Programme of the 9th DOAS Workshop 13–15 July 2020

Version date: 10 July 2020

Presentation times below are in UTC

Time differences for some locations:

Auckland:	UTC + 12	Toronto:	UTC – 4
Melbourne:	UTC + 10	Mexico City:	UTC – 5
Seoul:	UTC + 9	Boulder:	UTC – 6
Hefei:	UTC + 8	Los Angeles:	UTC – 7
De Bilt:	UTC + 2	Fairbanks:	UTC – 8

Oral presentations are 15 minutes + 5 minutes for discussion.
Poster pitches are 1 minute with 1 slide.

Day 1: Monday 13 July 2020

07:15 - 08:15	*Social event – coffee tables via Slack*	
08:30 - 08:40	Welcome *Gerard van der Steenhoven, director of KNMI*	
08:40 - 08:50	Logistics *Ankie Piters*	
Satellite Retrieval & Validation (part 1)	<u>*Chairs:*</u> **Pinhua Xie & Michel Van Roozendael**	
08:50 - 09:10	TROPOMI high-spatial resolution observations from space *Pepijn Veefkind*	
09:10 - 09:30	Status of the Geostationary Environment Monitoring Spectrometer (GEMS) NO_2 operational algorithm *Junsung Park*	page 30
09:30 - 09:50	Causes of low bias in TROPOMI satellite observations of tropospheric NO_2 column densities as explored with co-located MAX-DOAS and Pandora spectrometers at Yokosuka, Japan *Yugo Kanaya*	page 21
09:50 - 09:57	Poster pitches (6×1 min.) numbers: 40, 58, 9, 26, 27, 29	
09:57 - 10:20	*break*	
Satellite Retrieval & Validation (part 2)	<u>*Chairs:*</u> **Steffen Beirle & Ilse Aben**	
10:20 - 10:40	Sentinel-5p tropospheric NO_2 data assessment using MAX-DOAS and direct sun measurements *Gaia Pinardi*	page 31
10:40 - 11:00	TROPOMI NO_2 slant column retrieval: method, stability, uncertainties and comparisons with OMI *Jos van Geffen*	page 43

11:00 - 11:20	Retrievals of glyoxal tropospheric vertical columns from TROPOMI observations *Christophe Lerot*	page 25
11:20 - 11:40	Inhomogeneous scene effects in TROPOMI satellite data *Andreas Richter*	page 35
11:40 - 11:45	*In Memoriam Andreas Hilboll*	
11:45 - 12:40	*break*	

Satellite Retrieval & Validation (part 3)
Chairs: **Andreas Richter & Olga Puentedura**

12:40 - 13:00	Shipborne MAX-DOAS measurements for validation of TROPOMI NO_2 products *Ping Wang*	page 48
13:00 - 13:20	Uniform glyoxal and formaldehyde retrievals from S5P, OMI, GOME-2, and SCIAMACHY satellite instruments *Leonardo Alvarado*	page 7
13:20 - 13:40	Validation of the S5P formaldehyde L2 product using MAX-DOAS network observations *Isabelle De Smedt*	page 14
13:40 - 14:00	A global perspective on bromine monoxide composition in volcanic plumes derived from S5-P/TROPOMI *Simon Warnach*	page 49
14:00 - 14:06	Poster pitches (5×1 min.) numbers: 5, 6, 14, 22, 23	
14:06 - 14:30	*break*	

Radiative Transfer Modelling & Spectroscopy
Chairs: **Elena Spinei Lind & Jochen Stutz**

14:30 - 14:50	Quantitative comparison of measured and simulated O_4 absorption for one day with extremely low aerosol load over the tropical Atlantic *Thomas Wagner*	page 47
14:50 - 15:10	Sum over discernible absorption paths: a method to characterize radiative transfer effects on remote sensing of volcanic SO_2 *Santiago Arellano*	page 9
15:10 - 15:30	Optical closure of multispectral aerosol optical properties *Christopher Lee*	page 24
15:30 - 15:50	Spectrally resolved laboratory measurements of oxygen-oxygen collision induced absorption in the 308 – 500 nm range, including the 315, 328, 421, and 495 nm bands *Henning Finkenzeller*	page 15
15:50 - 15:57	Poster pitches (6×1 min.) numbers: 10, 33, 7, 4, 11, 12	
16:15 - 17:15	*Social event – coffee tables via Slack*	

Day 2: Tuesday 14 July 2020

07:15 - 08:15	*Social event – coffee tables via Slack*	
Atmospheric Measurements & Emissions (part 1)		
	Chairs: **Shanshan Wang & Yugo Kanaya**	
08:30 - 08:50	O_3 and OH production in Australia studied using MAX-DOAS measurements *Robert Ryan*	page 38
08:50 - 09:10	NO_X emission flux measuring by multiple mobile-DOAS instruments in Beijing *Yeyuan Huang*	page 19
09:10 - 09:30	Remote sensing of air pollution from satellite and MAX-DOAS network in China *Cheng Liu*	page 27
Satellite Retrieval & Validation (part 4)		
	Chairs: **MariLiza Koukouli & Thomas Wagner**	
09:30 - 09:50	First retrieval of aerosol effective height based on O_4 air mass factor at 477 nm: from TROPOMI onboard Sentinel-5P and GEMS onboard GK-2B *Wonei Choi*	page 13
09:50 - 09:58	Poster pitches (6×1 min.) numbers: 36, 45, 50, 51, 52, 54, 37	
09:58 - 10:20	*break*	
10:20 - 10:40	Experiments on high-detailed mapping of tropospheric NO_2 using GSA/Resurs-P observations: results, and validation with models and measurements *Oleg Postylyakov*	page 33
10:40 - 11:00	DOAS measurements of NO_2 and HCHO pollution in Kinshasa *Rodriguez Yombo Phaka*	page 50
11:00 - 11:20	Total column water vapour retrieval from S-5P/TROPOMI in the visible blue spectral range *Christian Borger*	page 11
11:20 - 11:40	Impact of 3D cloud structures on tropospheric NO_2 column measurements from UV-VIS sounders *Huan Yu*	page 51
11:40 - 11:47	Poster pitches (6×1 min.) numbers: 30, 34, 35, 44, 46, 48	
11:47 - 12:40	*break*	

New/Other Techniques & Concepts (part 1)
Chairs: **Alexander Cede & Johannes Lampel**

12:40 - 13:00	The "ideal spectrometer" for atmospheric observations *Ulrich Platt*	page 32
13:00 - 13:20	Discrete-Wavelength DOAS NO_2 slant column retrievals: feasibility and sensitivity analysis for a future instrument *Cristina Ruiz Villena*	page 37
13:20 - 13:40	High spectral resolution DOAS measurements with a novel compact spectrograph *Jonas Kuhn*	page 22
13:40 - 14:00	Operational ship emission monitoring using Long Path Differential Optical Absorption Spectroscopy *Stefan Schmitt*	page 39
14:00 - 14:07	Poster pitches (6×1 min.) numbers: 2, 17, 21, 41, 16, 59	
14:07 - 14:30	*break*	

Atmospheric Measurements & Emissions (part 2)
Chairs: **Isabelle de Smedt & Henning Finkenzeller**

14:30 - 14:50	Urban air pollution monitoring at micro, local and mesoscales *Elena Lind*	page 26
14:50 - 15:10	Comparison between DOAS and FTIR in different configurations: HCHO and SO_2 case studies in Central Mexico *Claudia Rivera Cárdenas*	page 36
15:10 - 15:30	Mini ozone holes due to dust release of iodine in the remote tropical free troposphere *Rainer Volkamer*	page 46
15:30 - 15:50	Biogenic and fire-sourced formaldehyde above various Arctic biomes in Alaska *William Simpson*	page 40
15:50 - 15:56	Poster pitches (6×1 min.) numbers: 3, 32, 38, 39, 20	
16:15 - 17:15	*Social event – coffee tables via Slack*	

Day 3: Wednesday 15 July 2020

07:15 - 08:15	*Social event – coffee tables via Slack*	
Atmospheric Measurements & Emissions (part 3)		
	Chairs: **Cheng Liu & Hanlim Lee**	
08:30 - 08:50	Monitoring air quality in Auckland NZ using MAX-DOAS *Jamie Halla*	page 17
08:50 - 09:10	Advanced mobile-DOAS techniuqes for locating and identifying urban area emission sources *Zhaokun Hu*	page 20
New/Other Techniques & Concepts (part 2)		
	Chairs: **Denis Pöhler & Anja Schönhardt**	
09:10 - 09:30	Imaging Fabry-Perot interferometer correlation spectroscopy – First measurements with a novel imaging technique of atmospheric trace gases *Christopher Fuchs*	page 16
09:30 - 09:50	Investigation of nighttime vertical distribution of HONO based on IBBCEAS technique *Fanhao Meng*	page 29
09:50 - 09:58	Poster pitches (7×1 min.) numbers: 47, 18, 24, 25, 28, 31, 55	
09:58 - 10:20	*break*	
10:20 - 10:40	The information content of skylight polarisation in MAX-DOAS trace gas- and aerosol profiling applications *Jan-Lukas Tirpitz*	page 42
Retrieval Methods, Uncertainties & Networks (part 1)		
	Chairs: **Udo Frieß & Ankie Piters**	
10:40 - 11:00	New MAX-DOAS retrieval method using WRF-Chem aerosol information for complex aerosol load condition *Qihua Li*	page 28
11:00 - 11:20	Impact of an elevation angle bias on MAX-DOAS profile retrievals *Steffen Beirle*	page 10
11:20 - 11:40	Accurate tropospheric NO_2 column retrieval based on combined direct-sun and zenith-sky twilight visible measurements *Michel Van Roozendael*	page 44
11:40 - 11:47	Poster pitches (6×1 min.) numbers: 1, 13, 15, 19, 49, 53	
11:47 - 12:40	*break*	

Retrieval Methods, Uncertainties & Networks (part 2)
Chairs: **Cristina Prados-Roman & Stefan Schreier**

12:40 - 13:00	Influence of horizontal inhomogeneity and noise on MAX-DOAS retrievals *Julia Remmers*	page 34
13:00 - 13:20	Uncertainty of the PGN total column NO_2 product *Alexander Cede*	page 12
13:20 - 13:40	The NDACC MAX-DOAS Central Processing Service *François Hendrick*	page 18

Atmospheric Measurements & Emissions (part 4)
Chairs: **Pepijn Veefkind & Christopher F. Lee**

13:40 - 14:00	Estimating real driving emissions from MAX-DOAS measurements at the A60 motorway near Mainz, Germany *Bianca Lauster*	page 23
14:00 - 14:06	Poster pitches (6×1 min.) numbers: 8, 42, 43, 56, 60	
14:06 - 14:30	*break*	
14:30 - 14:50	Long-term measurements of bromine monoxide and ozone in the Canadian high Arctic *Ramina Alwarda*	page 8
14:50 - 15:10	Remote sensing of radical precursors in wildfires plumes: Synergies between aircraft and satellites *Kyle Zarzana*	page 52
15:10 - 15:30	Expanding CU SOF data products for evaluating the impacts of biomass burning emissions during the 2018 Pacific Northwest wildfire season: emission fluxes and enhancement ratios of CO, NH_3, C_2H_4, C_2H_6, HCN, HCHO, HCOOH, CH_3OH and PAN *Rainer Volkamer*	page 45
15:30 - 15:50	Mini-DOAS observations of biomass burning plumes during FIREX-AQ *Jochen Stutz*	page 41
15:50 - 16:00	*Closing remarks & Adjourn*	
16:15 - 17:15	*Social event – coffee tables via Slack*	

Abstracts of oral presentations

The abstracts of the oral presentations are given on the following pages, sorted alphabetically on the presenters last name; page numbers of the abstracts are listed in the above programme.

