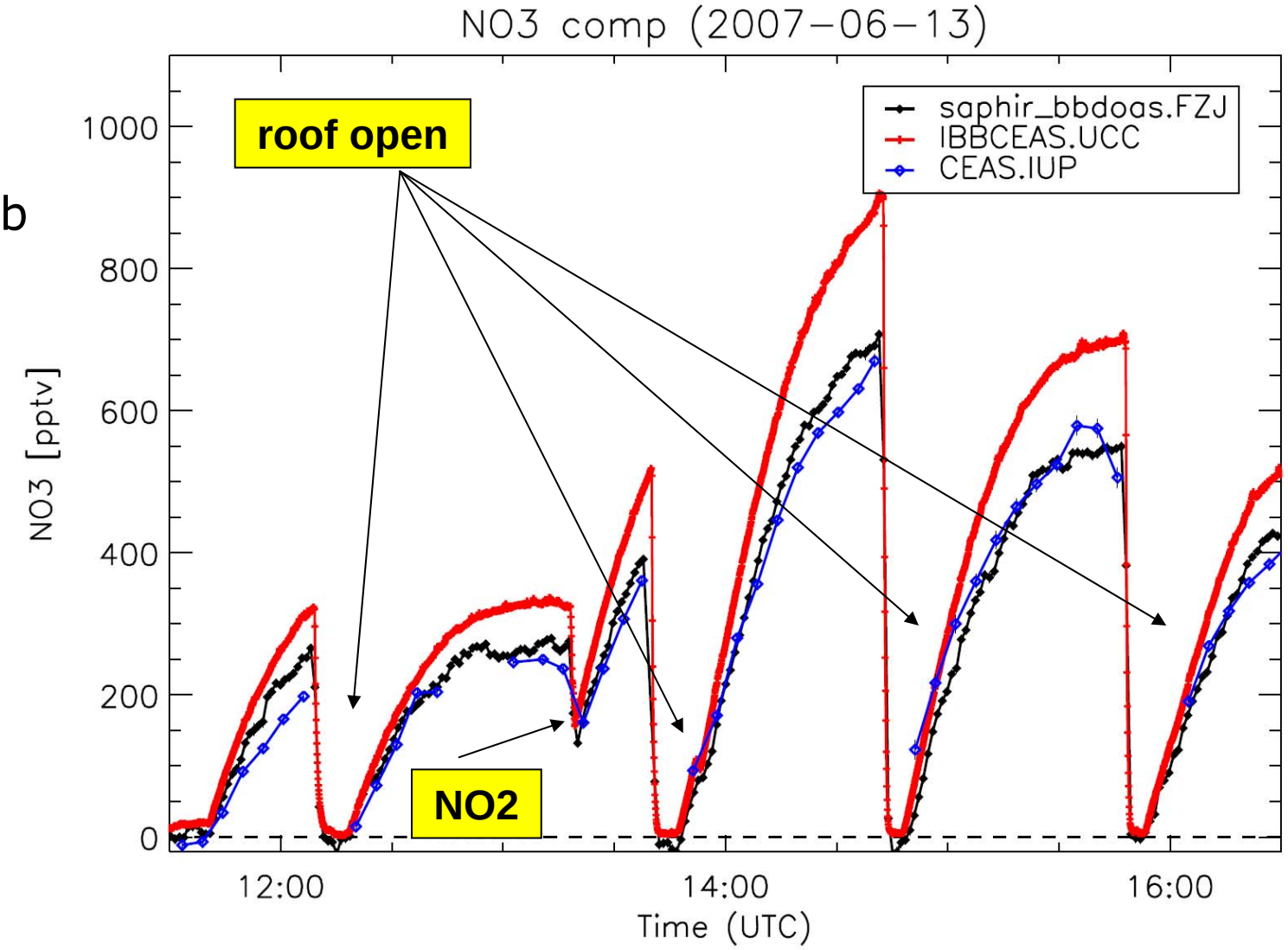
NO3 N2O5 Intercomparison SAPHIR

Instruments	Group	Species
CEA-DOAS	IUP Heidelberg	NO3
IBB-CEAS	**UC Cork**	**NO3**
BB-DOAS	**FZ Jülich**	**NO3**
Pulsed CRDS	NOAA Boulder	NO3, N2O5, NO2
BroadBand CRDS	U Leicester	NO3, N2O5
off-axis CRDS	UA Fairbanks	NO3, N2O5
CRDS / CEAS	MPI Mainz	NO3, N2O5
Thermal Conv LIF	Tokyo MU	N2O5
LIF	UC Berkeley	NO3, N2O5
LOPAP	**BU Wuppertal**	N2O5+HNO3

NO3 N2O5 Intercomparison SAPHIR

NO3 photolysis O3~170ppb

Poster!

