

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

Version date: 10 July 2020

Poster are listed below, sorted alphabetically on the last name of the presenter.

Poster pitches of 1 minute with 1 slide are organised as follows (times are in UTC; see also the main programme):

Day 1: Monday 13 July 2020

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14:00 - 14:06 Poster pitches (5 × 1 min.) numbers: 5, 6, 14, 22, 23

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Day 2: Tuesday 14 July 2020

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11:40 - 11:47 Poster pitches (6 × 1 min.) numbers: 30, 34, 35, 44, 46, 48

14:00 - 14:07 Poster pitches (6 × 1 min.) numbers: 2, 17, 21, 41, 16, 59

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Abstracts of poster presentations

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The Mainz Profile Algorithm MAPA

Steffen Beirle*, Steffen Dörner and Thomas Wagner

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Presenter: Steffen Beirle

Abstract:

The MAInz Profile Algorithm (MAPA) derives vertical profiles of aerosol extinction and trace gas concentration from MAX-DOAS measurements. Within MAPA, vertical profiles are parameterized by (1) the integrated column, i.e. AOD (aerosols) or VCD (trace gases), (2) the layer height, and (3) a parameter determining the profile shape. As forward model, a look-up-table is used (calculated with the radiative transfer model McArtim) relating these parameters to corresponding DSCDs for different observation geometries. Best matching parameters and the corresponding profiles are determined by a Monte Carlo approach. MAPA v0.98 is described in detail in Beirle et al., AMT, 2019. Here we present the current MAPA version and discuss recent and future extensions and improvements.

Aircraft-based 2- and 3D trace gas measurements with HAIDI (Heidelberg Airborne Imaging DOAS Instrument) – Results of the EMeRGe missions

Katja Bigge*, Udo Frieß, Denis Pöhler, Ulrich Platt

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Presenter: Katja Bigge

Abstract:

Today, the majority of humanity lives in urban areas. Accordingly, these are a significant source of a multitude of atmospheric emissions from human activity such as traffic to heating, industry or power generation. Pollutants directly impact the local inhabitants' health, but are also transported to neighbouring areas, undergo chemical evolution and can have an impact on climate. To understand and assess effective measures for reducing the effects, it is important to determine the source locations and strengths as well as relevant chemical processes.

Aircraft-based measurements can cover the gap between long-term ground-based and globe-covering satellite instruments with its high temporal and spatial coverage during flight time. Remote sensing methods in particular allow a fast and wide-spread probing of atmospheric trace gas distributions. Within this context, the HAIDI (Heidelberg Airborne Imaging DOAS Instrument) instrument has been designed to provide trace gas distributions of extremely high temporal and spatial resolution (40 m x 40 m at 1.5 km flight altitude, 266 m x 266 m at 10 km flight altitude, at 10 ms temporal resolution) in 2D and 3D during overflight.

We present results of HAIDI measurements during the EMeRGe (Effect of Megacities on the Transport and transformation of Pollutants on the Regional to Global Scales) missions, where the instrument was part of the comprehensive set of measurement equipment installed on the research airplane HALO (High Altitude and Long range re-search aircraft) of the DLR (German Aerospace Center). The EMeRGe missions targeted the emission outflows of megacities to investigate their compositions and the atmospheric impact of urban pollution. One mission part was conducted in Europe (July 2017) and aimed at areas around Paris, London, the Po area, Madrid and the Benelux area. The second mission part was based in Taiwan (March 2018) and investigated Taiwan cities, Bangkok, Manila, Japanese cities and the outflow of pollutants from mainland China.

HAIDI has derived a number of trace gases such as NO₂, SO₂ and HCHO. It was possible to obtain high-resolution 2D data of NO₂ and SO₂ from megacity areas and plumes of megacities, power plants and ships, and to estimate their emission rates. The instrument setup also allows the retrieval of 3D concentrations using inverse modelling based on 3D radiative transfer calculations.

NO₂ profiling using Pandora instruments in Toronto, Canada

Kristof Bognar*, Xiaoyi Zhao, Ramina Alwarda, Steffen Beirle, Vitali Fioletov, Udo Frieß, Kimberly Strong

*) Department of Physics, University of Toronto, Toronto, ON, Canada; kbognar@physics.utoronto.ca

Presenter: Kristof Bognar

Abstract:

Pandora instruments form a global network of UV-Visible spectrometers focused on providing consistent long-term measurements of atmospheric composition. Total column data of NO₂ and other trace gases are valuable for satellite validation, while the instruments also perform elevation scans that might be used to investigate local air pollution. The most useful data for air quality studies are surface concentrations and vertical profiles, quantities not readily available from Pandora measurements. Here we use Environment and Climate Change Canada's network of Pandora instruments in the Greater Toronto Area (GTA) to retrieve vertical profiles of aerosols and NO₂. We process the Pandora elevation scans as MAX-DOAS data, and retrieve profiles using a parametric and an optimal estimation algorithm. Collocated instruments show very good agreement when azimuth viewing angles are similar, and comparisons to in situ measurements of NO₂ indicate that even short scans (4 elevation angles) provide useful data. Profile retrievals are performed on the entire time series of several instruments, in order to build a dataset to study the distribution and variability of NO₂ in the GTA.

Comparison of measured and simulated NO₂ and HCHO integral content in the atmospheric boundary layer in Moscow region

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Presenter: Alexander Borovski

Abstract:

Moscow megacity is among the world's 20 largest megacities. Intensive air emissions of pollutants affect the air quality of the regional atmosphere. To obtain diagnostic and predictive assessments of this impact intensive measurements of air pollutants as well as chemical transport simulations are developed. Important task continue to be agreement of parameters used in chemical transport models (CTMs) with experimental results.

We present preliminary results of the comparison of the measured by DOAS technique and simulated by SILAM and COSMO-Ru7-Art NO₂ and HCHO integral contents (IC) in the atmospheric boundary layer (ABL) at Zvenigorod Scientific Station (ZSS) located in 38 km west from Moscow. The comparison covers January and July of 2014 when background and polluted by Moscow air mass observed at ZSS.

The measured NO₂ IC in the ABL observed at ZSS does not exceed 0.5×10^{16} molec cm⁻² in background conditions of the atmosphere when non-east wind direction dominated. It grows up to 5.4×10^{16} molec cm⁻² when polluted air masses come from Moscow megacity. Simulated NO₂ IC has similar behavior. As a whole, a good agreement between measured and simulated datasets is observed. Some underestimation of the NO₂ emission presents for sources located to the south, south-east and south-west from ZSS and overestimation ones for sources located to the north, north-east and north-west from ZSS.

The measured HCHO IC in the ABL does not exceeds 6×10^{16} molec cm⁻² in background conditions and shows significant temperature trend. Statistically significant difference is observed between data obtained during east and west wind directions. This effect points to Moscow megacity influence on the air quality at the regional atmosphere. Simulated HCHO IC using both CTMs is much less that measured one, but simulations reproduce the main patterns of measured HCHO IC variations.

This study was supported by Russian Science Foundation grant number 16-17-10275.

The FDR4ATMOS project and its use for the DOAS community

Tim Bösch*, Stefan Noël, Klaus Bramstedt, Tina Hilbig, Andreas Richter, Heinrich Bovensmann, Günter Lichtenberg, Melanie Coldewey-Egbers, Mourad Hamidouche, John P. Burrows

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Presenter: Tim Bösch

Abstract:

The aim of the ESA funded FDR4ATMOS (Fundamental Data Records in the domain of satellite Atmospheric Composition) project is the creation and validation of Fundamental Data Records (FDR) of GOME and SCIAMACHY Level 1 radiances and irradiances. An FDR consists of a continuous, harmonized record of calibrated, geolocated, uncertainty-quantified sensor observations in geophysical units, together with all ancillary and underlying data used to calibrate the observations and estimate uncertainty. It can be used by the scientific community as a common starting point for further analyses to enable a better traceability of uncertainties and differences between individual data products.

Here we shortly introduce the project itself and describe the individual steps from the creation of GOME and SCIAMACHY Level 1 FDRs to their final publication, which will be the first FDR of spectrally resolved radiances and irradiances.

Since there is a need for quality assessment and control when creating a FDR, it follows that the FDR have to be validated to ensure a maximum in accuracy and integrity of the final product. Here, especially the FDR validation process is of interest for the DOAS community as Level 1 data is planned to be validated with the help of Level 2 products. This procedure is described on the example of NO₂, which is derived using the DOAS method. Special emphasis is placed on analyzing the differences between both instruments (e.g. spatial and spectral resolution), such that a consistent NO₂ time series can be created.

The DOAS community can benefit from the FDR products and the methods developed to derive them (e.g. improved error characterization, combination of time series of different sensors). Especially, problems to be faced within the validation step of the FDR will have a strong similarity to the everyday work of the DOAS community (e.g. handling of correlative data sets, definition of quality criteria, definition of proper ground scenes and times).