Uniform glyoxal and formaldehyde retrievals from S5P, OMI, GOME-2, and SCIAMACHY satellite instruments

Leonardo M. A. Alvarado*, Andreas Richter, Mihalis Vrekoussis, Nikos Daskalakis, and John P. Burrows

*) Institute of Environmental Physics, University of Bremen; lalvarado@iup.physik.uni-bremen.de

Presenter: Leonardo Alvarado

Abstract:

Glyoxal (CHOCHO) and formaldehyde (HCHO) are intermediate products in the tropospheric oxidation of the majority of volatile organic compounds (VOCs). CHOCHO is also a precursor of secondary organic aerosol (SOA) in the atmosphere. CHOCHO and HCHO are released from biogenic, anthropogenic, and pyrogenic sources. CHOCHO and HCHO tropospheric lifetimes are typically considered to be short (e.g. several hours), as they are rapidly removed from the atmosphere by their photolysis, oxidation by OH, and uptake on particles or deposition. Since many years the number of retrievals of formaldehyde and glyoxal abundances from space-borne instruments using the Differential Optical Absorption Spectroscopy (DOAS) method has been increasing. Most recently, some studies focused on improving the retrieval of glyoxal and formaldehyde from different satellite measurements in order to reduce the uncertainties in their columns and in estimation of VOC emissions. This study focuses on a new homogenized glyoxal and formaldehyde retrievals using air mass factors computed based on profiles simulated with the TM5 chemistry transport model. This retrieval algorithm is applied to (a) the SCIAMACHY, (b) the OMI, (c) the three GOME-2 (on MetOp-A, -B and -C), and (d) TROPOMI. Overall, the retrieved formaldehyde and glyoxal column amounts from the homogenized retrieval algorithm show similar seasonal and temporal behavior among the instruments over selected regions. In addition, the combination of six instruments provides more than 16 years of measurements, which are used for the investigation of emission and temporal variability of VOC on a global scale, but also over specific regions.

This study is dedicated to the memory of our friend and colleague, Andreas Hilboll.

Long-term measurements of bromine monoxide and ozone in the Canadian high Arctic

Ramina Alwarda*, Kristof Bognar, Kimberly Strong

*) Department of Physics, University of Toronto, Toronto, ON, Canada;
ramina.alwarda@mail.utoronto.ca

Presenter: Ramina Alwarda

Abstract:

Two ground-based spectrometers located at the Polar Environment Atmospheric Research Laboratory (PEARL) in Eureka, Nunavut (80°N, 86°W, 610 masl) are used to retrieve ozone and nitrogen dioxide (NO2) total columns and bromine monoxide (BrO) partial columns, utilizing zenith-sky DOAS and MAX-DOAS approaches, respectively. This presentation will provide an overview of these measurements, with a focus on the springtime Arctic stratosphere and troposphere. Springtime zenith-sky measurements started in 1999 provide information about year-to-year variability over the past two decades, including stratospheric ozone depletion events. Until this year, the smallest springtime ozone and NO2 columns were measured in 2011, when Eureka was inside the unusually persistent and cold polar vortex that year. However, in spring 2020, ozone columns reached a record low of 200 DU, compared to the minimum of 250 DU observed in 2011. Minima in the NO2 columns were also observed in these two years, with smaller values in 2011 rather than 2020. During the Arctic spring, periodic release of bromine from sea salt aerosols and snowpack on sea ice triggers ozone depletion events (ODEs) in the troposphere. A four-year MAX-DOAS dataset (2016-2019) of springtime BrO partial columns, aerosol observations, and weather data are used to investigate bromine source contributions and the role of meteorological conditions. Back-trajectory calculations reveal that while only air mass contact with first-year ice correlates to increased BrO, multi-year ice may also act as a source of bromine. In-situ aerosol measurements show that accumulation mode aerosols have no correlation with BrO while coarse mode aerosols are required for enhanced BrO observations. This supports the idea that sea salt aerosols are a direct bromine source in the Arctic troposphere.

Sum over discernible absorption paths: a method to characterize radiative transfer effects on remote sensing of volcanic SO2

Santiago Arellano*, Bo Galle, Christoph Kern

*) Chalmers University of Technology; santiago.arellano@chalmers.se

Presenter: Santiago Arellano

Abstract:

We introduce a method to characterize radiative transfer effects on remote sensing of volcanic SO2 using spectroscopic methods in the near UV region. The method is related to previous approaches using the distribution of photon paths but it does not assume any specific form for the distribution, as it has been previously done for cloud remote sensing with high-resolution spectrometers. We derive the contributions of "dilution" and multiple scattering and determine the "straight optical path" for different measurement scenarios. The method is tested against a Monte-Carlo radiative transfer code and field measurements using stationary scanning-DOAS and mobile-DOAS from a UAS on different volcanoes. This method can be easily extended to different measurement platforms from ground, air or space.

Impact of an elevation angle bias on MAX-DOAS profile retrievals

Steffen Beirle*, Steffen Dörner, Sebastian Donner, Vinod Kumar, Julia Remmers, and Thomas Wagner

*) Max-Planck-Institut für Chemie, Mainz, Germany; steffen.beirle@mpic.de

Presenter: Steffen Beirle

Abstract:

MAX-DOAS measurements, i.e. DOAS measurements under different elevation angles (EAs), provide information on vertical profiles of aerosols and trace gases. DSCDs can vary strongly as function of EAs (up to about 20% for a change of 1° at low EAs). Thus, MAX-DOAS profile retrievals are expected to be strongly affected by a systematic bias in EAs. The calibration of EAs is not trivial (Donner et al., AMT, 2020). Even with best practice procedures, the remaining uncertainties are about 0.1°-0.3°. Here we investigate the impact of an EA bias on aerosol and trace gas profile retrievals using the MAinz Profile Algorithm (MAPA), investigating both synthetic and real data. We apply a systematic bias to the true or nominal EAs and analyze the impact on profile parameters, profiles, the O4 scaling factor, the fit residue, and the quality flags provided by MAPA. This allows to provide more realistic errors of profiles gained from MAX-DOAS measurements. In addition, it might be possible to detect and maybe even correct for a large EA offset by e.g. systematic artefacts in the difference between measured and simulated DSCD sequences.

Total column water vapour retrieval from S-5P/TROPOMI in the visible blue spectral range

Christian Borger*, Steffen Beirle, Steffen Dörner, Holger Sihler, Thomas Wagner

*) Max Planck Institute for Chemistry; christian.borger@mpic.de

Presenter: Christian Borger

Abstract:

Atmospheric water plays a key role for the Earth's energy budget and temperature distribution via radiative effects (clouds and vapour) and latent heat transport. Thus, the distribution and transport of water vapour are closely linked to atmospheric dynamics on different spatio-temporal scales. In this context, global monitoring of the water vapour distribution is essential for numerical weather prediction, climate modeling and a better understanding of climate feedbacks.

Here, we present a total column water vapour (TCWV) retrieval using the absorption structures of water vapour in the visible blue spectral range. The retrieval consists of the common two- step DOAS approach: first the spectral analysis is performed within a linearized scheme. Then, the retrieved slant column densities are converted to vertical column densities (VCDs) using an iterative scheme for the water vapour a priori profile shape which is based on an empirical parameterization of the water vapour scale height.

We apply this novel retrieval to measurements of the TROPOspheric Monitoring Instrument (TROPOMI) onboard ESA's Sentinel-5P satellite and compare our retrieved H_2O VCDs to a variety of different reference data sets. Furthermore, we present a detailed characterization of this retrieval including theoretical error estimations for different observation conditions. In addition, we investigate the impact of different input data sets (e.g. surface albedo) on the retrieved H_2O VCDs.

Uncertainty of the PGN total column NO2 product

Alexander Cede*, Martin Tiefengraber, Manuel Gebetsberger, Moritz Müller

*) LuftBlick, Austria; alexander.cede@luftblick.at

Presenter: Alexander Cede

Abstract:

As a network of ground-based standardized Pandora spectrometer systems, the Pandonia Global Network (PGN) delivers total and tropospheric column amounts of several trace gases in an automated way. Total NO2 columns from direct sun observations are already extensively used to validate satellite data, also because they can give accurate vertical columns, especially since the air mass factor (AMF) is well defined and therefore possible errors when converting the measurements from slant columns to vertical columns are small. However the exact value for the PGN data accuracy is always a question in the validation efforts, since it is not explicitly given in the data up to the current processor version 1.7. This presentation describes our plan to include the accuracy in the next processor version 1.8. It focuses on the influence of the AMF, the effective NO2 temperature and the determination of the slant column amount in the reference spectrum.

First retrieval of aerosol effective height based on O4 air mass factor at 477 nm: from TROPOMI onboard Sentinel-5P and GEMS onboard GK-2B

Wonei Choi*, Hanlim Lee

*) Pukyong National University; cwyh3338@gmail.com

Presenter: Wonei Choi

Abstract:

We, for the first time, retrieved aerosol effective height (AEH) based on O4 air mass factor (AMF) at 477 nm from TROPOMI onboard Sentinel-5 Precursor satellite. In this present study, AEH was retrieved by performing online radiative transfer calculations to account for a variety of O4 VCD values. In addition, aerosol type classification algorithm using TROPOMI CO and AI with their new threshold values was introduced to determine the aerosol types of smoke, dust, and sulfate. The AEHs were retrieved over various aerosol source regions including northeast Asia (complicated aerosol sources), South African (biomass burning smoke aerosols), and Sahara desert (dust aerosols). Finally, the TROPOMI-based AEH retrievals were compared with those from ground-based lidar measurement over northeast Asia from January 2018 to June 2019. Meanwhile, in this present study, we also discuss the AEH retrieval from hyperspectral radiance obtained from Geostationary Environment Spectrometer (GEMS) during the period of in orbit test. GEMS onboard GK-2B satellite was successfully launched in February 2020.

Validation of the S5P formaldehyde L2 product using MAX-DOAS network observations

Isabelle De Smedt*, G. Pinardi, C. Vigouroux, B. Langerock, S. Compernolle, K.U Eichman, N. Theys, C. Lerot, H. Yu, J. Vlietinck, F. Romahn, P. Hedelt, Z. Cheng, J.C. Lambert, D. Loyola, M. Van Roozendael and NIDFORVAL HCHO team

*) BIRA-IASB; isabelle.desmedt@aeronomie.be

Presenter: Isabelle De Smedt

Abstract:

The Sentinel-5 Precursor (S5P) was launched on the 13th of October 2017, with on board the TROPOspheric Monitoring Instrument (TROPOMI). The formaldehyde (HCHO) L2 product is operational since the end of 2018. The prototype of the tropospheric HCHO retrieval algorithm is developed at BIRA-IASB and implemented at the German Aerospace Center (DLR) in the S5P operational processor (De Smedt et al., 2018). In this work, we investigate the quality of the HCHO tropospheric column product and its validation within the MPC framework (Mission Performance Center) and the S5PVT NIDFORVAL project (S5P NItrogen Dioxide and FORmaldehyde VALidation). Within NIDFORVAL, the S5P HCHO product has been validated using the full FTIR and MAXDOAS dataset (Vigouroux et al., 2020). Validation results have been assessed against reported product uncertainties taking into account the full comparison error budget, showing that the product quality reaches its requirements. Here, we focus on satellite-satellite comparison based on the OMI QA4ECV HCHO product and on ground-based validation using MAX-DOAS and Pandora network observations. About 15 HCHO measuring stations are involved, providing data corresponding to a wide range of observation conditions at mid and low latitudes, and covering remote, sub-urban, and urban polluted sites. Comparison results show usually negative biases for large HCHO columns, while a positive offset is observed for the lowest columns. For the MAX-DOAS stations providing vertical profile retrievals, the impact of a priori profiles on the comparison is assessed. The dataset allows to discuss validation results as a function of emission source. Seasonal and diurnal variations are compared. Long term variation are also monitored using the OMI and MAX-DOAS QA4ECV dataset. NIDFORVAL HCHO team Alkis Bais, Sebastian Donner, Theano Drosoglou, Michel Grutter, Jay R. Herman, Hitoshi Irie, Dimitris Karagkiozidis, Cheng Liu, Ankie Piters, Claudia Rivera, Julia Remmers, Thomas Wagner, François Hendrick, Alfonso Saiz-Lopez, Nader Abuhassan, Alexander Cede, Martin Tiefengraber Vigouroux et al.: TROPOMI/S5P formaldehyde validation using an extensive network of ground-based FTIR stations, Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2020-30, in review, 2020.