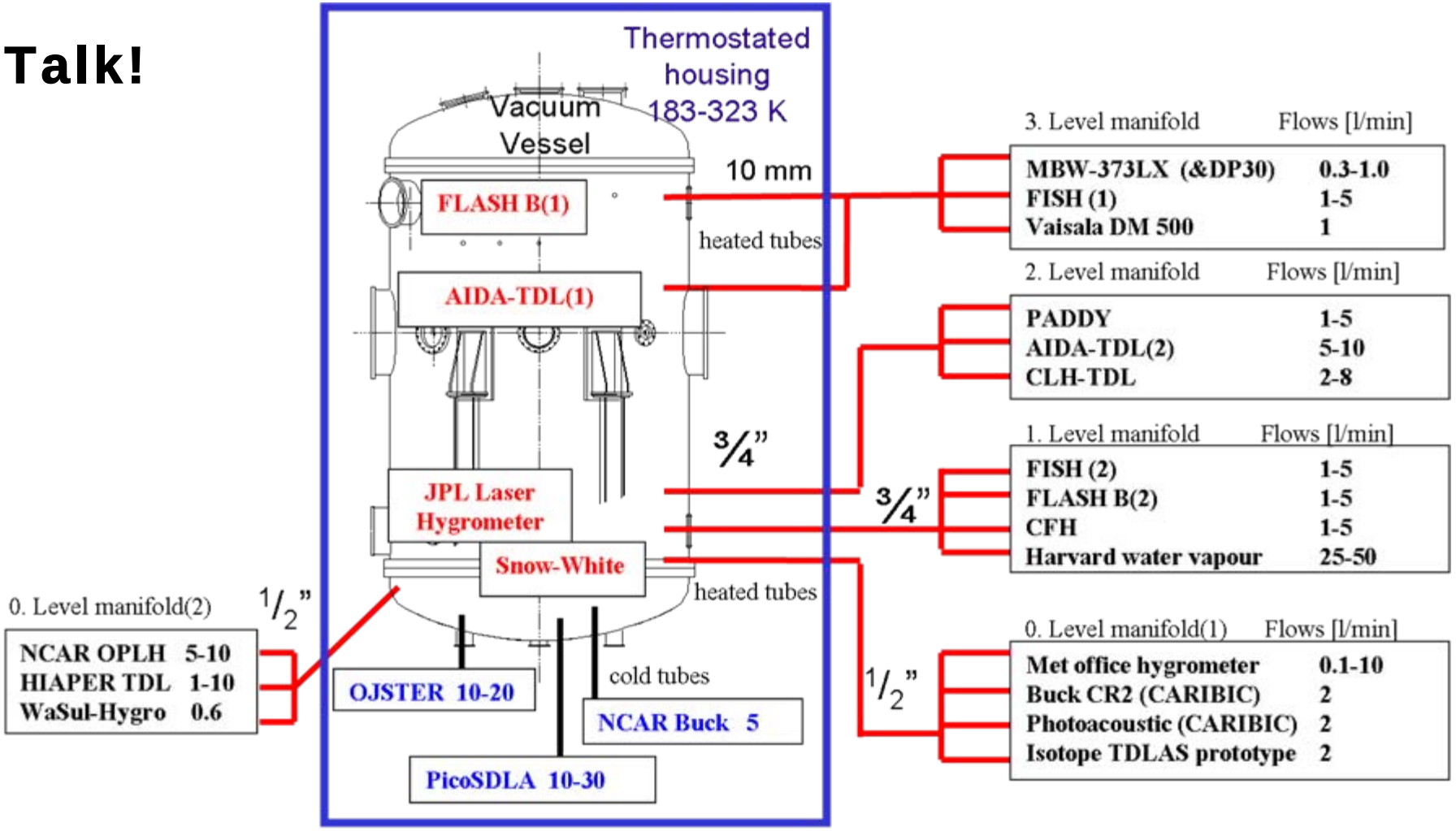


AquaVIT H2O Intercomparison AIDA (groups)

Participants	Institute	Instrument
Harald Saathoff	Forschungszentrum Karlsruhe (IMK-AAF)	AIDA TDL, MBW-373LX (FP)
Volker Ebert	University of Heidelberg	AIDA TDL
Cornelius Schiller	Forschunszentrum Jülich (ICG-1)	FISH-1 (Ly-α), FISH-2 (Ly-α), MBW-DP30 (FP)
Robert L. Herman, Robert F. Troy	JPL, Caltech	JPL-Laser-Hygrometer (TDL)
Holger Vömel	University of Colorado	CFH (FP)
Elliot Weinstock, Jessica Smith	Harvard University	Harvard Ly-α
Sergey Khaykin, Leonid Korshunov	Central Aerological Observatory	FLASH-A (Ly-α), FLASH-B (Ly-α)
Linnea Avallone, Sean Davis	University of Colorado	CLH (TDL)
Teresa Campos, Frank Flocke, Dennis Krämer	NCAR Boulder	NCAR OPLH (TDL)
Mark Zondlo	Southwest Science, Inc.	HIAPER VCSEL (TDL)
Martina Krämer	Forschunszentrum Jülich (ICG-1)	Ojster TDL
George Durry	University of Reims & INSU/CNRS	PicoSDLA (TDL)
Debbie O'Sullivan	UK Met Office	Met Office (Ly-α)
Theo Brauers, Rolf Häseler	Forschungszentrum Jülich (ICG-2)	Vaisala Sensor DM 500
Zoltán Bozóki, Arpad Mohacsi	University of Szeged	WaSul-Hygro (PA)
Andreas Zahn, Julia Keller, Christoff Dyroff	Forschungszentrum Karlsruhe (IMK-ASF)	CARIBIC (Buck FP, PA), Isotope TDL
Frank Wienhold, Ulrich Krieger, Martin Brabec	ETH Zürich	Snow-White (FP)
Ulrich Bundke	University of Frankfurt	PADDY (FP)
Peter Mackrodt	PTB Braunschweig	Water permeation source
Referees		
David Fahey, Ru-Shan Gao	NOAA, Boulder	
Ottmar Möhler	Forschungszentum Karlsruhe (IMK-AAF)	

AquaVIT H2O Intercomparison AIDA (setup)