Validation of SO₂ layer height from TROPOMI as a part of OPAS Engage-KTN SESAR project

Hugues Brenot*, Nicolas Theys, Scott Wilson, Rory Clarkson, Lieven Clarisse, Stefano Corradini, Riccardo Biondi, Pierre-Yves Tournigand, Giuseppe Salerno, Klaus Sievers, Christophe Lerot, Jeroen van Gent, Michel Van Roozendael

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Presenter: Hugues Brenot

Abstract:

Volcanic ash and gas is, like sulphur dioxide (SO₂), a major risk for air traffic. To mitigate this risk and to improve situational awareness for air traffic management (ATM), OPAS Engage-KTN project targets the creation of a new service using the SWIM (System Wide Information System Management) Yellow Profile. This new service provides early warnings of volcanic SO₂ layer height (SO₂LH) retrievals from 3 satellite instruments (TROPOMI, IASI-A and IASI-B). The implementation of this service is part of OPAS – Operational alert Products for ATM via SWIM – project, a KTN (Knowledge Transfer Network) Engage Catalyst funded project (Thematic Challenge 3; <https://engagektn.com>) of SESAR JU (Single European Sky ATM Research Joint Undertaking; <https://www.sesarju.eu>). We present the TROPOMI SO₂LH algorithm and the uses of inverse modelling and external observations from satellites and ground-based instruments to validate TROPOMI SO₂LH products for recent eruptions that impacted air traffic (i.e. Etna in Dec. 2018, Raikoke in June 2019, Ubinas in July 2019). Cross-comparison with the satellite instruments CALIOP (Cloud-Aerosol Lidar with Orthogonal Polarization), IASI (Infrared Atmospheric Sounder Interferometer), with GNSS (Global Navigation Satellite System) radio-occultations, and with retrievals from FLAME MAX-DOAS network is shown. This study will also highlight the point of view of an aircraft manufacturer (Rolls-Royce) directly in relation with airlines and ATM for the avoidance of flights through volcanic plumes and SO₂ clouds. This is due to engine susceptibility to aerosols and the risk of sulphidation. The development of our new SO₂LH products from TROPOMI contributes to an existing early warning system, so called SACS (Support to Aviation Control Service; <http://sacs.aeronomie.be>). This system is dedicated to support aviation and ATM, and was recently upgraded in the frame of EUNADICS-AV project (European Natural Airborne Disaster Information and Coordination System for Aviation; <http://www.eunadics.eu>), with many other alert products related to natural airborne hazard affecting air traffic (e.g. volcanic ash column and layer height, smoke from forest fires and desert dust).

Evaluating the effect of aerosols on OMI NO₂ retrievals using airborne in-situ and direct-sun measurements during KORUS-AQ

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Presenter: Stephen Broccardo

Abstract:

During the KORUS-AQ airborne field campaign in Korea in 2016, a payload of in-situ aerosol and trace-gas instrumentation, as well as the 4STAR airborne sun-tracking spectrometer, were flown on the NASA DC-8 research aircraft. The latter instrument measures the direct solar irradiance at high spectral resolution, allowing retrieval of the NO₂ column density. Flight profiles included several vertical profile measurements co-incident with OMI overpasses, over both land and ocean. We compare NO₂ column measurements by 4STAR (upward looking) and OMI (downward looking), and attempt to explain the discrepancies based on total-column and in-situ aerosol measurements accompanied by a radiative-transfer modelling approach.

Tomographic view of gas emissions using an improved algorithm with adaptive regularization

Nicolás Casaballe*, Matías Di Martino, Erna Frins

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Presenter: Nicolás Casaballe

Abstract:

The combination of passive multi-axis DOAS observations enables the tomographic reconstruction of gas distributions in the atmosphere emitted from different sources. Due to the nature of this type of observations, the reconstruction algorithms have been adapted to produce the most accurate and precise results using a limited sampling of the system under study.

We have developed a new algorithm based on a regularized minimization approach, specialized in retrieving a plume cross-section that was scanned through. Our algorithm embeds some of the physical characteristics of the plume to constrain the inversion [1].

A recent improvement for this algorithm takes into account that the spatial sampling, resulting from the scanning instruments, is not homogeneous. Therefore, we introduced an adaptive approach, with an enhanced regularization that has a locally tuned weight according to the uncertainty levels introduced by the sampling scheme [2]. We tested this approach on reconstructions of simulated gas distributions for different configurations applicable to Multi-Axis DOAS.

In this presentation we will summarily review the basics of the method and possible applications, such as the retrieval of the NO_2 distribution within the plume emitted from a group of stacks of a power plant in Montevideo city.

[1] N, Casaballe, M. Osorio, M. Di Martino, & E. Frins, (2017). Comparison between regularized optimization algorithms for tomographic reconstruction of plume cross sections in the atmosphere. *Earth and Space Science*, 4, 723–736. <https://doi.org/10.1002/2017EA000341>

[2] N. Casaballe, M. Di Martino, M. Osorio, J. A. Ferrari, T. Wagner, and E. Frins, "Improved algorithm with adaptive regularization for tomographic reconstruction of gas distributions using DOAS measurements," *Appl. Opt.* 59, D179-D188 (2020). <https://doi.org/10.1364/AO.383584>

The characteristics of NO₂ concentrations retrieved from MAX-DOAS during the summer of 2014 at Raoyang station in China

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Presenter: Siyang Cheng

Abstract:

Ground-based Multi-AXis Differential Optical Absorption Spectroscopy (MAX-DOAS) measurements were performed during the summer of 2014 at Raoyang, a rural site in the North China Plain. The tropospheric NO₂ vertical column densities (VCDs) and vertical profiles were retrieved to investigate the rural pollution condition of the Beijing-Tianjin- Hebei developed economic circle in China. The average daytime diurnal variation of NO₂ VCD_{Trop} with a peak at 8:00 local time is apparent, presenting the minimum in the afternoon and the higher values in the morning and evening. The diurnal pattern at Raoyang station is distinct from the ones at the urban or polluted stations. The NO₂ volume mixing ratios (VMRs) in a 200-m vertical layer adjacent to the surface are compared to the results measured by in-situ observations on the ground, which indicates a strong correlation between them. Based on the vertical distribution of NO₂ VMRs, the lifted layers are observed at higher altitudes, probably related to the long-range transport. These results are beneficial to further study NO₂ pollution features and ozone secondary formation in chemical simulation model in the North China Plain.

Measurements of the water vapor absorption cross sections in the blue-violet spectral range by cavity-enhanced extinction spectroscopy

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Presenter: Randall Chiu

Abstract:

The absorption cross sections of water vapor in the blue-violet spectral range (415–460 nm) are currently not well known. In particular, many weak spectral lines are not included in either the High resolution TRANsmission molecular absorption (HITRAN) database or its High TEMPerature companion, HITEMP. Direct measurements of weak absorption cross section lines of water vapor have been limited by the slant column density (SCD) of gaseous water molecules that is achievable under well controlled conditions in a laboratory setting. We use cavity-enhanced extinction spectroscopy (CE-ES) to generate water vapor SCDs of $1\text{--}7 \times 10^{23} \text{ molec cm}^{-2}$ in a temperature controlled laboratory set-up; these SCDs are comparable to those measured in remote sensing field measurements. A pair of high-reflectivity ($R > 0.99995$) mirrors are separated by 80–90 cm to realize effective path lengths up to 16 km; water vapor is generated from deionized water in an aerosol-free double-bubbler system. A heat exchanger surrounding the optical cavity provides temperature control between $-80 \text{ }^\circ\text{C}$ and $+90 \text{ }^\circ\text{C}$, though the vapor pressure of water limits signal-to-noise to temperatures of approximately $-5 \text{ }^\circ\text{C}$ or higher. An LED with a peak intensity at 455 nm is used to measure multiple lines at moderately high spectral resolution (currently $\sim 0.15 \text{ nm}$ FWHM optical resolution). Here we present H₂O spectra measured at $59 \text{ }^\circ\text{C}$, $29 \text{ }^\circ\text{C}$, $14 \text{ }^\circ\text{C}$, and $3 \text{ }^\circ\text{C}$, and compare these spectra with available cross-sections in the literature, as well as field observations. The spectra acquired to date exhibit a small but non-negligible baseline that requires further investigation. Ongoing work also seeks to improve the optical resolution to well below 0.1 nm. Our goal is to refine available line lists for gas-phase water by combining laboratory measurements with quantum chemical calculations.

Horizontal distribution of tropospheric NO₂ derived from dual-scan multi-wavelength MAX-DOAS measurements in Uccle (Belgium)

Ermioni Dimitropoulou*, F. Hendrick, M. M. Friedrich, G. Pinardi, F. Tack, A. Merlaud, C. Fayt, C. Hermans, M. Van Roozendael

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Presenter: Ermioni Dimitropoulou

Abstract:

Ground-based Multi-Axis Differential Optical Absorption Spectroscopy (MAX-DOAS) measurements of aerosols and tropospheric nitrogen dioxide (NO₂) have been carried out in Uccle, Brussels, during two years (March 2018 – March 2020). The MAX-DOAS instrument has been operating in both UV and visible (Vis) wavelength ranges in a dual-scan configuration consisting of two sub-modes: (1) an elevation scan in a fixed viewing azimuthal direction (the so-called main azimuthal direction) pointing and (2) an azimuthal scan in a fixed low elevation angle (2 deg.). By analyzing the O₄ and NO₂ DSCDs in five different wavelengths along every azimuthal direction and by applying a new Optimal-Estimation-based horizontal distribution inversion approach, the distribution of the NO₂ near-surface concentrations (VMRs) and vertical column densities (VCDs) are retrieved along ten different azimuthal directions. The corresponding NO₂ horizontal field show a clear seasonal cycle and allow the identification of the main NO₂ hotspots in the Brussels area. An important application of those dual-scan multi-wavelength MAX-DOAS measurements is the validation of satellite missions with high spatial resolution, such as TROPOMI/S5P. Measuring the horizontal distribution of tropospheric NO₂ VCDs in different azimuthal directions is shown to improve the spatial collocation with satellite measurements leading to a better agreement between both ground-based and satellite datasets.