Spectrally resolved laboratory measurements of oxygen-oxygen collision induced absorption in the 308 – 500 nm range, including the 315, 328, 421, and 495 nm bands

Henning Finkenzeller*, Rainer Volkamer

*) University of Colorado Boulder & CIRES, Boulder, CO, USA; henning.finkenzeller@colorado.edu

Presenter: Henning Finkenzeller

Abstract:

Oxygen-oxygen collision induced absorption accounts for significant absorption of solar radiation in the atmosphere. It needs to be considered in the interpretation of spectra in absorption spectroscopy. If not represented correctly, it interferes in the retrieval of other trace gases. Quantitative measurements of oxygen-oxygen collision induced absorption, combined with the oxygen concentration vertical profile, allow to constrain radiative transfer processes in the atmosphere. No spectrally resolved cross section data of the bands below 335 nm wavelength, at 421 nm, and at 495 nm have been available. This study presents spectrally resolved gas-phase laboratory measurements of the oxygen-oxygen collision induced absorption in the ultraviolet and blue spectral range (308 – 500 nm), including the 315, 328, 421, and 495 nm bands, acquired with Cavity Enhanced Absorption Spectroscopy under atmospherically relevant conditions. While the newly acquired data generally agree with existing data on the strong bands, significant differences consist in a higher signal to noise ratio, a non-zero baseline between bands, and a different band shape of the 344 nm band. This presentation discusses the laboratory setup and analysis scheme used to determine the cross section, and first applications of the cross section to atmospheric data sets.

Imaging Fabry-Perot interferometer correlation spectroscopy – First measurements with a novel imaging technique of atmospheric trace gases

Christopher Fuchs*, Jonas Kuhn, Nicole Bobrowski, Ulrich Platt

*) Institute of Environmental Physics, Heidelberg University, Germany; cfuchs@iup.uni-heidelberg.de

Presenter: Christopher Fuchs

Abstract:

Imaging of trace gases by optical remote sensing can provide insights in the dynamics of physical and chemical processes within the atmosphere. However, dispersive techniques are not able to resolve many processes on their intrinsic spatial and temporal scale, e.g. Imaging DOAS. Non-dispersive imaging techniques, e.g. SO_2 cameras, reach high spatial and temporal resolution, but due to their strongly restricted spectral information are limited to SO_2 only.

We describe a imaging technique for atmospheric trace gases, based on the application of a Fabry-Perot interferometer (FPI). The periodic transmission pattern of the FPI is matched to the periodic variation (usually due to the vibrational structure) of the absorption cross section of the target molecule. The increase of spectral information for the detection of trace gases reduces cross sensitivities, greatly reduces the measurement time, and allows the application of the technique to other species e.g., HCHO, BrO.

We present the first measurement for SO_2 with an imaging Fabry-Perot correlation spectroscopy (IFPICS) prototype with a detection limit of $\approx 5 \times 10^{17}$ molec/cm^2. Additionally, we will present sensitivity studies of further trace gases, supported by first laboratory measurements.

Monitoring air quality in Auckland NZ using MAX-DOAS

Jamie D Halla*, Richard Querel

*) Defence Technology Agency; j.halla@dta.mil.nz

Presenter: Jamie Halla

Abstract:

New Zealand is often thought of as a pristine environment with very low levels of air pollution. Although for the most part this may be true, its largest city Auckland has a population ∼1.5 million and several large emission sources including industry, the shipping ports and traffic from vehicles. Multiple sites were used to examine the pollution distribution in Auckland and examine current trends using MAX-DOAS coupled with other ground-based instruments. This talk will focus on results from these measurements and examine any differences between normal operations and the relatively clean period where the city was shut down due to the COVID-19 outbreak.

The NDACC MAX-DOAS Central Processing Service

François Hendrick*, C. Fayt, M. Friedrich, S. Beirle, U. Friess, A. Richter, T. Bösch, K. Kreher, A. Piters, T. Wagner, J.-L. Tirpitz, A. Bais, M. Navarro-Comas, C. Prados-Roman, O. Puentedura, A. Cede, E. Lind, A. Dehn, S. Casadio, P. Castracane, and M. Van Roozendael

*) Royal Belgian Institute for Space Aeronomy (BIRA-IASB); francois.hendrick@aeronomie.be

Presenter: François Hendrick

Abstract:

Since it provides vertically-resolved information on atmospheric gases at a horizontal scale approaching the one from nadir backscatter satellite sensors, the ground-based MAX-DOAS technique has been recognized as a valuable source of correlative data for validating space-borne observations of air-quality-related species such as NO2, HCHO, SO2, O3, etc. In this context, the ESA Fiducial Reference Measurements for Ground-Based DOAS Air- Quality Observations (FRM4DOAS) project is aiming at developing a near-real-time (6-24h latency) central processing system for the delivery of harmonized, quality-controlled, and fully traceable data products from MAX-DOAS instruments. The first phase of the project has been dedicated to the development of a prototype version of this processing system for 3 key products (NO2 vertical profiles, total O3 columns, and tropospheric HCHO profiles) and its demonstration at 11 project partners MAX-DOAS stations. In this presentation we will describe the efforts carried out during the last months to develop the first MAX-DOAS central processing service to be operated within the Network for the Detection of Atmospheric Composition Change (NDACC). The main aspects of the service development will be presented, like the FRM4DOAS prototype algorithm optimisation, operationalisation, and validation, and the establishment of MAX-DOAS NDACC instrument and data retrieval certification procedures, user data policy, datasets DOI, etc. This operational service will be launched end of April 2020 for a dozen of MAX-DOAS instruments. The resulting data sets will be stored in the NDACC and ESA EVDC data handling facilities. This activity and its future upscaling in terms of stations and data products will ensure that MAX-DOAS observations at a FRM quality level will be made available for the validation of present and future satellite missions like the Copernicus atmospheric Sentinels (5p, 4, 5). First comparison results with S5p/TROPOMI NO2 and HCHO column data will be presented in the companion abstract by Friedrich et al.

NOx emission flux measuring by multiple mobile-DOAS instruments in Beijing

Yeyuan Huang*, Ang Li, Pinhua Xie, Zhaokun Hu, Jin Xu, Xiaoyi Fang, Hongmei Ren, Bing Dang

*) Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Sciences; yyhuang@aiofm.ac.cn

Presenter: Yeyuan Huang

Abstract:

Measurements of the NOx emissions in Beijing are of great significance because they aid in the understanding of the development of NOx pollution in mega-cities of China. However, the NOx emissions of the mega-cities are very difficult to measure due to the changes of the wind patterns and roads' moving sources during the measurement. In order to get good spatial coverage of the different ring roads in Beijing in a short amount of time, 2 mobile-DOAS instruments were used to measure the NOx emission flux in April. In addition, a wind profile radar provided simultaneous measurements of the wind field for the altitudes between 50 m and 1 km. We first determined the NOx emission flux of different ring roads using the wind field averaging from the measured wind data. The results show that NOx emission flux of Beijing 5th Ring road, representing the urban part, varies from (20.09±6.05) ×1024 molec./s to (38.02±14.79) ×1024 molec./s. It was found that on April 20th, NOx emission flux of the 3rd Ring were slightly higher than that of the 4th Ring, because the two ring roads were measured at different time periods. We then analyzed the NOx emission flux error budget and error sensitivity. The main error source was the wind field uncertainty. But for some measurements, the main emission flux error source was either the wind speed uncertainty or the wind direction uncertainty, rather than the both. As Beijing's NOx emissions come from road vehicle exhaust, we found that the emission flux error has a more diverse sensitivity to the wind direction uncertainty and this improves our knowledge on this topic. NOx emission flux error sensitivity study indicates that more accurate measurements of the wind field are crucial to effective NOx emission flux measuring in the mega-cities of China. Having the actual time and high resolved wind measurements is a big advantage for mega-cities' NOx emission flux measuring. We used 2 mobile-DOAS sets and a wind profile radar to measure the NOx emission flux in Beijing for the first time. These 2 modifications for the mobile-DOAS measurements improved the quality of the emission flux measuring results. This approach can be applied in many other mega-cities in China.

Advanced mobile-DOAS techniuqes for locating and identifying urban area emission sources

Zhaokun Hu*, Ang Li, Pinhua Xie

*) Hefei Institutes of Physical Science, CAS; zkhu@aiofm.ac.cn

Presenter: Zhaokun Hu

Abstract:

Pollutant concentration distribution and emission are important ways to understand regional pollution. To investigate the distribution characteristics and identify individual sources rapidly, a new mobile passive differential optical absorption spectroscopy (DOAS) instrument has been developed, which set two angle telescopes (90°,30°) to receive the scattered light respectively, and set two mechanical shutters to switch the optical path quickly in the mobile platform. The instrument collected the zenith scattered light in the UV or visible region and it was used to derive the vertical column density of trace gases above the measurement route. The slant column density in two different viewing directions were detected, and combined with the geometric approximation, the vertical column density of trace gas was obtained. After obtaining the column concentration distribution, the data were analyzed by semi variance analysis combined with geographical information. Monte Carlo simulation was used to reconstruct the high spatial resolution pollutant concentration distribution, combined the wind field data during the observation, the high spatial resolution emission flux in the area can be quickly obtained. A field experiment was performed in Beijing and some industrial area. The distribution information of vertical column density along the route was derived, the concentration distribution of NO2 at 200m*200m resolution and the 0.01°*0.01° resolution emission flux data are obtained further. The scheme can provide a new method to verify pollutant concentration distribution and emission source inventory.