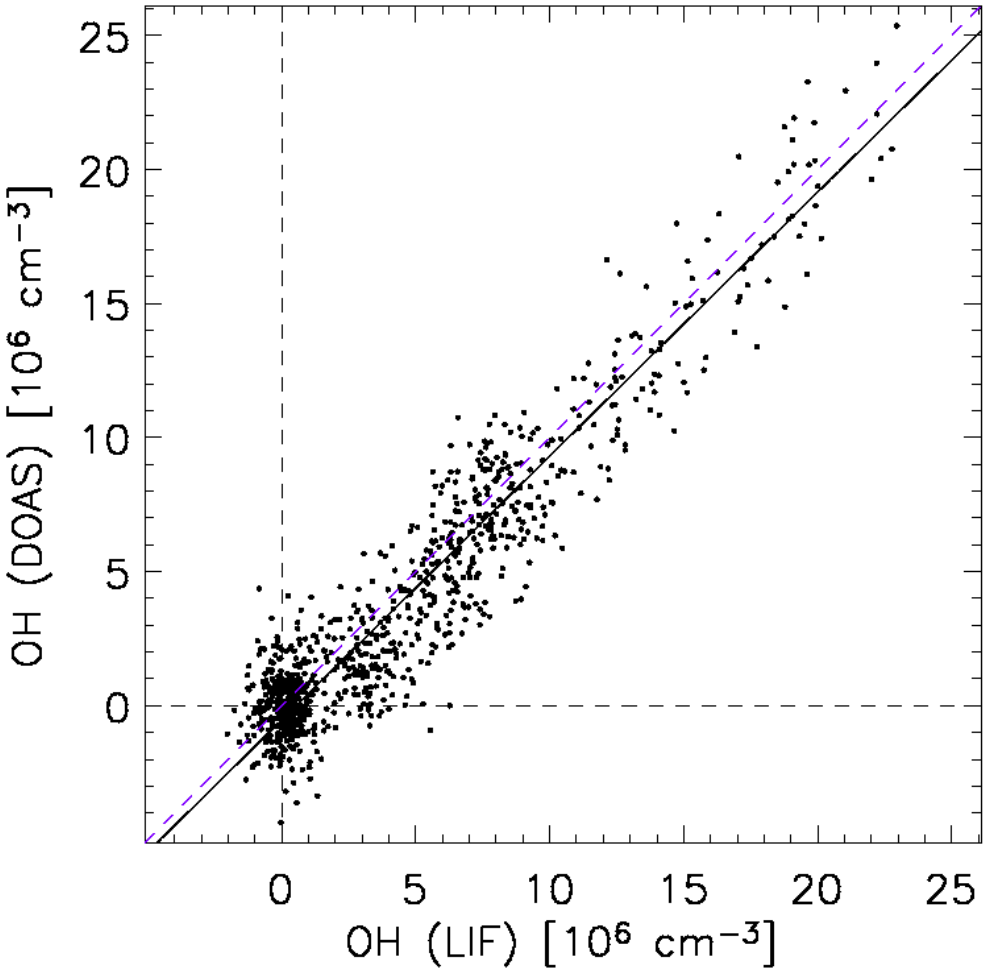
Talk!



Informal OH intercomparison at SAPHIR

Schlosser et al., J. Atmos. Chem. 56, doi:10.1007/s10874-006-9049-3, 2007

2003: 26.–31.5., 2.–12.6., 16.–30.9. (13d)



FITEXY: y = a + bx

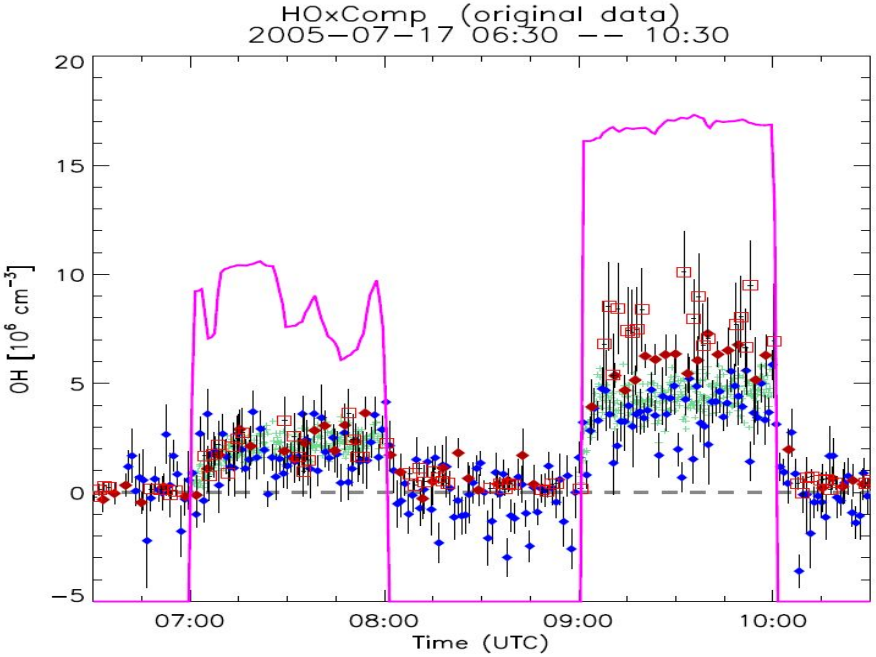
a = −0.5333
b = 0.9842
σ(a) = 0.0726
σ(b) = 0.0118
χ² = 1.03E+003
q = 0.00235