Monitoring of SO₂ and BrO in volcanic gas plumes via MAX-DOAS: the Network for Observation of Volcanic and Atmospheric Change (NOVAC) exemplified for Masaya volcano from 2014-2020

Florian Dinger*, Nicole Bobrowski, Timo Kleinbek, Ulrich Platt, Thomas Wagner

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Presenter: Florian Dinger

Abstract:

Monitoring magnitude or chemical composition of volcanic gas emissions can help to forecast volcanic eruptions. Furthermore, volcanic gas plumes are highly interesting study objects for complex atmospheric chemistry. Founded in 2005, the Network for Observation of Volcanic and Atmospheric Change (NOVAC) monitors the SO₂ and BrO emissions of (as today) 42 volcanoes using scanning UV-spectrometers and the MAX-DOAS technique. We present SO₂ emission fluxes and BrO/SO₂ molar ratios in the gas plume of Masaya volcano (Nicaragua) from 2014-2020 retrieved from NOVAC. Volcanoes emit bromine actually as HBr which is then partially converted in the volcanic gas plume to BrO via the destruction of atmospheric ozone. Variations in the BrO/SO₂ time series can thus originate from variations in the magmatic system or in the surrounding atmospheric conditions.

We observed an annual cyclicity in the BrO/SO₂ time series and suggest that this might be a manifestation of meteorological cycles. In particular, a strong anti-correlation (-51%) between the BrO/SO₂ molar ratios and the ambient water vapour concentration has been observed. As a possible explanation, variations in the generally high ambient humidity may result in a dilution of the bromide concentration in the aerosol phase causing an early stop of the autocatalytic bromide to BrO conversion. No systematic dependency between the BrO/SO₂ molar ratios and the plume age has been observed for an age range of 2-12 min after the release from the volcanic edifice.

Our time series cover the latest activity cycle of Masaya's lava lake which exhibited a period of enhanced activity from late 2015 - May 2018. When corrected for the annual cyclicity, we observed further variations in the long-term trends in the gas data which coincide with the general volcanological variations. The BrO/SO₂ molar ratios showed no significant long-term trend prior to the period of enhanced activity with a long-term mean of $2.9 \cdot 10^{-5}$, but exhibited a persistent step increase of $0.7 \cdot 10^{-5}$ in November 2014 followed by trends of $1.2 \cdot 10^{-5}$ per year from November 2014 - May 2018 and $-0.8 \cdot 10^{-5}$ per year from May 2018 - March 2020. In contrast, the SO₂ emission fluxes had mean daily maxima of $(2.5 \pm 1.1) \text{ t d}^{-1}$ prior to the period of enhanced activity, were hardly effected by the onset of this period, but dropped to mean daily maxima of $(1.5 \pm 0.7) \text{ t d}^{-1}$.

Sensitivity study for the fit settings for the retrieval of HCHO slant column densities from MAX-DOAS measurements using synthetic and measured spectra

Sebastian Donner*, Steffen Dörner, Janis Pukite, Steffen Beirle, Thomas Wagner

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Presenter: Sebastian Donner

Abstract:

Together with international partners, we operate six stationary MAX-DOAS instruments located in Mainz/Germany, Bayfordbury/United Kingdom, Greater Noida/India, Basra/Iraq, at the Amazonian Tall Tower Observatory (ATTO) measurement site/Brasil and in Guangzhou/China. The meteorological and environmental conditions for all these measurements are very different. The measurements from these stations will be used to study the geographic and seasonal variation of tropospheric HCHO. It also constitutes a valuable data base for global satellite validation. However, so far not all of these data are always analysed in a consistent way. Since HCHO is sometimes less abundant and its absorption structures are rather weak compared to other gases such as NO₂ the retrieval result can strongly depend on the chosen DOAS fit settings.

Therefore, a sensitivity study was performed to find the most suitable DOAS fit settings which can be used for the retrieval of HCHO slant column densities for all/most MAX-DOAS instruments. For that purpose, both measured and synthetic spectra were used. The synthetic spectra were simulated at high spectral resolution (and including Raman scattering) for a large variety of scenarios using the radiative transfer model SCIATRAN (Rozanov et al., 2014).

Here, we present the main findings of this study. We give recommendations for the fit interval and the use of the so-called Pukite terms for NO₂ and O₃. In addition, the sensitivity to various fit settings will be listed.

One year of MAX-DOAS measurements of tropospheric trace gases and aerosols in the suburban area of London

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Presenter: Sebastian Donner

Abstract:

Multi-AXis (MAX)-DOAS instruments record spectra of scattered sun light under different elevation angles. From such measurements tropospheric vertical column densities (VCDs) and vertical profiles of different atmospheric trace gases and aerosols can be determined for the lower troposphere. These measurements allow a simultaneous observation of multiple trace gases (e.g. HCHO, CHOCHO, NO₂, etc.) with the same measurement setup. Since November 2018, a MAX-DOAS instrument is operated at the Bayfordbury Observatory, which is located approximately 30 km north of London. This measurement site is operated by the University of Hertfordshire and equipped with an AERONET station, a LIDAR and multiple instruments to measure meteorological quantities and solar radiation. Depending on the prevailing wind direction the air masses at the measurement site can be dominated by the pollution of London (SE to SW winds) or rather pristine air (northerly winds). Therefore, this measurement site is well suited to study the influence of anthropogenic pollution on the atmospheric composition and chemistry at a rather pristine location in the vicinity of London, a major European capital with 9.8 million inhabitants and 4 major international airports.

In this study, trace gas and aerosol profiles are retrieved using the MAInz Profile Algorithm MAPA (Beirle et al., 2018) with a focus on tropospheric formaldehyde (HCHO) which plays an important role in tropospheric chemistry. The HCHO results are combined with the results of other trace species such as NO₂, CHOCHO and aerosols in order to identify different chemical regimes and pollution levels.

Using NDACC MAX-DOAS Central Processing System data for TROPOMI NO₂ and HCHO column validation: first results

Martina M. Friedrich*, François Hendrick, Gaia Pinardi, Caroline Fayt, Michel Van Roozendael, Alkis Bais, Steffen Beirle, Tim Bösch, Stefano Casadio, Paolo Castracane, Angelika Dehn, Sebastian Donner, Udo Friess, Dimitris Karagkiozidis, Karin Kreher, Mónica Navarro-Comas, Ankie Piters, Richard Querel, Julia Remmers, Andreas Richter, J. Lukas Tirpitz, Thomas Wagner, Margarita Yela

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Presenter: Martina Friedrich

Abstract:

We present complementary validation of TROPOMI NO₂ and HCHO products using tropospheric vertical columns (and profiles) obtained from measurements from ground-based MAX-DOAS stations that were processed with the new NDACC (Network for the Detection of Atmospheric Composition Change) MAX-DOAS central processing system. This facility, developed within the ESA FRM4DOAS (Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations) project, provides analysis from spectra to vertical profiles using state-of-the-art retrieval algorithms (see companion abstract from Hendrick et al.). During the last months, it underwent a thorough testing exercise before going live by the beginning of May. Much of the data presented here, is reprocessed data from this testing period using the latest version of the system for reprocessing. There are two main goals of the exercise presented in this contribution: The demonstration of the usefulness of such a central processing system for satellite validation; testing and preparation of the data for automatic ingestion into validation servers

HeiDOAS: A new framework for DOAS applications

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Presenter: Udo Friess

Abstract:

We present our newly developed, python based library HeiDOAS for the analysis of DOAS measurements, with the main goal of a physically correct simulation of scattered light observations. HeiDOAS consists of a library with the following main features:

- Processing of common spectra file formats, easy implementation of new file formats
- Numerous mathematical operations on spectra
- Fast Fourier transform convolution using various pre-defined instrument line shape functions, user-defined functions or measured slit functions
- Built-in tool for the wavelength calibration with simultaneous determination of instrument line shape parameters using a high resolution Fraunhofer spectrum
- Simulation of Raman spectra
- Fit of instrument line shape functions to measured atomic emission lines, including overlapping lines
- Physically correct forward modelling of spectra based on high-resolution Fraunhofer spectrum and cross sections, including polynomial, Raman signal, etc.
- Novel DOAS fit routine with the following features:
 - Unlimited number of cross sections
 - Shift/squeeze of cross sections and measured spectra either individually or in groups
 - Non-linear offset represented either as polynomial or user-defined function
 - Optionally non-linear fit of Raman spectrum as intensity offset instead of Ring spectrum
 - Fit either using the traditional DOAS approach with pre-convoluted cross sections, or in fully non-linear mode on high resolution using computationally efficient fast Fourier convolution
 - Retrieval of instrumental line shape parameters during the fit
- Easy to use plotting routines for spectra and for DOAS fit results

HeiDOAS can be used either as stand-alone application or as an integral part of our novel profile and aerosol retrieval algorithm that is currently under development (see presentation of Jan-Lukas Tirpitz et al.). We will present the main features of HeiDOAS and show some exemplarily applications using both simulated spectra and field data.