Causes of low bias in TROPOMI satellite observations of tropospheric NO2 column densities as explored with co-located MAX-DOAS and Pandora spectrometers at Yokosuka, Japan

Yugo Kanaya*, Hisahiro Takashima, Takashi Sekiya, Kazuyuki Miyazaki, Henk Eskes, Gaia Pinardi, Daniel Santana Diaz, Moritz Müller, Alexander Cede, Hiroshi Tanimoto

*) Japan Agency for Marine-Earth Science and Technology (JAMSTEC); yugo@jamstec.go.jp

Presenter: Yugo Kanaya

Abstract:

Satellite observations of NO2, a key atmospheric pollutant, were remarkably improved with TROPOMI (Sentinel-5P), launched in 2017, achieving a spatial resolution of 5.5×3.5 km. However, there is still a fundamental issue of low bias in the determined tropospheric NO2 column densities (e.g., 25-50spectroscopic observations such as MAX-DOAS. Our results of validation at Yokosuka (32.32°N, 139.65°E), located on the south edge of Tokyo metropolitan area, during winter 2018-19 were consistent; TROPOMI (within 0.1°) had a low bias by a factor of 1.6 against ground-based MAX-DOAS. Here we demonstrate that such a large gap could be quantitatively explained by the combination of (1) uncertainty in the MAX-DOAS observations including (2) spatial inhomogeneity of NO2 (15-28%), (3) biased vertical profile shapes assumed for satellite retrievals (11%), and (4) effects from co-present aerosols and/or biased surface albedo (20%). For (1), a co-located Pandora instrument in direct-sun mode was used to evaluate the uncertainty of MAX-DOAS. Part of the bias likely originated from spatial inhomogeneity (term (2)), as pollution levels were higher in the northeast with the line of sight for MAX-DOAS than in south for Pandora. The term (3) was evaluated by considering vertical profiles from MAX-DOAS with the satellite's averaging kernels. The term (4) was evaluated with OMI QA4ECV products, where surface albedo in the NO2 fitting window was high (∼0.1) in winter and suspected to be contributed from aerosols; too large reflectance assumed at the bottom surface might have resulted in a too high air mass factor and then a low NO2 from OMI. We will also discuss potential validation strategies for the new satellites including GEMS and Japanese GOSAT-GW.

High spectral resolution DOAS measurements with a novel compact spectrograph

Jonas Kuhn*, Ulrich Platt, Nicole Bobrowski, Thomas Wagner

*) Institute for Environmental Physics, Heidelberg University, Germany, Max Planck Institute for Chemistry, Mainz, Germany; jkuhn@iup.uni-heidelberg.de

Presenter: Jonas Kuhn

Abstract:

Usually DOAS-type remote sensing of atmospheric trace gases in the UV and visible is performed at spectral resolutions of some hundreds of pm up to a nm. This is usually sufficient, since many trace gases (e.g. SO2, NO2, H2O, O3, HCHO, CHOCHO, BrO, OClO, IO, etc.) exhibit structured absorption (due to vibro-electronic transitions) on a nm wavelength scale. The intrinsic spectral resolution of many atmospheric trace gas absorption cross sections and also of spectral structures in the solar spectrum are, however, on the order of several pm in this wavelength range. Spectral artefacts resulting from measurements with low spectral resolution are corrected by using a recorded reference spectrum and highly resolved literature data of Fraunhofer lines and trace gas absorption cross sections. This type of DOAS measurements can easily be performed with compact grating spectrographs.

In some cases, however, higher spectral resolution is desired: 1) When absorption cross sections of different trace gases overlap on the nm scale they can still be distinguished on a higher resolution. 2) When the absorption cross section is only structured on higher resolution, e.g. single sharp absorption lines. 3) If evaluation without a recorded reference spectrum is desired, spectra on the intrinsic resolution of the Fraunhofer lines and absorption cross sections are required.

Grating spectrographs with resolution of a pm scale are typically very bulky instruments and hardly practical for field measurements. Here we report the development of a high resolution spectrograph based on a high finesse Fabry Perot Interferometer. A spectral resolution of about 2-5 pm is reached with an instrument design, which is comparable in size, weight and stability to widely used low resolution grating spectrometers. A series of applications for active and passive remote sensing are discussed, including precise water vapour measurements in the visible range, oxygen column measurements for the determination of atmospheric photon path lengths or quantification of OH radicals.

Estimating real driving emissions from MAX-DOAS measurements at the A60 motorway near Mainz, Germany

Bianca Lauster*, Steffen Dörner, Steffen Beirle, Sebastian Donner, Sergey Gromov, Katharina Uhlmannsiek, Thomas Wagner

*) Max Planck Institute for Chemistry; b.lauster@mpic.de

Presenter: Bianca Lauster

Abstract:

Nitrogen oxides ($NO_X = NO + NO_2$) have a direct and indirect impact on human health. Therefore, the World Health Organization recommends limiting the concentration of nitrogen dioxide (NO_2) in the atmosphere. Nevertheless, these limits are regularly exceeded. Especially, fossil fuel combustion from road traffic is a major contributor to the emission of NO_X.

Multi Axis-Differential Optical Absorption Spectroscopy (MAX-DOAS) is able to measure trace gases in the lower troposphere. Here, this remote sensing method was used to measure NO_X emissions at a highly frequented motorway. Two MAX-DOAS instruments were set up on both sides of the A60 motorway close to Mainz, Germany. The parallel viewing direction allows measuring the background signal at the upwind side and the background plus traffic emissions on the downwind side. Together with the effective wind speed perpendicular to the motorway, it is thus possible to retrieve the total traffic emissions. Compared to the expected emissions calculated from the European emission standards, the derived emissions of NO_X are by a factor 11 ± 7 higher.

In this study, first measurement results are presented and the method is evaluated with regard to the practicability and error margin.

Optical closure of multispectral aerosol optical properties

Christopher F. Lee*, T. K. Koenig, I. Ortega, E. Kassianov, L. K. Berg, K. Lantz, J. Michalsky, R. Ferrare, J. Hair, C. Hostetler, and R. Volkamer

*) Dept Chemistry & CIRES, University of Colorado at Boulder, USA; christopher.f.lee@colorado.edu

Presenter: Christopher Lee

Abstract:

Aerosols and clouds remain a major source of uncertainty in the global radiative budget. Optical closure studies that combine vertically resolved measurements of aerosol size distributions and refractive index are needed to assess our understanding of multispectral aerosol optical properties (extinction profile, g-parameter, aerosol optical depth) inferred from active and passive remote-sensing measurements. A fundamental sampling challenge to assess optical closure consists of the different spatial, spectral, and temporal scales at which remote sensing and in-situ instruments characterize aerosol optical properties. A major step towards overcoming this sampling challenge is the development of NASA's airborne multi-wavelength High Spectral Resolution Lidar (HSRL-2) that provides measurements of aerosol extinction profiles at 355nm, 532nm, and 1064nm. We investigate the suitability of these measurements as a-priori information to constrain aerosol profile retrievals at 360nm and 477nm, two popular wavelengths in the DOAS community due to prominent O2-O2 absorption bands.

The dataset we use is from the Two-Column Aerosol Project (TCAP) in July 2012, which actively tackled the sampling challenge by deploying two research aircraft above the DoE ARM mobile facility at Cape Cod, MA. Specifically, the following facilities and instruments were deployed: 1) DoE G1 aircraft equipped with in-situ measurements of aerosol size distributions (harmonized from UHSAS, PCASP, CAS sensors; Kassianov et al., 2015) and aerosol chemical composition to constrain refractive index (AMS, SP2); 2) the NASA King Air research aircraft equipped with nadir-looking HSRL-2 (measures below aircraft to the surface). Both aircraft regularly passed/profiled over 3) the DoE ARM surface site equipped with the following instruments: a) the University of Colorado 2-D MAX-DOAS (measured aerosol phase function parameter, g; aerosol optical depth at 360nm and 477nm inferred from O2-O2, and at 430nm from Raman Scattering Probability; Ortega et al., 2016a,b), b) AERONET Cimel sun photometer, c) two visible Multi Filter Rotating Shadow Band Radiometers. This comprehensive data set is re-analyzed here to assess the uncertainty introduced into the aerosol extinction profile, and the perceived effects on O2-O2 and RSP, if the wavelength dependence is based on either i) vertically resolving in-situ measurements (G1 aircraft), ii) HSRL-2, or iii) ground-based column sensors (Aeronet, MFRSR).

Retrievals of glyoxal tropospheric vertical columns from TROPOM observations

Christophe Lerot*, Isabelle De Smedt, Nicolas Theys, Huan Yu, Jonas Vlietinck, Michel Van Roozendael, Jenny Stavrakou, Jean-François Müller, Leonardo Alvarado, Andreas Richter, Christian Retscher

*) BIRA-IASB; christophe.lerot@aeronomie.be

Presenter: Christophe Lerot

Abstract:

Since its launch in October 2017, TROPOMI records earthshine radiances in spectral ranges from the ultraviolet to the shortwave infrared regions at an unprecedented spatial resolution (3.5 x 7 km^2 and 3.5 x 5.5 km^2 after August 2019). A suite of L2 operational products provide key information for the understanding and monitoring of the Earth-atmosphere system, and more particularly of aspects related to ozone layer protection, air quality and climate change. The ESA S5p+ Innovation activity aims at further exploiting the capability of the TROPOMI instrument by supporting the development of a number of additional scientific products, including glyoxal tropospheric column retrievals. The latter provide information on VOC emissions as glyoxal is mainly released in the atmosphere as an intermediate product of VOC oxidation, but also directly emitted from biomass burning events. We present here the BIRA-IASB S5p glyoxal product relying on a DOAS approach and its main features. We show how the large amount of TROPOMI data and its high resolution helps to better identify and localize VOC sources. The many intense fire events that occurred in the last years, e.g. in Northern America in 2018 or in Australia in 2019/2020, led to extreme levels of pollution and unprecedentedly high glyoxal columns are measured accordingly. We also highlight the excellent consistency between the TROPOMI and OMI glyoxal products, allowing thus to combine them in a 15-year data record. The validation of satellite glyoxal retrievals is difficult due to the scarcity of independent data and their own limitations caused by the low glyoxal optical depth. Nevertheless, a few ground-based data sets have been collected and preliminary comparisons with the S5p glyoxal product are presented.

Urban air pollution monitoring at micro, local and mesoscales

Elena Spinei Lind*, Jeffrey Geddes, Taylor Adams, Yun Dong

*) Virginia Tech; eslind@vt.edu

Presenter: Elena Lind

Abstract:

Increasing urbanization worldwide raise serious concerns about urban air quality and its effects on large human populations. This study presents application of Differential Optical Absorption Spectroscopy technique to multi scale urban air quality (NO2) monitoring using Pandora spectroscopic instruments (SciGlob Inc) in Boston, MA, USA (Sep 2019 - Jan 2020). Pandora instrument, located on top of 30 m building, performed over the roof sky scans (local to meso scales), into the street canyon "target" (micro-scale) and direct sun measurements. In situ NO2 measurements were also conducted on top of the roof (co-located with Pandora) and at the street level near the "target" building. NO2 spatial and temporal heterogeneity within different scales is discussed.

Remote sensing of air pollution from satellite and MAX-DOAS network in China

Cheng Liu*, Qihou Hu, Haoran Liu, Chengxin Zhang, Chengzhi Xing, Wei Tan, Wenjing Su, Fei Zhao, Congzi Xia, Xiangguang Ji, Hua Lin, Bo Li, Shuntian Wang

*) Department of Precision Machinery and Precision Instrumentation, University of Science and Technology of China, 230026 Hefei, China.; chliu81@ustc.edu.cn

Presenter: Cheng Liu

Abstract:

With the fast industrialization and urbanization in China, environmental pollution has become more serious and complex. Precise and real-time monitoring is the prerequisite for knowing the distribution characteristics and the evolution mechanism of the atmospheric pollutants. Over the last few years, we have successfully monitored atmospheric composition by using remote sensing from different platform, including satellite, ground and mobile vehicle, which have been validated to have good performance.

Remote sensing by satellite can describe the global distribution of various pollutants, which can also locate the emission point sources, such as factories etc. Ground-based MAX-DOAS monitor the vertical evolutions of these trace gases and aerosol at a fixed position, the column density of pollutants was divided into different layers, so we could detect transport plum in all altitude. Up to now, we have established a notional monitoring network with more than 30 MAX-DOAS, which could provide sufficient validation for satellite products and conduct scientific researches. Combining these two methods, which could provide precise horizontal and vertical distribution of pollutant, we could get a 3-D distribution of pollutants and the transport flux. Here, we analyzed the spatial distribution and temporal trends of satellite-observed air pollutants over eastern China during 2005–2017. We found significant decreasing trends in NO2 and SO2 since 2011 over most regions. Furthermore, we used the generalized additive models to clarify the relative contribution of local emissions and meteorological conditions. Our results show that meteorological determines daily changes in pollutants, while long-term, inter annual changes are determined by emissions. Emission reduction has played a decisive role in the recent reduction of the pollution!