Pearson linear corr.

r = 0.945
r² = 0.894
N = 908

accuracies:
DOAS: 6%
LIF: 10%

Formal OH / HO_2 instrument intercomparison, HOxComp (SAPHIR)



OH / $J(O^1D)$

LIF (5 instruments OH and HO2)
CIMS (1 instrument OH)
DOAS (1 instrument OH)
LIF (2 instruments OH-lifetime)

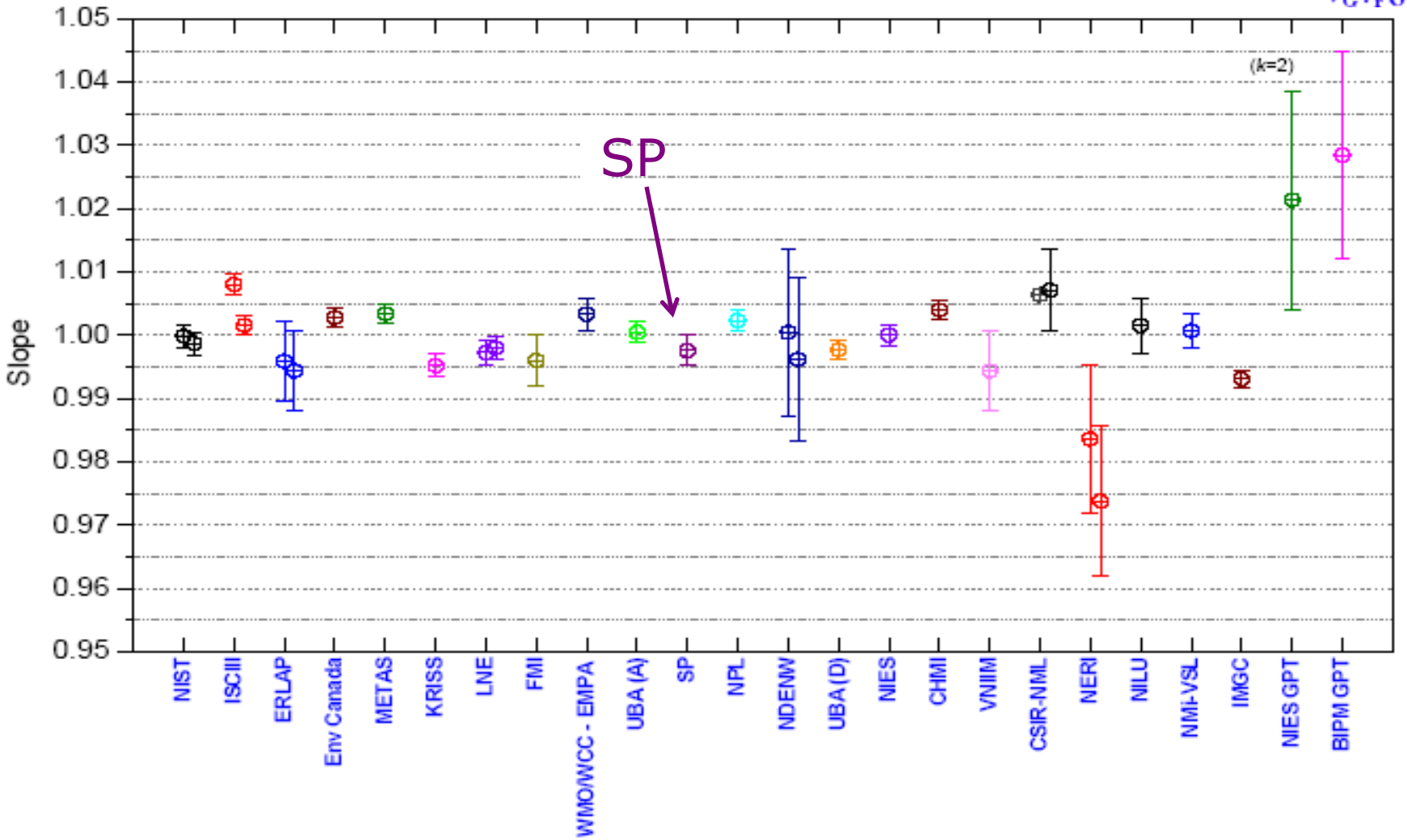
Duration: 2005
3 days outside (July 9 -11)
6 days in SAPHIR (July 17 – 23)