Trend analysis of stratospheric NO₂ and BrO measured by ground-based UV instruments over Kiruna, Sweden

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Presenter: Myojeong Gu

Abstract:

After the discovery that anthropogenic emissions of halogen compounds destroy the stratospheric ozone layer, the effect of the thinning ozone layer on human health and environment has attracted great attention. Very recent research reported that, while ozone depleting substances have been significantly reduced, strong ozone depletion is still observed in polar spring. There are many open questions about the underlying reasons. Stratospheric bromine compounds are known to contribute to the depletion of stratospheric ozone through catalytic cycles which also nitrogen oxides are involved. The abundances of both gases are intricately correlated depending on the measurement site, observation period, aerosol amount, atmospheric dynamics and the stratospheric temperature. Thus, investigating the relationship between stratospheric NO₂ and BrO, and their precursors are of great importance. Several efforts have been made to investigate the decadal trends of stratospheric NO₂ and BrO using satellite and ground-based measurements aided by computational models, but those have mainly focused on mid-latitudes and the southern hemisphere, and have not covered the most recent time period. This study shows the temporal variation of stratospheric NO₂ and BrO from 1997 to 2019 above Kiruna, Sweden by using ground-based zenith sky DOAS measurements, which extends the existing time series by several years. To estimate the linear trend of the stratospheric NO₂ and BrO, a linear least-squares algorithm is used. For NO₂ it was found that the amount has not significantly changed (+1.5%/decade) and for BrO a strong positive trend before 2001 and after 2005 a slight negative (-1.2 %/year) trend is found.

Advancements in iterative cavity enhanced DOAS instruments

Martin Horbanski*, J. Lampel, D. Pöhler, Oliver Fischer, Sven Riedner, Katja Bigge, U. Platt

*) Airyx GmbH / University of Heidelberg; martin.horbanski@airyx.de

Presenter: Martin Horbanski

Abstract:

Cavity Enhanced DOAS (CE-DOAS or BB-CEAS) allows to make in-situ measurements while maintaining the km-long light paths required. This technique has been successfully used for several years to measure in-situ atmospheric trace gases. A property of optical cavities is that in presence of strong absorbers or scatterers the length of the light path is reduced. Typical cavity evaluation schemes correct this effect using the measured total light intensity attenuation which is, however, also affected by other parameters, like light source stability or transmission variations of the optics and is thus prone to errors. An important DOAS advantage, to be independent of total light intensity, is actually lost.

The new ICAD (Iterative Cavity Enhanced DOAS) instruments use another approach, modelling the light path reduction from the derived absorbers in the optical resonator. It allows a sensitive and robust data analysis that does not depend on the total light intensity allowing a simpler and more compact instrument setup. The algorithm is discussed and simulations and validation measurements demonstrate its sensitivity and robustness. Our ICAD instrument is currently optimized to NO₂ measurements in the blue spectra range and for NO_x with a NO to NO₂ converter. The instruments are currently adapted to other trace gases. For the example of NO₂ we present an in depth analysis of attainable detection limits (0.02ppbv at 7min averaging time).

Furthermore we address the challenge to characterize the optical path length in cavity systems with ICOM (Integrated Calibration by means of Optical Modulation), a purely optical calibration technique without any mechanically moving parts. ICOM can avoid any gas calibration and makes the ICAD system thus fully self-calibrated and reduces the need for instrument maintenance to a minimum. A suitable compact spectrometer together with dedicated LED driver electronics was developed to implement this technique. The ICOM algorithm provides wavelength resolved path length curves. Its performance and accuracy are discussed and compared to other path length calibration methods.

We shortly outline the large range of new applications possible with this setup. These are for example mobile measurements to derive air pollution maps. Also Bicycle, car indoor, or work space measurements to derive personal NO₂ and NO_x exposure. The ICAD systems is also used to investigate direct vehicle emissions of NO_x.

Profiles of tropospheric ozone retrieved from MAX-DOAS and validation in China

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Presenter: Xiangguang Ji

Abstract:

The Multi Axis Differential Optical Absorption Spectroscopy (MAX-DOAS) is an effective instrument to monitor the vertical profiles of trace gases and aerosols in troposphere. Many trace gases which were mainly located in near surface, such as: Nitrogen dioxide (NO₂), Sulfur dioxide (SO₂) have been reported in many studies. However, it is difficult to retrieve the tropospheric ozone (O₃) profiles by using the MAX-DOAS due to the absorption of the stratospheric O₃. In this study, we used the stratospheric O₃ profile provided by Tropospheric Monitoring Instrument (TROPOMI), which were validated by Fourier Transform Spectrometer (FTS) in Hefei China, as external data sets to quantify the stratospheric component of O₃. Then the O₃ profiles were retrieved by using profile inversion algorithm. O₃ profiles in stratosphere were used to simulate the stratospheric O₃ differential slant column densities (dSCDs) by using radiative transfer models (RTM). The differences of stratospheric O₃ dSCDs simulated by various RTM and the corresponding influences to the retrieved O₃ profiles were analyzed. The obtained O₃ results were compared with independent O₃ measurements, the near-surface O₃ concentrations were shown to be consistent with in situ measurements, at the same time the vertical profiles were validated by ozone sounding in Beijing, China.

Uncertainty of PGN data products – current status and planned improvements

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Presenter: Karin Kreher

Abstract:

The Pandora Global Network (PGN) is a worldwide operating network of passive remote sensing Pandora spectrometer systems measuring atmospheric trace gases at high temporal resolution. Since a key objective of the PGN is the support of satellite validation, PGN instruments are homogeneously calibrated and the measured spectra are centrally processed in real-time. In this regard, in-depth understanding of the uncertainty in the PGN data products is also of great relevance. To investigate the uncertainty in the PGN data products further, as part of the ESA QA4EO project, a study to determine the hierarchy and magnitude of each of the uncertainty estimates for all data processing steps and parameters involved in the data analysis is undertaken. Here we provide an overview of this effort and present the first results of a qualitative study of the systematic uncertainties involved in all processing steps from raw data (Level 0, L0) via the corrected spectra (Level 1, L1) to the final products (Level 2, L2). This study is broken into several individual tasks, starting with the qualitative study of the systematic uncertainty of the L1 correction steps (including e.g. corrections for dark current, non-linearity, latency, flat field, temperature, stray light, sensitivity and wavelength) and includes a detailed investigation of the calibration processes involved.

MAX-DOAS measurements of BrO from the great Rann of Kachhach, India

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*) Max Planck Institute for Chemistry, Mainz, Germany; vinod.kumar@mpic.de

Presenter: Vinod Kumar

Abstract:

Active Bromine radicals (BrOx or Br+ BrO) can perturb the atmospheric oxidation capacity on local to regional scale. Measurement of BrO is used as a proxy for BrOx. Following the detection of BrO over the seasonal salt marsh of the Great Rann of Kachhach using satellite observations, we performed three weeks long ground-based MAX-DOAS measurements at two locations circa 70km far from each other and mobile measurements in the Great Rann of Kachhach during March- April 2019. Here we present measurements of BrO, NO₂, HCHO, AOD derived from MAX-DOAS and ozone derived from in situ measurements from the Great Rann of Kachhach. Very high BrO VCDs of more than 6×10^{13} molecules cm⁻² have been consistently observed during late afternoon hours, with the maximum reaching up to 4×10^{14} molecules cm⁻² at both stationary measurement locations. Similar diurnal trends and day to day variability were observed at both the sites indicating a small spatial variability in the BrO VCDs within the scope of our measurements. Generally, clear sky conditions with high aerosol load have been observed which indicate the possible role of aerosols on the activation and recycling of reactive bromine compounds. From the diurnal profiles, we find that the BrO enhancement kicks in at around noontime and reaches its maximum at late afternoon hours between 15:00 – 17:00 local time. Satellite borne sensors usually measure BrO only in the early afternoon hours, when enhancement of BrO just kicks in. Our measurements indicate that salt marshes like the great Rann of Kachhach can be a more substantial source of active bromine in the atmosphere than estimated by previous studies.

Early morning NO₂ VCDs of $\sim 5 \times 10^{15}$ molecules cm⁻² were found to decrease exponentially with the increase in BrO VCDs. In situ measurements show considerable ozone mixing ratio (~ 40 ppb) close to the surface throughout the day. A decrease in surface ozone mixing ratios is observed on several occasions, coinciding with an increase in BrO VCDs. However, unlike the previous studies, neither the surface ozone is completely destroyed, nor the decreased ozone mixing ratios persist for more than a few hours.

The Airyx 2D SkySpec instrument: MAX-DOAS measurements of tropospheric NO₂ and HCHO in Munich and the comparison to satellite observations

Johannes Lampel*, Ka Lok Chan, Denis Pöhler, Matthias Wiegner, Carlos Alberti, Ulrich Platt, and Mark Wenig

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Presenter: Johannes Lampel

Abstract:

We present the Airyx 2D SkySpec Instrument: A commercially available two-dimensionally scanning Multi-AXis Differential Optical Absorption Spectroscopy (MAX-DOAS) setup for the observations of trace gases using spectral measurements of scattered sun light and optionally also direct sun light. The waterproof design of the scanner unit is made for long-term outdoor deployment. Temperature stabilisation of the spectrometers and automatic calibration spectra measurement are used to ensure high-quality measurement data over months and years of observations.

We present the different available versions of the instrument and its technical properties as well as measurement data from field campaigns to show its robustness. In an outlook we summarize the upcoming developments and improvements regarding the mechanics and electronics of the SkySpec instrument family.

As an example for a long-term outdoor deployment, we show 2.5 years of measurements in Munich. Vertical columns and vertical distribution profiles of aerosol extinction coefficient, NO₂ and HCHO are retrieved from the 2D MAX-DOAS observations. The measured surface aerosol extinction coefficients and NO₂ mixing ratios are compared to in-situ monitor data. The retrieved surface NO₂ mixing ratios show good agreement with in-situ monitor data with a Pearson correlation coefficient (R) of 0.91. Similarly good agreement (R= 0.80) is also found for AOD when compared to sun-photometer measurements. Tropospheric vertical column densities (VCDs) of NO₂ and HCHO derived from the MAX-DOAS measurements are also used to validate OMI and TROPOMI satellite observations. Monthly averaged data show good correlation, however, satellite observations are on average 30% lower than the MAX-DOAS measurements. Furthermore, the 2D MAX-DOAS observations are used to investigate the spatio-temporal characteristic of NO₂ and HCHO in Munich. Analysis of the relations among aerosol, NO₂ and HCHO show higher aerosol to HCHO ratios in winter. The analysis also suggests that secondary aerosol formation is the major source of aerosols in Munich.