New MAX-DOAS retrieval method using WRF-Chem aerosol information for complex aerosol load condition

Qihua Li*, Cheng Liu, Chengzhi Xing, Ting Liu, Xiangguang Ji

*) Institutes of Physical Science and Information Technology, Anhui University, Heifei, 230601, China; lqh628@ahu.edu.cn

Presenter: Qihua Li

Abstract:

New MAX-DOAS retrieval method using WRF-Chem aerosol information for complex aerosol condition is presented. In many heavily polluted regions of the world, the aerosol loads can change very rapidly over a large range between clear days and heavily polluted days. The drastically changed aerosol load makes it difficult to give an appropriate a priori profile. The a priori profile has a significant impact on aerosol profile retrieval, thus should be a reasonable estimate of the true profile. WRF-Chem is the Weather Research and Forecasting (WRF) model coupled with Chemistry, can simulates aerosols for any MAX-DOAS site with the meteorology. WRF-Chem gives a coarse estimate of the true aerosol optical depth (AOD), and this AOD is used to generate the a priori profile. The retrieval is comprised of two steps, simulating AOD for MAX-DOAS instrument site via WRF-Chem method with The Global Forecast System GFS dataset and the aerosol retrieval with the a priori profile generated by simulated AOD. This method uses slant column densities retrieved by the QDOAS software. The aerosol retrieval uses constrained least square fitting with the Levenberg-Marquardt Method. VLIDORT is used for slant column density simulating and weighting function calculation. This method is applied to the retrieval of aerosol extinction profile with the spectra of the MAX-DOAS instrument located at the Chinese Academy of Meteorological Sciences (CAMS). The measured data from April 2018 to December 2018 is processed. The retrieved AOD is validated with the AERONET AOD at CAMS, and the retrieved surface extinction is validated with the surface PM2.5 concentration from the in site station in Guanyuan, Beijing. The total AOD ranges from 0.1 to 4.0 during the measurement. The result shows the improvement on the correlation between the MAX-DOAS results and the in site measurements on this complex aerosol load condition. This method is able to give quick and accurate retrieval result without the limitation of MAX-DOAS instrument location.

Investigation of nighttime vertical distribution of HONO based on IBBCEAS technique

Min Qin*, Fanhao Meng, Ke Tang, Jun Duan, Fang Wu, Pinhua Xie, Jianguo Liu, Wenqing Liu

*) Key Laboratory of Environmental Optics and Technology, Anhui Institute of Optics and Fine Mechanics, and Hefei Institutes of Physical Sciences, Chinese Academy of Science, Hefei 230031, China; mqin@aiofm.ac.cn

Presenter: Fanhao Meng

Abstract:

Nitrous acid (HONO), an important precursor of the hydroxyl radical (OH), plays an important role in tropospheric photochemistry. Despite the importance of HONO, the details of the formation processes of HONO in the atmosphere are debated for decades. The primary reaction surfaces for the nighttime HONO formation is still controversial, and the role of the aerosols in the heterogeneous production of HONO remains an open question. Here, we present the results of HONO and NO2 vertical profiles measured by the incoherent broadband cavity enhanced absorption spectroscopy (IBBCEAS). The primary sampling platform was the Beijing 325-m meteorological tower (BMT) [39°58'N, 116°23'E], equipped with an external container that was lifted on the side wiring of the tower. The IBBCEAS instrument was mounted in the movable container of the BMT for vertical measurements with a time resolution of IBBCEAS of 15s (vertical resolution of 2.4m for this work). Meanwhile, another IBBCEAS instrument was mounted in a temperature-stabilized container on the ground for simultaneous measurements. The vertical gradient of HONO was measured in combination with the two IBBCEAS instruments to investigate the source and sink of HONO at night. The different meteorological conditions were characterized throughout the measurement period, including clean episode and haze episode. Direct HONO emissions contributed an average of 29.3night. High resolution vertical profiles revealed (1) the ground surface dominated HONO production by heterogeneous conversion of NO2 during clean episodes, (2) the production of HONO on aerosol surface explained the HONO observations in the residual layer during E3, suggesting that the aerosol production was an important nighttime HONO source during haze episodes, (3) significant quantities of HONO were deposited to the ground surface at night. Acknowledgements. This work was supported by National Nature of Science Foundation of China (Grant Nos. 41875154, 41571130023, 91544104). Correspondence: Min Qin (mqin@aiofm.ac.cn)

Status of the Geostationary Environment Monitoring Spectrometer (GEMS) NO2 operational algorithm

Junsung Park*, Hyunkee Hong, Hanlim Lee

*) Pukyong National University; junsung2ek@gmail.com

Presenter: Junsung Park

Abstract:

We have developed the operational Nitrogen dioxide (NO2) retrieval algorithm for the Geostationary Environment Monitoring spectrometer (GEMS) which provides hourly radiance over Asia and West Pacific Ocean at wavelengths range from 300 to 500 nm with FWHM (Full Width Half Maximum) of 0.6. The GEMS operational NO2 algorithm consists of total NO2 column retrieval and tropospheric column estimation. First, the total NO2 column is retrieved based on Differential Optical Absorption Spectroscopy (DOAS) technique and Air Mass Factor (AMF) which is calculated using the linearized pseudo-spherical scalar and vector discrete ordinate radiative transfer code (VLIDORT, version 2.6) with inputs of Community Multiscale Air Quality (CMAQ) products are used. To produce total NO2 column density in real time, an AMF based on the Look-Up Table (LUT) is adopted. When total NO2 column density is obtained, the tropospheric NO2 column density is estimated using the Stratospheric and Tropospheric Separation (STS) method. The uncertainties of AMF and spectral fitting errors are calculated using synthetic radiance as a function of Aerosol Optical Depth (AOD), Single Scattering Albedo (SSA), Aerosol Peak Height (APH), measurement geometries and etc.,. APH is found to cause large uncertainties in both the NO2 SCD retrieval and AMF calculation. Given instrumental aspects, GEMS SNR and polarization effect cause the NO2 SCD retrieval errors up to 22% and 2%, respectively. We also discuss the IOT (In Orbit Test) results and the updates on our NO2 retrieval algorithm.

Sentinel-5p tropospheric NO2 data assessment using MAX-DOAS and direct sun measurements

Gaia Pinardi*, Steven Compernolle, Tijl Verhoelst, Michel Van Roozendael, François Hendrick, Henk Eskes, Ankie Piters, Alexander Cede, Martin Tiefengraber, Andreas Richter, Alkis Bais, Dimitris Karagkiozidis, Fani Gkertsi, Yugo Kanaya, Michel Grutter, Claudia Rivera, Sander Niemeijer, Panos Raptis, Stelios Kazadzis, Xiaoyi Zhao, Vitali Fioletov and the NIDFROVAL and PGN teams

*) BIRA-IASB; gaia.pinardi@aeronomie.be

Presenter: Gaia Pinardi

Abstract:

Owing to the multiple pointing geometries, the DOAS technique is sensitive to total, tropospheric and stratospheric NO2 content. MAX-DOAS measurements also allow to derive the surface concentration and, under favorable conditions, some information on the vertical distribution of NO2 in the first 4 kilometers above the surface. Such information is highly relevant for the validation of nadir UV-Vis sensors such as S5p/TROPOMI, that strongly rely on a-priori knowledge of the NO2 vertical distribution. Within the S5PVT NIDFORVAL project (S5P NItrogen Dioxide and FORmaldehyde VALidation using NDACC and complementary FTIR and UV-Vis DOAS ground-based remote sensing data) tropospheric NO2 data have been collected at about 20 MAX-DOAS stations. Pandora spectrometers measuring in direct sun mode are sensitive to the total NO2 columns. Data from about 20 stations coming from the Pandonia Global Network (PGN) are used in the MPC CalVal VDAF webserver (http://mpc-vdaf-server.tropomi.eu/no2) for the routine validation of S5p total NO2 columns. In this study, we investigate the consistency between the tropospheric NO2 validation results obtained using MAX-DOAS datasets and similar comparisons based on the direct sun PGN datasets. In the latter, the PGN tropospheric columns are derived by subtracting the S5p stratospheric content from the measured total columns. A special focus will be put on stations where both MAX-DOAS and direct sun measurements are performed, such as Cabauw, Athens, Xianghe, Yokosuka, Unam and the Toronto and Thessaloniki areas.

The "ideal spectrometer" for atmospheric observations

Ulrich Platt*, Thomas Wagner, Thomas Leisner

*) Heidelberg University; ulrich.platt@iup.uni-heidelberg.de

Presenter: Ulrich Platt

Abstract:

Spectroscopy of scattered-sunlight in the near UV to near IR spectral ranges has proven to be an extremely useful tool for the analysis of atmospheric trace gas distributions. A central parameter for the achievable sensitivity and spatial resolution of spectroscopic instruments is the light throughput (Étendue) of the instrument and the spectrometer, which is at the heart of the instrument. The Étendue of an instrument can be enhanced by (1) up-scaling the instrument dimensions or (2) by operating instruments in parallel. We present some new ideas and considerations how instruments for the spectroscopic determination of atmospheric gases could be optimized by using new possibilities in spectrometer design and manufacturing. Particular emphasis is on arrays of massively parallel instruments for observations using scattered-sunlight. We also discuss the optimal size of individual spectrometers in a spectrometer array. As example we discuss the design of a spectrometer system for use on a (low Earth orbit) satellite with sub-km ground pixel size.

Experiments on high-detailed mapping of tropospheric NO2 using GSA/Resurs-P observations: results, and validation with models and measurements

Oleg Postylyakov*, Alexander Borovski, Karim Shukurov, Alexandr Makarenkov, Marina Davydova, Yulia Muhartova

*) A.M. Obukhov Institute of Atmospheric Physics, Russian Academy of Science, Pyzhevsky per.3, Moscow, 119017, Russia; oleg.postylyakov@gmail.com

Presenter: Oleg Postylyakov

Abstract:

Experiments for the retrieval of the high-detailed spatial NO2 distribution in the troposphere using measurements of the GSA instrument onboard satellites of Resurs-P series were performed in 2016-2019. The authors developed an algorithm to obtain the tropospheric NO2 2D distribution with the horizontal spatial resolution reaching 2,4 km for the first time at the world level and provided on a grid with a step of 120 m. The high spatial resolution of the NO2 space measurements for the first time allowed the identification of local sources of NO2 pollution and their plumes. To validate the coarse structures in the obtained NO2 field we performed comparisons with OMI/Aura and TROPOMI/Sentinel-5P NO2 observations having the resolution of 13 km x 24 km and 7 km x 7 km. The comparison confirmed the reliability of the GSA NO2 fields in general. For the validation of fine structures detected in the NO2 fields of GSA/Resurs-P, we are developing methods based on comparisons with chemical transport models. The work was supported by Russian Foundation for Basic Research with grants 20-05-00826 and 18-29-10080.

Influence of horizontal inhomogeneity and noise on MAX-DOAS retrievals

Julia Remmers*, Steffen Beirle, Sebastian Donner, Thomas Wagner

*) Max Planck Institute for Chemistry, Mainz, Germany; julia.remmers@mpic.de

Presenter: Julia Remmers

Abstract:

MAX-DOAS measurements are widely used to retrieve vertical profiles of trace gases and aerosols. Usually a horizontal homogeneous distribution is assumed. We investigate the errors that are made due to this assumption on real and synthetic data. Furthermore a strategy is shown to retrieve noise levels from real measurements. This noise is then used on synthetic data to investigate the effects of noise on the retrievals. This study gives insight into the needed quality of real measurements for successful profile inversions in 1D and 3D.