Workshop, Nov 30 – Dec 2
first presentation of results, discussion
current: submission of paper

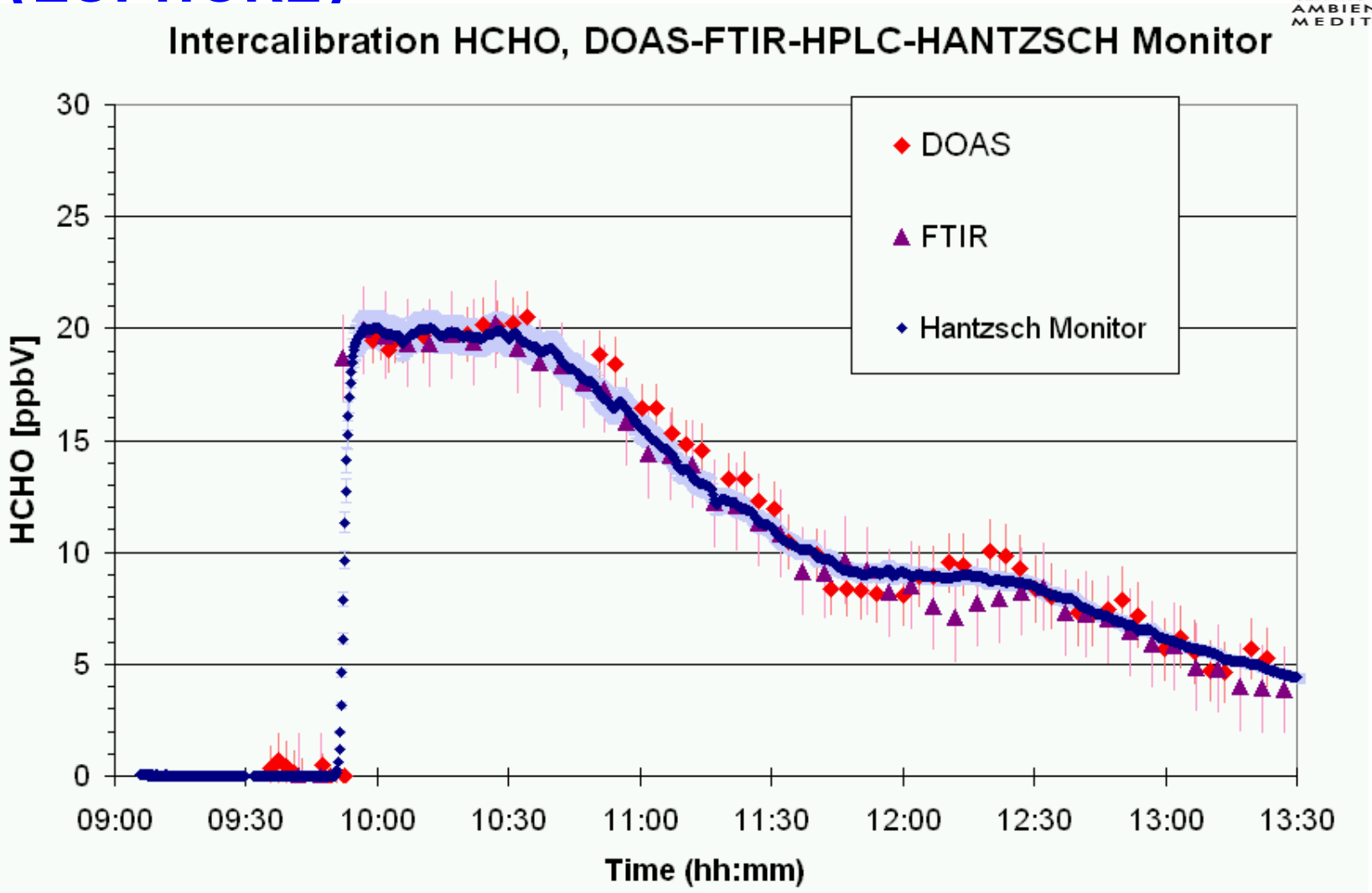