Variability of nitrogen oxide lifetimes and emission fluxes estimated by Sentinel-5P observations

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Presenter: Kezia Lange

Abstract:

Satellite observations of the high-resolution instrument TROPOMI on Sentinel-5P make it possible to measure nitrogen dioxide (NO_2) at city level and even to quantify the variability of nitrogen oxide (NO_x) emissions and lifetimes on a seasonal and daily basis.

NO_2 is an air pollutant and especially in cities of particular importance due to the large number and strength of emission sources in combination with people living nearby exposing their health to the polluted air. To quantify nitrogen oxide emissions and lifetimes with their high variability in space and time, satellite data is especially suited as it provides daily global coverage and large number of measurements. The Tropospheric Monitoring Instrument (TROPOMI) on the satellite Sentinel-5P, launched in October 2017, provides, thanks to its higher spatial resolution when compared to previous satellite instruments, the possibility of detailed investigations on lifetimes and emissions of air pollutants.

Two years of TROPOMI NO_2 data with a spatial resolution of up to 3.5 km x 5.5 km together with ECMWF ERA5 wind data are analyzed. The NO_2 data around a source is linked to the ERA5 wind data and rotated to a uniform wind direction to get clear emission patterns. Out of these twodimensional maps of the mean NO_2 distribution, one dimensional line densities are calculated by integration across wind direction.

Lifetimes and emission fluxes are calculated for different NO_x sources such as cities and power plants distributed over the world. They are compared among each other and to bottom-up emission inventories. Seasonal variability and weekday versus weekend effects in lifetimes and emissions are discussed.

Evaluation of TROPOMI cloud products for NO₂ retrievals

Miriam Latsch*, Andreas Richter, John P. Burrows, Thomas Wagner, Holger Silher, Michel van Roozendaal, Diego Loyola, Pieter Valks, Athina Argyrouli, Ronny Lutz, Pepijn Veefkind, Henk Eskes, Maarten Sneep, Ping Wang, Richard Siddans

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Presenter: Miriam Latsch

Abstract:

The first European Sentinel satellite for monitoring the composition of the Earth's atmosphere, the Sentinel 5 Precursor (S5p), carries the TROPospheric Monitoring Instrument (TROPOMI) on board to map trace species of the global atmosphere at high spatial resolution. Retrievals of tropospheric trace gas columns from satellite measurements are strongly influenced by clouds. Thus, cloud retrieval algorithms were developed and implemented in the trace gas processing chain to consider this impact.

In this study, different cloud products available for NO₂ retrievals from TROPOMI data are analyzed: the TROPOMI level 2 OCRA/ROCINN (Optical Cloud Recognition Algorithm/Retrieval of Cloud Information using Neural Networks) cloud products CRB (cloud as reflecting boundaries) and CAL (clouds as layers), the FRESCO (Fast Retrieval Scheme for Clouds from Oxygen absorption bands) cloud product, the VIIRS (Visible Infrared Imaging Radiometer Suite) cloud product, the O₂-O₂ cloud product, and the MICRU (Mainz Iterative Cloud Retrieval Utilities) cloud fraction. The cloud products are compared with regard to e.g. cloud fraction, cloud height, cloud albedo/optical thickness, flagging and quality indicators. In particular, difficult situations such as snow or ice, sun glint, and high aerosol load are investigated.

The eventual aim of this study is to better understand TROPOMI cloud products and their quantitative impacts on trace gas retrievals. Here, we present first results of a statistical analysis on a limited data set comparing currently existing cloud products and their approaches focusing on NO₂.

Effects of aerosol peak height on the PBL and volcanic AMFs for satellite based SO₂ retrievals

Hanlim Lee*, Wonei Choi, Jiwon Yang, Michel Van Roozendael, Ja-Ho Koo, Jun-sung Park, Daewon Kim

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Presenter: Hanlim Lee

Abstract:

We investigate effects of aerosol peak height (APH), and various parameters on the air mass factor (AMF) for SO₂ retrieval. Increasing aerosol optical depth (AOD) leads to multiple scattering within the planetary boundary layer (PBL) and an increase in PBL SO₂ AMF. However, under high AOD conditions, aerosol shielding effects dominate, which causes the PBL SO₂ AMF to decrease with increasing AOD. The height of the SO₂ layer and the APH are found to significantly influence the PBL SO₂ AMF under high AOD conditions. When the SO₂ and aerosol layers are of the same height, aerosol multiple scattering occurs dominantly within the PBL, which leads to an increase in the PBL SO₂ AMF. When the APH is greater than the SO₂ layer height, aerosol shielding effects dominate, which decreases the PBL SO₂ AMF. When the SO₂ and aerosol layers are of the same height under low AOD and solar zenith angle (SZA) conditions, increased surface reflectance is found to increase the PBL SO₂ AMF significantly. However, high AOD dominates the surface reflectance contribution to PBL SO₂ AMF. Under high SZA conditions, Rayleigh scattering contributes to a reduction in the light path length and PBL SO₂ AMF. For volcanic SO₂ AMF, high SZA enhances the light path length within the volcanic SO₂ layer, as well as the volcanic SO₂ AMF, because of the negligible photon loss by Rayleigh scattering at high altitudes. High aerosol loading and an APH that is greater than the SO₂ peak height lead to aerosol shielding effects, which reduce the volcanic SO₂ AMF. The SO₂ AMF errors are also quantified as a function of uncertainty in the input data of AOD, APH, and surface reflectance. The SO₂ AMF sensitivities and error analysis provided here can be used to develop effective error reduction strategies for satellite-based SO₂ retrievals.

Remote sensing of water vapor vertical distribution over Beijing with MAX-DOAS

Hua Lin*, Cheng Liu, Qihou Hu, Chengzhi Xing, Haoran Liu, Qihua Li, Zhuang Wang, Wei Tan, Xiangguang Ji, Qianqian Hong, Jianguo Liu

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Presenter: Hua Lin

Abstract:

Water vapor, which was listed as the most important greenhouse gas, increases strongly with temperature and amplifies the global warming process. Moreover, water vapor has a critical influence on secondary aerosol formation. Different from other greenhouse gas like CO₂, the variation of water vapor concentration can be relatively more severe. Thus, it is important to determine atmospheric water vapor vertical distribution in high spatial and temporal resolution. From 18 April to 30 September 2018, a longtime MAX-DOAS observation was conducted in Beijing, China. The vertical distributions of water vapor in this period were retrieved with Heidelberg profile retrieval algorithm (HEIPRO). The retrieved water vapor VCDs, surface concentrations and vertical profiles were compared with other independent datasets. The hourly averaged VCDs, surface concentrations were validated with colocated AERONET data and National Climatic Data Center (NCDC) data with R of 0.922 and 0.876, respectively. The vertical profiles of water vapor observed by MAX-DOAS agree well with Balloon-sonde measurements and the Pearson correlation coefficient R are larger than 0.9. What's more, a correlation analysis of the water vapor concentrations in the same height layers derived from MAX-DOAS and ECMWF- interim were conducted. A good agreement was found in the height layer below 2000m with R ranging from 0.702 to 0.881.

The influence of the spectral resolution of MAX-DOAS instruments on measurement errors

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Presenter: Haoran Liu

Abstract:

For the DOAS system, a better spectral resolution can improve the detection limit and the ability of the instrument to de-convolute overlapping bands of different species in theory. However, the selection of spectral resolution will usually be a compromise because the improvement of the resolution comes at the expense of light throughput (reduced the signal-to-noise ratio) and size (and therefore cost) of the instrumentation. Therefore, it's important to determine an optimal spectral resolution for the DOAS system, which will have a positive impact on trace gas retrieval and can also control the instrumentation's size and cost. However, there is currently little research in this area. In this study, we use the Vector Linearized Discrete Ordinate Radiative Transfer (VLIDORT) model to simulate the characteristic spectra with different resolutions (added various trace gas absorption component and corresponding noise). On the premise of avoiding hardware differences such as stray light and grating efficiency, the influence of spectral resolution on the retrieval of each gas was evaluated. In addition, we also designed parallel comparison experiments of instruments with different spectral resolutions to evaluate the effect of spectral resolution on the retrieval of each gas (including weak absorbers such as SO₂ and HONO) in actual observations. Combining the above experimental and simulation results, we explored better spectral resolution and inversion parameters.

Research of vertical profile of aerosol extinction based on measured O₄ of multi-elevation angles with MAX-DOAS

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Presenter: Suwen Li

Abstract:

A method for aerosol extinction profile retrieval using ground-based multi-axis differential optical absorption spectroscopy (MAX-DOAS) is studied, which is based on a look-up table algorithm. The algorithm uses parametric method to represent aerosol extinction profiles and simulate different atmospheric aerosol states by atmospheric radiation transfer model. Based on the method, aerosol extinction profile was obtained during six cloud-free days. The O₄ differential air mass factor (dAMF) measured by MAX-DOAS is compared with the corresponding model results under different atmospheric conditions ($R^2=0.78$). The aerosol optical thickness, aerosol weight factor in boundary layer, and the height of the boundary layer are obtained after the process of minimization and look-up table method. The retrieved aerosol extinction in boundary layer is compared with PM_{2.5} data measured by ground point instrument. The diurnal variation trend of the two methods is in good agreement. The correlation coefficients of the two methods are 0.71 when the aerosol optical thickness is smaller than 0.5. The results show that the look-up table method can obtain the aerosol state of the troposphere and provide validation for other instrument data.