Inhomogeneous scene effects in TROPOMI satellite data

Andreas Richter*, Andreas Hilboll, Abram Sanders, John P. Burrows

*) Institute of Environmental Physics, University of Bremen; richter@iup.physik.uni-bremen.de

Presenter: Andreas Richter

Abstract:

Ground-based DOAS observations usually rely on quartz fibres to achieve homogeneous filling of the instrument field of view. This is important as inhomogeneous filling of the spectrometer slit can lead to apparent spectral shifts, to apparent changes in instrument slit function and depending on the homogeneity of the detector response also to changes in linearity. Satellite instruments do not have fibres to homogenize the illumination of the slit, and in particular in the presence of clouds, the spectrometer slit is often illuminated unevenly.

During the QA4ECV project, analysis of OMI NO_2 data showed that scenes affected by inhomogeneous distribution of brightness not only have larger fitting residuals but also show systematic artefacts in the NO_2 slant columns. This effect was found in all available lv2 products albeit at different levels. A simple empirical correction was developed and could largely reduce the fitting RMS as well as the artefacts in the NO_2 slant columns.

In this presentation, IUP-UB TROPOMI retrievals for different absorbers (NO_2, BrO, HCHO, CHOCHO) are analysed for the effects of inhomogeneous scenes. Large signatures of scene inhomogeneity are found in fitting RMS for all absorbers and also clear artefacts in the products, but as in the case of OMI data, the magnitude of the effects depends on details of the analysis. The origins of the observed fitting problems are investigated and different approaches for compensation are evaluated, as well as the magnitude of problem remaining after correction.

Comparison between DOAS and FTIR in different configurations: HCHO and SO_2 case studies in Central Mexico

Claudia Rivera Cárdenas*, Wolfgang Stremme, Noemie Taquet, Martina M. Friedrich, Josué Arellano, Cesar Guarín, Alejandro Bezanilla, Diana Rivera, Cristina A. Mendoza Rodríguez, Michel Grutter

*) Centro de Ciencias de la Atmósfera, Universidad Nacional Autónoma de México, Mexico City, Mexico; claudia.rivera@atmosfera.unam.mx

Presenter: Claudia Rivera Cárdenas

Abstract:

We present data from two different Differential Optical Absorption Spectroscopy (DOAS) measurement configurations, direct sun (DS) and Multi AXis (MAX) DOAS, from two different monitoring sites in Mexico: at National Autonomous University of Mexico (UNAM) and at Altzomoni. We compare the products of these measurements, vertical column densities (VCDs) from the MAX-DOAS measurements and slant column density (SCDs) from the DS-DOAS, with data retrieved with the Direct Solar absorption Fourier Transform Infrared Spectroscopy (DS-FTIR) technique.

At the UNAM monitoring site (latitude 19.326, longitude -99.176, 2280 m a.s.l.), formaldehyde (HCHO) total column densities over the Mexico City Metropolitan Area (MCMA) were retrieved using the MAX-DOAS and DS-FTIR measurement technique. For the MAX-DOAS measurements, an Ocean Optics USB2000+ spectrometer was utilized and the software QDOAS was used to calculate differential Slant Column Densities (dSCDs) from the measured spectra, subsequently the Mexican MAX-DOAS Fit retrieval code (MMF) was used to convert from dSCDs to Vertical Column Densities using different types of datasets. For the DS-FTIR measurements, a spectrometer from Bruker Optics (model Vertex 80) that measures solar absorption spectra at different spectral regions with different detectors and band-pass filters placed on a rotating wheel, was used.

At the Altzomoni monitoring site (latitude 19.118, longitude -98.655, 3985 m a.s.l.), located 12 km north of the crater of the Popocatépetl volcano, both DS-FTIR and DS-DOAS measurement techniques were used to estimate the amount of sulfur dioxide (SO_2) molecules present in the volcanic plume. For this purpose, a solar tracker allows to track the sunlight and direct it towards a Bruker HR-125 spectrometer as well as towards an Ocean Optics S2000 spectrometer optimized for the ultraviolet-visible electromagnetic radiation range. From the measured spectra, SCDs of various atmospheric compounds were calculated. For the specific case of the Popocatépetl volcano plume, results of the temporal variability of the slant column density of SO_2 and the comparison between both measurement techniques are presented.

Discrete-Wavelength DOAS NO_2 slant column retrievals: feasibility and sensitivity analysis for a future instrument

Cristina Ruiz Villena*, Jasdeep S. Anand, Roland J. Leigh, Paul S. Monks, Claire E. Parfitt, David Spilling, Joshua D. Vande Hey

*) University of Leicester; crv2@leicester.ac.uk

Presenter: Cristina Ruiz Villena

Abstract:

The use of satellite NO_2 data for air quality studies is increasingly revealing the need for observations with higher spatial and temporal resolution. One way to achieve increased spatial resolution is to reduce the spectral information needed for the retrieval. Conventional satellite instruments measure continuous reflectance spectra at high spectral resolution and typically use a few hundred wavelengths to retrieve NO_2.

In this work we propose a variant of the Differential Optical Absorption Spectroscopy (DOAS) technique: Discrete- Wavelength DOAS (DW-DOAS), in which only 10 discrete spectral channels are used to retrieve NO2 slant column densities (SCDs). The feasibility of the technique is assessed using OMI and TROPOMI Level 1B data and validating the results against existing Level 2 datasets for these instruments (OMI: QA4ECV, TROPOMI: Operational), which use conventional DOAS algorithms. We find very good agreement between our algorithm and Level 2 data for both OMI (mean bias: < 5 %, uncertainty: 0.97×10^{15} molecules cm^{-2}) and TROPOMI (mean bias: < 11 %, uncertainty: 0.68×10^{15} molecules cm^{-2}).

The robustness of the technique is evaluated by means of a suite of sensitivity tests performed on synthetic data. The aim is to explore the effect of different phenomena such as noise or spectral shifts on the retrieval performance and find a suitable set of parameters for a potential future instrument. In this presentation we will give an overview of the DW-DOAS technique, outline the results of the feasibility and sensitivity tests, and discuss the implications for a potential application to a new instrument. The High-resolution Anthropogenic Pollution Imager (HAPI) instrument concept will be discussed as an option.

O3 and OH production in Australia studied using MAX-DOAS measurements

Robert Ryan*, Steve Rhodes, Matt Tully, Nicholas Jones, and Robyn Schofield

*) School of Earth Sciences, The University of Melbourne, Australia; rgryan92@gmail.com

Presenter: Robert Ryan

Abstract:

Tropospheric ozone plays a key role in oxidation chemistry through formation of OH radicals, as well as being a toxic pollutant and greenhouse gas. However, there are few observational constraints on tropospheric ozone and OH production mechanisms in the Australasian region. MAX-DOAS measurements can provide valuable information to inform our understanding of oxidation chemistry through measurements of NO2 and volatile organic compounds (VOCs, such as HCHO and glyoxal) which combine to form tropospheric ozone and HONO and HCHO which produce OH radicals. In this study we present a 2.5 year dataset of MAX- DOAS measurements of NO2, HONO, HCHO and glyoxal from Melbourne, Australia, which alongside meteorological measurements provide a detailed insight into key oxidation chemistry mechanisms. HONO photolysis is found to be the dominant source of OH radicals in all seasons in Melbourne, contributing on average between 45-70 % of OH production. We find photolysis of HCHO, which appears to be primarily derived from biogenic VOC emissions in rural Victoria, to be on par with ozone photolysis as an OH source here. We use the ratio of HCHO to NO2 to explore ozone production mechanisms; the ratio is predominantly less than one indicating VOC limited conditions. However, during high temperature episodes, formaldehyde and ozone levels are found to be high and during these high ozone episodes the production regime switches to NOx limited. These results highlight the importance of NOx reduction strategies to curb ozone pollution episodes, especially in a warming world.

Operational ship emission monitoring using Long Path Differential Optical Absorption Spectroscopy

Stefan Schmitt*, Denis Pöhler, Andreas Weigelt, Barbara Mathieu-Üffing, Lisa Kattner, André Seyler, Kai Krause, Folkard Wittrock, Johannes Lampel, Ulrich Platt

*) Airyx GmbH, Eppelheim, Germany; Stefan.Schmitt@airyx.de

Presenter: Stefan Schmitt

Abstract:

The well established active Long Path (LP)-DOAS method is applied in several scientific problems and also commercial systems for urban air pollution and stack emissions exist. However, due to the complex instrumental setup, the usually large footprint, the required infra-structure and operation man-power, the field of application for LP-DOAS instruments was limited. For example the direct monitoring of ship emissions was only possible with scientific instruments with large experimental setups.

We present a new commercial LP-DOAS prototype which fulfills the criteria required for easy set up and operation and is suitable for long light paths and fast measurements. With its high luminosity broad-band long-lifetime light source, compact sealed housing, autonomous alignment and data acquisition the new instrument extents the field of applications to long term operational monitoring tasks as well as short period campaigns. The recent system will be presented.

Currently, one of the main application is monitoring ship emissions of NO_2 and SO_2, which we conducted at the river Elbe close to Hamburg harbor, Germany, within a first 6-week measurement campaign in summer 2016. A prototype of the new LP-DOAS instrument was set up side by side to an MeSMarT in situ station with its measurement path crossing the highly frequented river (2.87km, one way). Emission signatures of a total of 5037 ship passes (of 1044 individual ships) were monitored while SO_2 and NO_2 detection limits of 80 pptv and 450 pptv, respectively, at time resolution of a few seconds were achieved. In comparison to the in situ station, which relies on meteorologic transport of the emission plume, the LP-DOAS technique has the advantage of measuring emissions in close proximity to the emission source and, thus, in a state of low plume dilution. While the in situ method detected 16% of the ships, the LP-DOAS was able to assign emission plumes to 41% of all passing ships primary limited by high traffic density and, thus, the difficulty to unambiguously assign recorded plumes to particular vessels, rather than to the sensitivity to the emission strength. The results of this study will be presented.

Further we aim to develop an instrumental extension for the additional measurement of NO and CO_2 which enables the direct measurement of NO_x and SO_2 emission factors of ships. A concept will be presented.

Biogenic and fire-sourced formaldehyde above various Arctic biomes in Alaska

William R. Simpson*, Jingqiu Mao, Tianlang Zhao

*) University of Alaska Fairbanks; wrsimpson@alaska.edu

Presenter: William Simpson

Abstract:

Formaldehyde, HCHO, is an atmospheric intermediate chemical produced by both fires and photochemical reactions of biological volatile organic compounds (BVOC), and thus is an important indicator of BVOC production and chemistry that is coupled to ozone and secondary organic aerosol formation. In this study, we present observations of HCHO via multiple axis differential optical absorption spectroscopy (MAX-DOAS) at two locations in Alaska in different years with different wildfire behavior. The summer of 2018 had much less wildfire than 2019, so the comparison allows identification of fire effects. Observations above Boreal forest ecosystems near Fairbanks, Alaska show HCHO increases nearly exponentially with increasing temperature during the summer and levels are low outside of the summertime biologically active period. We examine a three-year period at this Boreal forest site and find a large degree of interannual variability. In the summer of 2019, we deployed a second instrument to measure HCHO above Arctic tundra ecosystems at Toolik Field Station on the North Slope of Alaska. HCHO above the tundra is also observed to be a strong function of temperature, but levels of HCHO are lower at the tundra location than at the Boreal forest location. We compare the MAX- DOAS observations to Tropomi observations for 2018 and 2019.