Referee:
U.Schurath, FZK

Support:
ACCENT & EUROCHAMP

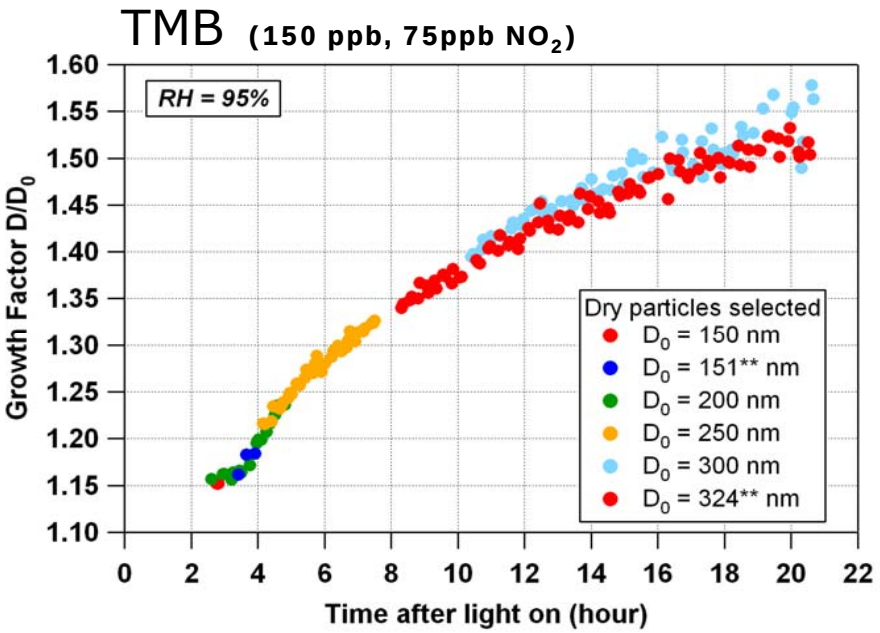
Formal Ozone intercomparison (BIPM)