Long-term observations of aerosol optical properties and vertical distribution at Hefei

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Presenter: Xiaomei Li

Abstract:

Long-term observation of aerosols by solar photometer and Multi-axial differential optical absorption spectroscopy (MAX-DOAS) were conducted at the Hefei site. The annual and seasonal characteristics of the solar photometer's aerosol optical depth (AOD) and Angstrom exponent (α) from 2015 to 2019 are analyzed. The average annual AOD from 2015 to 2019 is divided into 0.84, 0.73, 0.84, 0.65, and 0.63. The seasonal characteristics are the lowest in autumn and the highest in spring. The α is inversely proportional to the particle size, higher value indicates that fine particles are dominant, and vice versa. α shows a significant season variation, with the lowest value in spring and the highest value in summer, which may be related to northern transmission in spring and rainfall precipitation in summer. Using the aerosol profile data of MAX-DOAS, the seasonal characteristics of aerosols in vertical distribution are analyzed. And the differences in aerosol optical characteristics and vertical distribution under different pollution conditions are analyzed.

MAX-DOAS measurements of NO₂, SO₂, HCHO and BrO at the Mt. Waliguan WMO/GAW global baseline station in the Tibetan Plateau

Jianzhong Ma*, Jianzhong Ma, Steffen Dörner, Sebastian Donner, Junli Jin, Siyang Cheng, Junrang Guo, Zhanfeng Zhang, Jianqiong Wang, Peng Liu, Guoqing Zhang, Janis Pukite, Johannes Lampel, Thomas Wagner

Jianzhong Ma*, et al.

*) Chinese Academy of Meteorological Sciences; majz@cma.gov.cn

Presenter: Jianzhong Ma

Abstract:

Mt. Waliguan Observatory (WLG) is a World Meteorological Organization (WMO)/Global Atmosphere Watch (GAW) global baseline station in China. WLG is located at the north-eastern part of the Tibetan plateau (36.28° N, 100.0° E, 3816 m a.s.l.) and is representative of the pristine atmosphere over the Eurasian continent. We made long-term ground-based MAX-DOAS measurements at WLG during the period 2012–2015. In this study, we retrieve the differential slant column densities (dSCDs) and estimate the tropospheric background mixing ratios of different trace gases, including NO₂, SO₂, HCHO and BrO, using the measured spectra at WLG. Averaging of 10 original spectra is found to be an 'optimum option' for reducing both the statistical error of the spectral retrieval and systematic errors in the analysis. The dSCDs of NO₂, SO₂, HCHO and BrO under clear sky and low aerosol load conditions are extracted from measured spectra at different elevation angles at WLG. By performing radiative transfer simulations with the model TRACY-2, we establish approximate relationships between the trace gas dSCDs at 1° elevation angle and the corresponding average tropospheric background volume mixing ratios. Mixing ratios of these trace gases in the lower troposphere over WLG are estimated to be in a range of about 5 ppt (January) to 70 ppt (May) for NO₂, below 0.5 ppb for SO₂, between 0.3 and 0.7 ppb for HCHO, and lower than 0.3 ppt for BrO. Our study provides valuable information and data set for further investigating tropospheric chemistry in the background atmosphere and their links to anthropogenic activities.

On the added value of car-based Mobile-DOAS measurements for air quality model validation

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Presenter: Alexis Merlaud

Abstract:

Over the last years, a series of air quality-related field campaigns (e.g. MADCAT, AROMAT-1 and 2, AROMAPEX, and CINDI-2) involved car-based mobile-DOAS instruments from several research teams. Such mobile-DOAS measurements primarily focused on the horizontal variability of NO₂, SO₂, and H₂CO. They also enabled to validate airborne DOAS measurements of NO₂ above urban areas, and to quantify NO_x and SO₂ emissions from cities or power plants.

We first use coordinated Mobile-DOAS measurements performed during MADCAT, AROMAT-1, and CINDI-2 to intercompare different mobile-DOAS instruments. These instruments are based on compact UV-Visible spectrometers of different types. We discuss the performances of these compact spectrometers to measure slant columns of the three aforementioned chemical species. Regarding NO₂, we also compare retrievals of vertical columns, among the different Mobile-DOAS systems and with the high-performance static MAX-DOAS deployed in CINDI-2. Our parallel measurements enable us to disentangle algorithmic from instrumental differences.

This intercomparison study leads, for CINDI-2, to a database of harmonized Mobile-DOAS NO₂ vertical columns, recorded by 5 systems which followed different routes between Rotterdam and Utrecht. We compare these measurements with the Lotos-Euros CTM. We investigate the added value for the model validation of such mobile measurements compared to the static MAX-DOAS dataset.

Atmospheric aerosol detection based on MAX-DOAS

Zhiqiang Ning*

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Presenter: Zhiqiang Ning

Abstract:

Multi-axis differential optical absorption spectroscopy (MAX-DOAS) measurements were performed in the urban environment of Madrid, Spain, from March to September 2015. The O₄ absorption in the ultraviolet (UV) spectral region was used to retrieve the aerosol extinction profile using an inversion algorithm. The results show a good agreement between the hourly retrieved aerosol optical depth (AOD) and the correlative Aerosol Robotic Network (AERONET) product, with a correlation coefficient of $R = 0.87$. Higher AODs are found in the summer season due to the more frequent occurrence of Saharan dust intrusions. The surface aerosol extinction coefficient as retrieved by the MAX-DOAS measurements was also compared to in situ PM_{2.5} concentrations. The level of agreement between both measurements indicates that the MAX-DOAS retrieval has the ability to characterize the extinction of aerosol particles near the surface. The retrieval algorithm was also used to study a case of severe dust intrusion on 12 May 2015. The capability of the MAX-DOAS retrieval to recognize the dust event including an elevated particle layer is investigated along with air mass back-trajectory analysis

Daytime HCHO and NO₂ observations from MAX-DOAS measurements in Eastern Los Angeles

Peter Peterson*, Leslie Tanaka, Lisa Hernandez

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Presenter: Peter Peterson

Abstract:

Despite continued emission reductions in Southern California, regular ozone exceedances remain a prevalent issue. To improve our understanding of these issues through vertically resolved measurements of ozone precursors, a MAX-DOAS instrument was deployed in Whittier, California, ≈ 20 km southeast of downtown Los Angeles. Continuous measurements of HCHO, NO₂, and aerosol extinction over the spring of 2020 are presented. Comparisons of MAX-DOAS NO₂ measurements with in-situ measurements from a nearby California Air Resources Board monitoring site and tropospheric NO₂ retrievals from the Ozone Monitoring Instrument (OMI) are also discussed.

Deriving an NO absorption cross section for deep UV active DOAS measurements

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Presenter: Denis Pöhler

Abstract:

Active DOAS measurements can also be applied in the deep UV spectral region between 200 and 300nm. Several gases feature strong absorption structures in this region and can directly be identified like NO (nitrogen oxide), NH₃ (ammonia), SO₂ (sulfur dioxide), NO₂ (nitrogen dioxide) and many aromatic compounds. The direct measurement of NO and NH₃ is relevant for monitoring e.g. emissions and air pollution.

Some commercial emission measurement systems based on deep UV DOAS exist; they typically use calibration gases. Also some long-path measurements were performed for NO detection using older NO literature absorption cross sections. We observed that these literature absorption cross sections are inaccurate and can result in an overestimation of the NO concentration by a factor of 10. The literature cross sections tend to have a too low spectral resolution and ignored significant saturation effects in its spectrum. In order to generate a high resolution NO absorption cross section (198 – 230nm) we combined high resolution laboratory measurements with LIFBASE scale-free absorption line simulations. The simulations can only generate an arbitrary unit cross section due to many unknown parameters. We, therefore, developed a method to convert the LIFBASE data to absolute absorption cross sections using our high resolution lab measurements. Besides the standard temperature of 293K, we could also simulate the cross section for higher temperatures.

The resulting absorption cross section was then validated and compared to other publications. The partly large differences between the various literature absorption cross sections are investigated. Simulations and laboratory measurements show that the used NO absorption cross section and the consideration of the saturation effect has a very large influence on the derived NO concentration and can not be ignored even at rather low concentrations.

2019 Antarctic stratospheric sudden warming – a DOAS perspective from three NDACC sites

Margarita Yela*, C. Prados-Roman, J.A. Adame, M. Navarro-Comas, H. Ochoa, O. Puertedura

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Presenter: Cristina Prados-Roman

Abstract:

As a result of troposphere-stratosphere synoptic coupling, during some polar winters the strong cyclonic winds of the polar vortex weakens or even reverses, yielding a Stratospheric Sudden Warming (SSW). These sorts of events are particularly rare in the southern hemisphere where upwards propagating planetary waves (PW) are less frequent than in the northern counterpart because of weaker PW forcing due to smaller topographical differences and land-sea contrasts. Because chlorine catalyzed chemical ozone loss in the polar winter lower stratosphere depends strongly on temperatures and vortex confinement, the varying polar vortex is reflected in large variations in ozone loss. In 2019 an SSW took place over Antarctica, resulting in a 60-90° S zonal mean temperature anomaly of over +25 K (10 hPa) by mid-September as compared to the 1979-2018 mean, even a stronger temperature anomaly than in the major Antarctic 2002 SSW for the same period. Within the framework of the nationally funded project of VHODCA (VOCs, Halogens, Ozone and nitrogen Dioxide in Antarctic Atmosphere), this work presents a latitudinal overview of the 2019 SSW based on the zenith-sky DOAS observations of NO₂, O₃, BrO and OClO performed from the NDACC sites of Belgrano II (77° S), Marambio (64° S) and Ushuaia (55° S). In order to investigate the anomalies occurred in the stratosphere due to the 2019 weakened polar vortex, these DOAS observations are compared with the ones from the 2018 season.