Mini-DOAS observations of biomass burning plumes during FIREX-AQ

Jochen Stutz*, Katie Tuite, Nathaniel Brockway

*) Department of Atmospheric and Oceanic Sciences, University of California Los Angeles; jochen@atmos.ucla.edu

Presenter: Jochen Stutz

Abstract:

The UCLA mini-DOAS instrument performed remote sensing measurements of HCHO, HONO, NO_2, SO_2, and aerosol proxies in and above biomass burning plumes during the FIREX-AQ field experiment onboard NASA's DC8 aircraft. The mini-DOAS scanners/telescopes were pointed at different elevations angles, depending on the flight conditions of the DC8. During plume overpasses the mini-DOAS measured in the nadir, while it pointed in the limb or zenith during plume transects. The collected spectra were analyzed using the DOAS technique with out-of-plume solar reference spectra to retrieve differential slant column densities (DSCDs) of the various trace gases. The goal of our FIREX-AQ observations is to study HONO emissions from forest fires as well as secondary HONO chemistry in the plume.

Here we will present examples of the FIREX-AQ observations and discuss the unique conditions encountered when observing biomass burning plumes using the DOAS technique. We will discuss examples of interpretation strategies to derive emission factors and to study plume chemistry. We will compare preliminary HONO, NO_2, and HCHO emission factors from fires in the Western United States to available literature values.

The information content of skylight polarisation in MAX-DOAS trace gas- and aerosol profiling applications

Jan-Lukas Tirpitz*, Udo Frieß, Ulrich Platt

*) Institute of Evironmental Physics, University of Heidelberg; jan-lukas.tirpitz@iup.uni-heidelberg.de

Presenter: Jan-Lukas Tirpitz

Abstract:

Multi-AXis Differential Optical Absorption Spectroscopy (MAX-DOAS) is a well-established ground-based measurement technique for the detection of atmospheric aerosol and trace gases: ultra-violet and visible radiation spectra of skylight are analyzed to obtain information on different atmospheric parameters. An appropriate set of spectra recorded under different viewing geometries ("Multi-Axis") allows retrieval of aerosol and trace gas vertical distributions by applying numerical inversion methods. Currently one of the method's major limitations is the limited information content in the measurements that reduces the sensitivity particularly at higher altitudes. It is well known but not yet used in MAX-DOAS profile retrievals that measuring skylight of different polarisation directions provides additional information: the degree of polarisation for instance strongly depends on the atmospheric aerosol content and the aerosol properties and – since the light path differs for light of different polarisation – the set of geometries available for the inversion is extended. We present a novel polarization-sensitive MAX-DOAS instrument and a corresponding inversion algorithm, capable of using polarization information. Further, in contrast to existing MAX-DOAS algorithms consisting of separate aerosol and trace gas retrieval modules, our novel inversion scheme simultaneously retrieves aerosol and trace gas profiles of several species in a single step. The improvement over "unpolarised" MAX-DOAS approaches will be discussed, based on both, synthetic data and real measurements.

TROPOMI NO_2 slant column retrieval: method, stability, uncertainties and comparisons with OMI

Jos van Geffen*, Folkert Boersma, Henk Eskes, Maarten Sneep, Mark ter Linden, Marina Zara, Pepijn Veefkind

*) Royal Netherlands Meteorological Institute (KNMI), De Bilt, The Netherlands;
jos.van.geffen@knmi.nl

Presenter: Jos van Geffen

Abstract:

The Tropospheric Monitoring Instrument (TROPOMI), aboard the Sentinel-5 Precursor (S5P) satellite provides measurements of atmospheric trace gases and of cloud and aerosol properties. The retrieval of nitrogen dioxide (NO_2) concentrations is a three-step procedure: slant column density (SCD) retrieval, separation of the SCD in its stratospheric and tropospheric components, and conversion of these into vertical column densities. This presentation focusses on the TROPOMI NO_2 SCD retrieval: the DOAS retrieval method used, the stability of the SCDs and the SCD uncertainties, as well as a comparison with the Ozone Monitoring Instrument (OMI) OMI NO_2 SCDs.

The statistical uncertainty, based on the spatial variability of the SCDs over a remote Pacific Ocean sector is very stable over time and some 30% less than the long-term average over OMI/QA4ECV data (since the pixel size reduction on 6 Aug. 2019 TROPOMI uncertainties are $\sim 8\%$ larger). The SCD uncertainty reported by the DOAS fit is about 10% larger than the statistical uncertainty, while for OMI/QA4ECV the DOAS uncertainty is some 20% larger than its statistical uncertainty. Comparison of the SCDs themselves over the Pacific Ocean, averaged over one month, shows that TROPOMI is about 5% higher than OMI/QA4ECV, which seems to be due mainly to the use of the so-called intensity offset correction in OMI/QA4ECV but not in TROPOMI. The row-to-row variation in the SCDs of TROPOMI is af factor of ~ 2 (~ 5) larger than OMI in 2005 (2018); still, a so- called stripe correction of this non-physical across-track variation is useful for TROPOMI data.

In short, TROPOMI shows a superior performance compared with OMI/QA4ECV and operates as anticipated from instrument specifications.

Accurate tropospheric NO2 column retrieval based on combined direct-sun and zenith-sky twilight visible measurements

Michel Van Roozendael*, François Hendrick, Martina Friedrich, Ermioni Dimitropoulou, Caroline Fayt, Christian Hermans, Gaia Pinardi, Tijl Verhoelst, Ting Wang, Pucai Wang

*) Royal Belgian Institute for Space Aeronomy; michelv@aeronomie.be

Presenter: Michel Van Roozendael

Abstract:

Ground-based UV-visible measurements using the Differential Optical Absorption Spectroscopy (DOAS) are well suited for the monitoring of nitrogen dioxide (NO2) in the atmosphere. Current observation systems deployed in networks exploit the zenith-sky twilight geometry to retrieve stratospheric NO2 columns (e.g. the SAOZ network), the direct-sun geometry to retrieve the total column (e.g. the Pandonia/PGN network) and the Multi-Axis DOAS (MAX-DOAS) geometry to retrieve tropospheric columns and surface concentrations (e.g. the FRM4DOAS/NDACC network). For the validation of space nadir sensors such as Sentinel-5P/TROPOMI, the primary product of interest is the tropospheric column. In this work, we investigate how direct-sun total column measurements and zenith-sky twilight measurements performed with the same instrument can be combined to retrieve highly accurate tropospheric columns. We show that properly accounting for the diurnal cycle of the stratospheric NO2, the accuracy of the retrieved residual tropospheric columns is better than 10 percent under moderately polluted conditions, such as encountered during the CINDI-2 intercomparison campaign. We then compare the results of three different retrieval approaches using measurements from the CINDI-2 campaign: a) the proposed approach, b) MAX-DOAS tropospheric column retrievals, c) tropospheric column retrievals using the temperature dependence of the NO2 cross-section. Using measurements in Xianghe (China), we also discuss the case of highly polluted sites where twilight zenith-sky observations can be significantly contaminated by the tropospheric pollution.

Expanding CU SOF data products for evaluating the impacts of biomass burning emissions during the 2018 Pacific Northwest wildfire season: emission fluxes and enhancement ratios of CO, NH3, C2H4, C2H6, HCN, HCHO, HCOOH, CH3OH and PAN

Natalie Kille*, Kyle J Zarzana, David Thomson, Christopher Lee, Teresa L. Campos, Larry D. Oolman, David M. Plummer, Eric C. Apel, Ilana B. Pollack, Jacob Lindaas, Emily V. Fischer, Wade Permar, Lu Hu, Frank Flocke, Rebecca Hornbrook, Alan Hills, Amy Sullivan, Rainer Volkamer

*) University of Colorado Boulder; natalie.kille@colorado.edu

Presenter: Rainer Volkamer

Abstract:

Column measurements of absorption along the direct solar beam present an underutilized, yet powerful, approach to quantify trace gas emissions from distributed sources such as wildfires. Measurements of vertical column densities (VCDs), unlike in situ measurement, are independent of boundary layer height, do not require inlets, and average over inhomogeneities present in the column, providing a unique perspective unachievable using in situ sensors alone. Furthermore, a single instrument can accurately measure both quantitative emission mass fluxes on the scale of a wildfire, and enhancement ratios of multiple chemically-important trace gases. Enhancement ratios provide a means to compare the VCD and in situ measurement approaches – two measurement techniques that sample on different spatial scales – and to assess calibrations and plume inhomogeneities. In this work we present measurements using the University of Colorado Solar Occultation Flux (CU SOF) instrument and measurement technique to quantify VCDs, emission fluxes and enhancement ratios of infrared absorbing trace gases from wildfires including but not limited to CO, NH3, C2H4, C2H6, HCN, HCHO, HCOOH, CH3OH and PAN. We present the airborne SOF measurements and quantify emission fluxes from a variety of fuel types, locations, and fire intensities, measured during the July-September 2018 Pacific Northwest wildfire season within the context of the BB-Flux project. We also present coordinated SOF measurements with an in situ payload within the context of the WE-CAN project; enhancement ratios are used for intercomparison and validation of the SOF and in situ techniques. The presented SOF technique, with its diversity of chemically-important trace gases emitted from wildfires, provides detail to evaluate plume chemistry and emission fluxes, ultimately providing crucial constraints for the interpretation of atmospheric models trying to better understand wildfire impacts.

Mini ozone holes due to dust release of iodine in the remote tropical free troposphere

Rainer Volkamer*, Theodore Koenig, Sunil Baidar, Barbara Dix, James F. Bresch, Edwin W. Eloranta, Bruce Morley, Scott Spuler, Samuel R. Hall, Kirk Ullmann, Ru-Shan Gao, J. Michael Reeves, Alfonso Saiz-Lopez, Carlos Cuevas, Rafael Fernandez

*) Dept Chemistry & CIRES, University of Colorado at Boulder, USA; rainer.volkamer@colorado.edu

Presenter: Rainer Volkamer

Abstract:

Significant enhancements of iodine have been observed in Sahara dust events in form of methyl iodide (CH_3I) and iodine monoxide (IO) radicals, but atmospheric models currently do not consider dust as a source of iodine. Dust plumes are often accompanied by significant ozone loss, which is commonly attributed to reactive uptake of O_3 and other odd oxygen species (i.e., N_2O_5, HNO_3) on dust surfaces. However, laboratory experiments struggle to reproduce the large reactive uptake coefficients needed to explain field observations, and do not consider iodine chemistry. We present first observations of "mini ozone holes" in the remote (Southern Hemisphere) tropical free troposphere west of South America (TORERO field campaign), and show IO is elevated in otherwise unpolluted (low NO_x) dust layers that originate from the Atacama and Sechura Deserts. Ozone concentrations inside these elevated dust layers are often 10-20 ppb, and as low as 3 ppb. Ozone depletion is found to be widespread, i.e., dust layers extend thousands of km along the coast, up to 6 km altitude, and 500 km over the open ocean. IO radical concentrations inside decoupled dust layers are higher than in the marine boundary layer, and exceed nearby free tropospheric IO background concentrations by as much as a factor 6, indicating vigorous gas-phase ozone destruction by iodine chemistry inside the dust layers. We use field measurements of IO and BrO radicals, CH_3I, NO_2, photolysis frequencies, aerosol size distributions, and high-spectral resolution lidar aboard the NSF/NCAR Gulfstream 5 aircraft, in conjunction with cloud resolving back trajectories and chemical model simulations to estimate the iodine source from dust, and investigate the mechanisms responsible for the "mini ozone holes". The implications for surface air quality, oxidative capacity, and climate are briefly discussed.