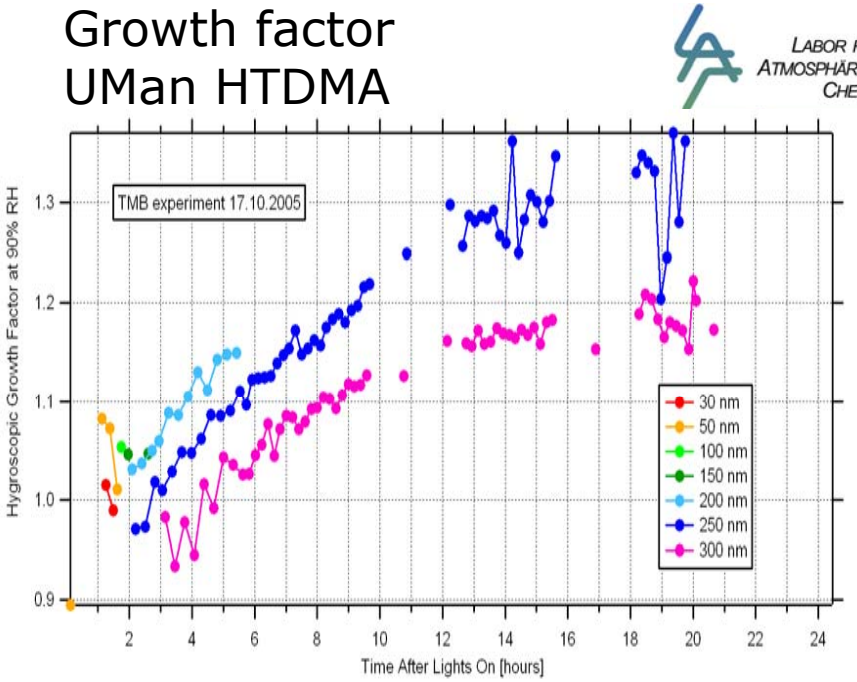


Informal HCHO intercomparison (EUPHORE)



Intercomparison of 2 HTDMAs





PSI instrument & UMan instrument
October 2005
Photooxidation of trimethylbenzene (TMB) and α-pinene
UMAN instrument does dry the aerosol before the first DMA, which results in a low hygroscopic growth factor for larger particles

Instrument Intercomparison Achievements and Outlook

- 12 different instrument intercomparison campaigns have been performed at different chamber within the Eurochamp project
  - radicals: OH, HO2, NO3, N2O5
  - inorganic gases: H2O, HONO, O3
  - organics: OVOCs, HCHO
  - particles: ice, SOA
- 3 intercomparison activities planned:
  - species: HONO, O3
  - publications:
    - several activities published and under review
  - **datasets need to be included in the database when papers are accepted.**

Quality Assured Raw Data (experiment)

- well defined and documented procedures from raw data (spectra, chromatograms, voltage, ...) to time series (concentrations, physical parameters)
- calibration factors must trace back to well defined calibration procedures
- complete description of a data point:

  time, interval, parameter(s), error(s)

- exchange of experimental and model data is only possible through an open, plattform independent, extendable, downward compatible, and easy to read and write format
- disk space is not limiting → ASCII (text) files

Dataset requirements – edf format

- Time (TZ, interval ..)
- Chamber (exactly specified)
- Instrument[s] (Manufacurer, S/N, calibration, ...)
- Operator[s] (Name[s], email[s], ...)
- measured quantities (value[s], precision, accuracy, ...)
- no data selection (i.e. don‘t remove values at det.limit)
- example:
  - header

    global attributes (where, who, what, ...)

    data attributes (description of data columns)
  - data (records)

    time, interval, val1, std1 [, val2, std2 ..]

    .....

    .....

EUROCHAMP Data Format - edf

- For use for the EUROCHAMP data base.
  primarily supports time series as recorded in most chambers, e.g. concentration profiles.
- **PDF-description** of the edf-format: http://saphir.fz-juelich.de/eurochamp/
- **Manual:** **How to create edf files**.
- Within N1 a number of **Programs** were developed to help creating edf-files.
  Browser based operation
- **edf template generator**
  - creates a edf header template
  - provides file for download
- **edf file checker**
  - upload your edf file to the FZJ server
  - tests edf file for errors
  - log file output
  - Plot data (ps-figures for download)
- **edf file creator** (under construction)
  Creates an edf-file from submitted data.
- **edf file merger** (under construction)
  combines a number of edf files into one edf file with a common time axis.
- **edf file correlator** (under construction)
  analyzes the columns of an edf file with a common time axis.
- **edf idl routines**
  - Provided for download
  - test phase, current version 0.9

N1 – what needs to be done in Eurochamp-2?

- **raw data handling:**
  - update the format
  - update the tools for the edf files

- **instrument intercomparisons:**
  - evaluate dataset and publish results
  - encorporate original data in the EUROCHAMP database (N2)
  - aerosol formation and generation

- **chamber characterization:**
  - update chamber overview table
  - compare similar experiments in different chambers
  - report spectra, turbulence, etc.

- **standard experiments:**
  - report standard experiments as aquality record within database