OCIO as observed by TROPOMI on Sentinel 5P

Janis Pukite*, Christian Borger, Steffen Dörner, Myojeong Gu, Thomas Wagner

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Presenter: Janis Pukite

Abstract:

The TROPospheric Monitoring Instrument (TROPOMI) is an UV-VIS-NIR-SWIR instrument on board of the Sentinel-5P satellite developed for monitoring the Earth's atmosphere. It was launched on 13 October 2017 in a near polar orbit. It measures spectrally resolved earthshine radiances at an unprecedented spatial resolution of around 3.5×7.2 km² (3.5×5.6 km² starting from 6 Aug 2019) (near nadir) with a total swath width of ~ 2600 km on the Earth's surface providing daily global coverage. From the measured spectra high resolved trace gas distributions can be retrieved by means of differential optical absorption spectroscopy (DOAS). Chlorine dioxide (OCIO) is a by-product of the ozone depleting halogen chemistry in the stratosphere. Although being rapidly photolysed at low solar zenith angles (SZAs) it plays an important role as an indicator of the chlorine activation in polar regions during polar winter and spring at twilight conditions because of the nearly linear relation of its formation to chlorine oxide (ClO). Here we present a new DOAS retrieval algorithm of the slant column densities (SCDs) of chlorine dioxide (OCIO), compare this TROPOMI OCIO signal with ground based zenith sky measurements and correlate it with meteorological data for both Antarctic and Arctic regions.

Estimation of NO_x, SO₂ and HCHO emissions from the megacity of Lahore, Pakistan using car MAX-DOAS observations and comparison with regional model and TROPOMI satellite data

Maria Razi*, Steffen Dörner, Vinod Kumar, Sebastian Donner, Christian Borger, Noor Ahmad, Steffen Beirle, Thomas Wagner

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Presenter: Maria Razi

Abstract:

Lahore, megacity of Pakistan with more than 11 million inhabitants is a strong emission source of atmospheric pollutants. We present results of a top-down emission procedure for NO_x and SO₂ for Lahore, based on car multi-axis differential optical absorption spectroscopy (car-MAX-DOAS) observations. Additionally, the total flux of HCHO from the city is determined which can be seen as an indicator for VOC emissions. Results from two extensive campaigns, which took place in summer 2017 and spring 2018 will be presented. From the measured spectra, we retrieve the vertically integrated concentration (the so-called tropospheric vertical column density, VCD) of the trace gases along the driving route by using the so-called geometric approximation method. By combining these observations with ECMWF Re-Analysis wind data, the total fluxes of NO_x, SO₂ and HCHO from the city of Lahore are estimated. From both measurement campaigns, we also analyzed the seasonal variability of the above-mentioned species.

Derived NO_x and SO₂ emissions are compared to the bottom-up emission inventory EDGAR 4.3.2. Spatial distributions of the tropospheric NO₂ and SO₂ VCDs observed by car MAX-DOAS are compared with those simulated using a coupled regional-global model system (MECO(n)). We find that, the model is able to account for the spatial variability but the VCDs are systematically underestimated by the regional model. Finally, derived NO_x emissions are also compared to the emissions estimated from TROPOMI satellite observations.

The vertical distribution of NO₂ and HONO in winter at a rural site of Hefei based on the Multi-Axis Differential Absorption Spectroscopy

Bo Ren*, Pinhua Xie, Jin Xu, Ang Li, Xin Tian, Zhaokun Hu, Xiaomei Li

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Presenter: Bo Ren

Abstract:

HONO, as one of the sources of OH free radicals in the atmosphere, affects the oxidative capacity of the atmosphere. Some studies have shown that HONO plays an important role in the generation of haze in winter. The conversion of NO₂ is considered to be one of the important sources of HONO, so it is very important to explore the vertical distribution of HONO and NO₂ in the atmosphere for understanding the formation of air pollution. The Multi-Axis Differential Absorption Spectroscopy (MAX-DOAS) method is a passive remote sensing technology that can quickly and effectively obtain the three-dimensional distribution characteristics of trace gas in the atmosphere. In this study, the MAX-DOAS instrument was used to perform spacial distribution measurement of HONO and NO₂ of Science Island in Hefei during December 2017, and the vertical distribution of these two gases were obtained by the PriAM algorithm. The results showed that the volume mixing ratio (VMR) and vertical column density (VCD) of NO₂ within 10m near the ground during the observation period were 2-80 ppb and $6.0 \times 10^{15} - 5.5 \times 10^{16}$ molec./cm², respectively. In addition, the near-ground results obtained by MAX-DOAS instrument were consistent with the NO₂ concentration of the China National Environment Monitoring Station (the correlation coefficient was 0.71 and slope was 0.96). However, the VMR and VCD of HONO were 0.01-2ppb and $3.5 \times 10^{14} - 7.0 \times 10^{15}$ molec./cm², respectively. Moreover, the concentration of HONO mainly concentrated within 100m near the surface and decreased obviously with the increase of the altitude. The average HONO/NO₂ ratio was 2.38% (VMR) and 4.88% (VCD), and the correlation between HONO and NO₂ was 0.62, indicated that HONO was mainly derived from NO₂ conversion during the study period. The transfer from the urban area of Hefei was the main source for the HONO and NO₂ in the study area during the pollution period by combining the analysis of the wind field. Besides, sources from the northern and northwestern of Anhui also had a significant effect for the study area.

Measurement of water vapor in blue light band based on MAX-DOAS and seasonal correlation analysis of water vapor and aerosol extinction in Qingdao

Hongmei Ren*, Ang Li, Zhaoku Hu, Yeyuan Huang, Jin Xu, Pinhua Xie, Hongyan Zhong

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Presenter: Hongmei Ren

Abstract:

Obtaining the vertical column density (VCD) and profile of atmospheric water vapor is of great significance for the study of water vapor transport and weather conditions, and water vapor plays an important role in the formation and accumulation of PM_{2.5}. In this paper, multi-axis differential optical absorption spectroscopy (MAX-DOAS) is used to measure the water vapor and aerosol extinction simultaneously, and the water vapor and aerosol extinction profiles are retrieved. The convolution method with the instrument's slit function was used to obtain the effective absorption reference section of water vapor, and then DOAS fitting was performed (the water vapor fitting band was 434nm ~ 453.5nm, and the O₄ fitting band was 338nm ~ 370nm) to obtain the slant column density (SCD). Calculate AMF through atmospheric radiation transmission model, then calculate water vapor VCD and AOD according to SCD and AMF, finally use PriAM algorithm based on optimal estimation method to retrieve aerosol extinction profile and water vapor profile (0 ~ 4km). The monthly mean profile data of the European Centre for Medium-Range Weather Forecasts (ECMWF) is used as the prior profile for water vapor retrieve in the current month. This inversion method was applied to the monitoring data of Qingdao MAX-DOAS site from March 4, 2019 to March 31, 2019, and correlation analysis was performed between the water vapor VCD result retrieve from MAX-DOAS and the ECMWF vertical column density daily mean data, $R^2 = 0.93$; comparing the profile data of MAX-DOAS and ECMWF, the 50m, 200m, 400m, and 600m water vapor mixing ratio data retrieve from MAX-DOAS and the 35m, 196m, 405m, and 570m data download from ECMWF, the coefficient of determination R^2 are of 0.70, 0.83, 0.88, and 0.88, respectively. The results verify the feasibility of retrieve water vapor VCD and profile based on MAX-DOAS in the blue light band. Using the observation data of Qingdao MAX-DOAS site from March 4, 2019 to March 3, 2020, retrieve VCD of water vapor and AOD, and linear regression analysis was performed on AOD and water vapor VCD every month. The monthly AOD and water vapor VCD have a good linear relationship, and the correlation is higher in winter and autumn, and lower in summer and autumn.

Retrieving the spatial distribution of trace gases using measurements of three ground-based MAX-DOAS instruments and vertical concentration profiles

Michael Revesz*, Stefan F. Schreier, Philipp Weihs, Tim Bösch, Kezia Lange, Andreas Richter, Mihalis Vrekoussis, Alois W. Schmalwieser

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Presenter: Michael Revesz

Abstract:

A method to retrieve the spatial distribution of trace gases using data from three ground-based MAX-DOAS instruments was developed within the project VINDOBONA (VIenna horizontal and vertical Distribution OBServations Of Nitrogen dioxide and Aerosols). The method was applied and evaluated on the example of NO₂. At three different locations around the inner districts of Vienna, Austria, MAX-DOAS measurements are performed in the visible and partially in the UV spectral range. Each instrument is set up to determine the column densities in different azimuthal directions and at low elevation angles within approximately a horizontal plane. The different lines of sight of the three instruments intersect horizontally and can be used to estimate the horizontal spatial distribution of trace gases.