Quantitative comparison of measured and simulated O4 absorption for one day with extremely low aerosol load over the tropical Atlantic

Thomas Wagner*, Steffen Dörner, Sebastian Donner, Steffen Beirle, Stefan Kinne

*) MPI for Chemistry, Mainz, Germany; thomas.wagner@mpic.de

Presenter: Thomas Wagner

Abstract:

Measurements of the atmospheric absorption of the oxygen dimer O4 are often used to characterize the atmospheric light paths, e.g. to derive properties of clouds and aerosols. Some recent studies indicated discrepancies between measurements and simulations of the atmospheric O4 absorption, while others found exact quantitative agreement. One difficulty in these studies was to correctly represent the aerosol properties in the radiative transfer simulations. In this study we investigate MAX-DOAS measurements of the atmospheric O4 absorption during a ship cruise in April and May 2019 over the tropical Atlantic. The elevation angle of the instruments telescope is automatically stabilized in order to compensate the motion of the sea. We select measurements on one day with extremely low aerosol optical depth (between about 0.03 and 0.05 at 360 nm). For such conditions the atmospheric scattering processes are dominated by Rayleigh scattering on air molecules. Besides the MAX-DOAS measurements, also measurements by a ceilometer and sun photometer are available, which are used to constrain the atmospheric aerosol properties. The radiative transfer simulations are carried out with the full spherical radiative transfer model MCARTIM. We find that the measured O4 absorptions overestimate the simulated O4 absorptions by 10 to 15%.

Shipborne MAX-DOAS measurements for validation of TROPOMI NO2 products

Ping Wang*, Ankie Piters, Jos van Geffen, Olaf Tuinder, Piet Stammes, Stefan Kinne

*) Royal Netherlands Meteorological Institute (KNMI), De Bilt, The Netherlands; ping.wang@knmi.nl

Presenter: Ping Wang

Abstract:

Tropospheric NO_2 and stratospheric NO_2 vertical column densities are important TROPOMI data products. In order to validate the TROPOMI NO_2 products, KNMI MAX-DOAS instruments have measured NO_2 on ship cruises over the Atlantic and the Pacific oceans. The MAX-DOAS instruments have participated in five cruises on-board RV Sonne (in 2017 and 2019) and RV Maria S. Merian (in 2018). The MAX-DOAS measurements were acquired in 7 months and spanned about 300° in longitude and 90° in latitude. During the cruises there were also aerosol measurements from Microtops sun-photometers. The MAX-DOAS measured stratospheric NO_2 columns between 1.5×10^{15} and 3.5×10^{15} molec. cm^{-2}, and tropospheric NO_2 up to 0.6×10^{15} molec. cm^{-2}. The MAX-DOAS stratospheric NO_2 vertical column densities have been compared with TROPOMI stratospheric NO_2 vertical column densities and the stratospheric NO_2 vertical column densities simulated by TM5-MP model. Good correlation is found between the MAX-DOAS and TROPOMI and TM5 stratospheric NO_2 vertical column densities, with a correlation coefficient of 0.93 or larger. The TROPOMI and TM5 stratospheric NO_2 vertical column densities are about 0.4×10^{15} molec. cm^{-2} (19%) higher than the MAX-DOAS measurements. The TROPOMI tropospheric NO_2 has also good agreement with the MAX-DOAS measurements. The tropospheric NO_2 vertical column density is as low as 0.5×10^{15} molec. cm^{-2} over remote oceans.

A global perspective on bromine monoxide composition in volcanic plumes derived from S5-P/TROPOMI

Simon Warnach*, et al.

*) Max-Planck-Institut für Chemie, Mainz, Germany; s.warnach@mpic.de

Presenter: Simon Warnach

Abstract:

Bromine monoxide (BrO) is a halogen radical altering the atmospheric ozone chemistry, e.g. in polar regions, the stratosphere as well as volcanic plumes. In particular, the molar bromine to sulphur ratio in volcanic gas emissions is characteristic to the magmatic composition of a volcano. The high spatial resolution of S5-P/TROPOMI (up to 3.5x5.5km^2) and daily coverage offer the potential to detect BrO even during minor eruptions and determine BrO/SO_2 ratios during continuous passive degassing. Here, we present a global overview of BrO/SO_2 molar ratios in volcanic plumes derived from a systematic investigation of two years (2018 and 2019) of TROPOMI data. We retrieved BrO column densities as well as SO_2 column densities using Differential Optical Absorption Spectroscopy (DOAS) and calculated mean BrO/SO2 molar ratios for each volcano. The calculated BrO/SO_2 molar ratios differ strongly between different volcanoes ranging between several 10^{-5} and 10^{-4}. The data are classified and discussed with regard to several volcanic parameters – more specific the volcanic region, volcano type (i.e. subduction zone, hotspot etc.) as well as activity level.

DOAS measurements of NO2 and HCHO pollution in Kinshasa

Rodriguez Yombo Phaka*, Alexis Merlaud, Gaia Pinardi, Caroline Fayt, Martina Friedrich, François Hendrick, Lars Jacob, Michel Van Roozendael, Emmanuel Mahieu, Richard Bopili Mbotia Lepiba, Jean-Pierre Mbungu

*) University of Liège, Liège, and University of Kinshasa; rodriguez.yombophaka@student.uliege.be

Presenter: Rodriguez Yombo Phaka

Abstract:

Recent studies show that air pollution also affects by Africa. Air quality is worsening in large cities with growing populations. Satellite observations over some Central African cities seem to confirm this pollution for species such as NO2, HCHO and aerosols. The sources of pollution are generally different from those found in Europe for example. In Central Africa, particularly in the Congo Basin, the main sources of NO2 and HCHO emissions are forest fires and the use of embers in cooking. Kinshasa, the capital of the Democratic Republic of Congo, a large megalopolis of about 11 million inhabitants, like several other large cities in Africa, lack ground-based atmospheric measurement systems. To improve this situation, the researchers of the University of Kinshasa (Unikin) in collaboration with the UV-Vis group of the Belgian Institute for Space Aeronomy (IASB) have set up a first installation of a simple atmospheric observation equipment. This equipment was installed on the roof of the Faculty of Sciences of Unikin (-4.42°S, 15.31°E) in May 2017 and has operated until November 2019. The instrument is based on a compact AVANTES spectrometer covering the spectral range 290 - 450 nm with 0.7 nm resolution. The spectrometer is a Czerny-Turner type with an entry slit of 50 μm wide, and an array of 1200 l/mm. A 10 m long and 600 μm thick diameter optical fiber is connected to the spectrometer to receive the incident light beam from the sky. Measurements were mainly made by looking in a fixed direction. In November 2019, a Multi-Axis DOAS instrument (MAX-DOAS) has been installed to replace the first instrument. The measurements clearly show the signature of polluting species such as NO2 and HCHO in Kinshasa's atmosphere. In this study, we therefore show all the different steps of the algorithm we used to obtain the vertical columns from the observations of the instrument installed in Kinshasa. We present a first comparison of these ground-based observations of NO2 in Kinshasa with those from the OMI and TROPOMI satellites for clear days between May and November 2017.

Impact of 3D cloud structures on tropospheric NO2 column measurements from UV-VIS sounders

Huan Yu*, Arve Kylling, Claudia Emde, Bernhard Mayer, Michel Van Roozendael, Kerstin Stebel, Ben Veihelmann

*) Royal Belgian Institute for Space Aeronomy; huan.yu@aeronomie.be

Presenter: Huan Yu

Abstract:

Operational retrievals of tropospheric trace gases from space-borne spectrometers are made using 1D radiative transfer models. To minimize cloud effects generally only partially cloudy pixels are analysed using simplified cloud contamination treatments based on radiometric cloud fraction estimates and photon path length corrections based on oxygen collision pair (O2-O2) or O2A-absorption band measurements. In reality, however, the impact of clouds can be much more complex, involving scattering of clouds in neighbouring pixels and cloud shadow effects. Therefore, to go one step further, other correction methods may be envisaged that use sub-pixel cloud information from co-located imagers. Such methods require an understanding of the impact of clouds on the real 3D radiative transfer. We quantify this impact using the MYSTIC 3D radiative transfer model. The generation of realistic 3D input cloud fields, needed by MYSTIC (or any other 3D radiative transfer model), is non-trivial. We use cloud data generated by the ICOsahedral Non-hydrostatic (ICON) atmosphere model for a region including Germany, the Netherlands and parts of other surrounding countries. The model simulates realistic liquid and ice clouds with a horizontal spatial resolution of 156 m and it has been validated against ground-based and satellite-based observational data. As a trace gas example, we study NO2, a key tropospheric trace gas measured by the atmospheric Sentinels. The MYSTIC 3D model simulates visible spectra, which are ingested in standard DOAS retrieval algorithms to retrieve the NO2 column amount. Spectra are simulated for a number of realistic cloud scenarios, snow free surface albedos, and solar and satellite geometries typical of low-earth and geostationary orbits. The retrieved NO2 vertical column densities (VCD) are compared with the true values to identify conditions where 3D cloud effects lead to significant biases on the NO2 VCDs. A variety of possible mitigation strategies for such pixels are then explored.

Remote sensing of radical precursors in wildfires plumes: Synergies between aircraft and satellites

Kyle J Zarzana*, Kyle J. Zarzana, Natalie Kille, Theodore K. Koenig, Christopher F. Lee, Nicolas Theys, Christophe Lerot, Isabelle De Smedt, Michel Van Roozendael, Christoph Knote, Johana Romero, Ben Howard, David Thomson, Larry Oolman, David Plummer, Rainer Volkamer

*) University of Colorado Boulder; kyle.zarzana@colorado.edu

Presenter: Kyle Zarzana

Abstract:

Biomass burning plumes are thick, complex mixtures of gases and particles that vary rapidly in space and time. Detailed chemical measurements can be made by flying instrumented research aircraft through these plumes, but due to hazardous conditions near the fire, these flights typically must be conducted several tens of kilometers downwind, and thus may not observe short-lived radical species. Satellite-borne instruments are not bound by these limitations and can make measurements directly over the fire source. While satellites provide snapshots in time of plume spatial distributions, aircraft can be deployed to capture changes in the temporal evolution of emissions. For optically thick plumes satellites primarily probe the top of the smoke, and may miss chemistry in the regions of the plume where smoke is the thickest. The 2018 BB-FLUX campaign (Biomass Burning Fluxes of Trace Gases and Aerosols) was conducted during the summer of 2018 in the Western United States, and provides a unique dataset for examining the synergy between aircraft and satellite measurements. A suite of upward pointing remote sensing instruments, including several spectrometers measuring scattered light in the ultraviolet (330-375 nm) and visible (425-490 nm) and a Fourier transform infrared spectrometer (700-5000 cm-1) measuring along the direct solar beam, were deployed on a research aircraft that performed over 100 plume underpasses, measuring columns of species such as CO, HONO, HCHO, and NO2. Several species were simultaneously measured in both the direct sun and zenith sky geometry, enabling measurements of air mass factors for optically thick plumes. Many of the species measured from the plane can also be measured from space by the TROPOspheric Monitoring Instrument (TROPOMI) instrument on the Sentinel-5 Precursor satellite, often using similar or identical retrieval settings as those used on the plane. Several flights were coordinated with satellite overpasses to provide near simultaneous measurements from the plane and from space. The combination of satellite measurements over a large spatial scale with localized aircraft measurements over several hours provides a unique dataset for examining satellite retrievals, plume chemistry, and budgets of radical precursors such as HONO and HCHO.