In this method, the intersections of the different lines of sight from the three MAX-DOAS instruments define segments along the slant columns. From the measured slant column densities and the segment lengths the mass concentration for all intersecting segments can be estimated. Since the three instruments in Vienna were set up at different altitudes and are performing lowest horizontal measurements at different elevation angles, corrections are required to account for changes in trace gas concentration with altitude. A suitable "concentration scaling"-factor can be derived from the known vertical profiles for the chosen trace gas.

A few difficulties were identified: Evaluation of the new method using in-situ measurement data appears to be difficult as those measurements may sense localised peaks in trace gas concentration. Further, possibly larger uncertainty of the vertical profiles in ground-proximity has a significant impact on the retrieved spatial distribution of trace gases. Car-DOAS measurements are expected to improve the evaluation of the new method.

Mapping NO₂ at the University of Colorado Boulder: a DOAS Educational Experience

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Presenter: Margarita Reza

Abstract:

Differential Optical Absorption Spectroscopy (DOAS) is widely used to quantify atmospheric trace gas concentrations on local and global scales. This presentation describes a NO₂ mapping experiment using zenith scattered solar photons (zenith sky DOAS) as part of a graduate level course in Analytical Atmospheric Spectroscopy (CHEM5161) at the University of Colorado Boulder. This exercise aims to familiarize 1st year graduate students with the operation of a spectrometer, wavelength calibration, collection of field measurements (zenith scattered light spectra), retrieval of NO₂ dSCDs using the QDOAS software, and to practice data analysis skills. Students have the opportunity to evaluate the effects of viewing geometry by varying the elevation angle as they collect data at the University of Colorado Boulder main campus. With the integration of GPS data, students then generate a map showing how NO₂ varies temporally and spatially. Enhancements of NO₂ were observed along the CU Boulder East District and West District energy plants, a construction site, and a parking lot. Evaluation of wind data in context of the location of these NO_x sources (NO_x = sum of NO and NO₂) is used to corroborate the validity of the spatial NO₂ distributions. The emission flux of NO_x is then calculated using the divergence flux method, correlating NO₂ enhancements over the background with the location of power plants on campus, after consideration of chemical sinks, transport times, and NO_x partitioning. The NO₂ mapping experiment serves as a powerful educational experience that aids in students' understanding of the DOAS method and facilitates discussion of satellite applications to pinpoint NO_x emissions from space (e.g., Beirle et al., 2019). The experiment employs relatively low cost Avantes USB-2 spectrometers, along with Avantes AvaSoft 8 software and a GPS smartphone application, both of which are free. This practical experiment can easily be modified to study different research questions relevant to graduate students of atmospheric chemistry. Current limitations in the available hardware, and potential adaptations for the undergraduate curriculum in analytical chemistry, environmental studies, physics, or engineering are also discussed.

Towards emission fluxes from wildfires: evaluation of divergence fluxes of inert and reactive gases

Jake P. Rowe*, Christoph Knote, Natalie Kille, Kyle J. Zarzana, Johana Romero, Theodore K. Koenig, Christopher F. Lee, Nicolas Theys, Christopher Lerot, Isabel de Smedt, Michel van Roozendaal and Rainer Volkamer

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Presenter: Jake Rowe

Abstract:

The Biomass Burning Fluxes of Trace Gases and Aerosols (BB-FLUX) field campaign was carried out during the summer of 2018 with the primary goal of quantifying emission fluxes of trace gases such as CO, NH₃, and others from wildfires. To characterize these emission fluxes, the University of Colorado Solar Occultation Flux (CU SOF) instrument was deployed to measure vertical trace gas columns through biomass burning plumes along the direct solar beam. While these methods have proved successful from an aircraft for individual wildfires, satellites could enable emission flux characterizations on a global scale. The Sentinel-5 Precursor (S5P) satellite, which houses the TROPOspheric Monitoring Instrument (TROPOMI), provides a unique opportunity to quantify and validate emission fluxes from space due to its higher spatial resolution and signal to noise as compared to previous satellites. This allows one to observe area sources such as wildfires and measure reactive trace gases such as NO₂, HCHO, CHOCHO, and more recently also HONO. The satellite swath has broad spatial coverage, but limited temporal coverage. By contrast the aircraft has broader temporal coverage of individual wildfires for any given day. This presentation actively bridges between these different temporal and spatial sampling scales to study the evolution of the wildfire plume using the FLEXible PARTticle Dispersion Model (FLEXPART). The columns measured from the aircraft, as well as aerosol profiles and in situ wind measurements are used to assess the model performance in the context of plume injection heights, modeled wind profiles, and ultimately their impacts on emission fluxes derived from the divergence flux approach. Once the wind field is well-established, we also apply it to S5P/TropOMI satellite maps of selected trace gases. The temporal flux evolution will be evaluated, comparing the aircraft perspective with that extracted from stationary 2D satellite images, and a total error budget will be determined.

MAX-DOAS HCHO measurements: comparison with TROPOMI and FTIR in Australasia

Robert Ryan*, Jeremy Silver, Richard Querel, Dan Smale, 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:

Measurements of volatile organic compounds (VOCs) are lacking from Australasia, a region with large isoprene emission hotspots. Here we present two and a half years of formaldehyde (HCHO) measurements from Melbourne, Australia and Lauder, New Zealand (December 2016 – May 2019). We compare MAX-DOAS formaldehyde measurements in the remote rural environment of Lauder to co-located FTIR HCHO measurements. The HCHO vertical column measurements from the MAX-DOAS and FTIR have similar seasonality and magnitude. Furthermore, MAX-DOAS measurements at Melbourne and Lauder are compared against coincident TROPOMI HCHO measurements. TROPOMI performs very well over Melbourne, with summertime daily comparison yielding a linear regression slope of 1.0 and R² of 0.59. Over one year of monthly average results the regression slope was 1.0 with R² of 0.90, a vast improvement over OMI results which did not capture any season HCHO variation at this location. Over Lauder, TROPOMI observes the seasonality and magnitude of HCHO vertical columns (as measured by the ground-based instruments). Regions of high HCHO production corresponding with forested and rural areas around Melbourne can be identified using TROPOMI, highlighting the importance of these results for future VOC studies in Australasia.

Real driving NO_x emission measurements of vehicles and detection of manipulated emission control systems with ICAD-NO_x-instruments for plume chasing

Christina Schmidt*, D. Pöhler, T. Engel, U. Roth, M. Horbanski, J. Lampel, T. Bütler, J. Janssen, N.E. Ligterink, J.-P. Lollinga, P.A.J. Tilanus and U. Platt

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Presenter: Christina Schmidt

Abstract:

Poor air quality in urban areas is mainly caused by nitrogen oxides (NO_x) emissions from vehicles, which are regulated by the EURO norm (EURO V: 2000mg/kWh, EURO VI: 400mg/kWh). Existing possibilities to measure if the vehicles comply with the regulations (e.g. PEMS: Portable Emission System) are rare and costly. With the Plume Chasing (PC) method, it is possible to easily and accurately measure the emissions of a vehicle in real driving situations by analysing the diluted emission plume behind the investigated vehicle. With this, it can be perfectly used for the detection of malfunctioning or illegally manipulated emission control systems (ECS). For PC the ICAD-NO_x+CO₂-instrument has many advantages in comparison to other instruments. The fast measurement with high accuracy and mobile applicability allows relatively simple emission studies. We focus especially on trucks on roads all over Europe. Some of the latest studies are presented.

In 2018 and 2019 studies on German and Austrian highways showed that among several hundreds of trucks up to 35% of the EURO V trucks and up to 25% of the EURO VI trucks showed consistently high emissions above the EURO norm, which provides strong evidence for a high number of defect or manipulated ECS. With the help of the police, manipulated ECS could be found in some of the trucks with very high emissions.

To further validate PC and optimise the measurement setup, studies with PEMS on board of the measured vehicles took place in Sweden and the Netherlands in Nov 2019 and Feb 2020. During a 3-day study in Sweden, PC of a EURO V and a EURO VI truck for several hours in different geographic conditions was performed with and without the emission cleaning system being activated. The derived PC NO_x emission values even for short measurement times of 1 and 2 minutes showed very good agreement with the averaged PEMS NO_x data of the trucks. The study demonstrated the robustness of the PC method to investigate high emitter trucks. In the EU project CARES, PC is further developed. Therefore a PC measurement bus from TNO, Netherlands, is fully equipped with different instruments including several ICAD-NO_x+CO₂-instruments, LICORs for CO₂ or CPCs for particles. Different measurement configurations are tested and optimised together with improved data analysis algorithms. The main goal is to develop PC for institutional operation, e.g. by the police. First results will be presented.

Spatial variability of vertical NO₂ and aerosols profiles in Vienna observed by three ground-based MAX-DOAS instruments

Stefan F. Schreier*, Andreas Richter, Tim Bösch, Kezia Lange, Michael Revesz, Mihalis Vrekoussis, Philipp Weihs, Alois W. Schmalwieser, John P. Burrows

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Presenter: Stefan Schreier

Abstract:

Since December 2016, April 2017, and August 2018, three ground-based MAX-DOAS instruments continuously record daytime spectral UV/vis measurements in the urban environment of Vienna, Austria. The three instruments are operating in two configurations: (1) elevation scans at fixed azimuthal directions and (2) azimuthal scans at fixed elevation angles. In the present work, we investigate the spatial variability of vertical NO₂ and aerosol profiles over the urban environment of Vienna by analyzing long-term measurements obtained with the former configuration. The retrieval of vertical profiles is based on BOREAS (Bremen Optimal estimation REtrieval for Aerosols and trace gaseS). Additional BOREAS retrieval results such as near-surface NO₂, near-surface aerosol extinction coefficient, and AOD are compared with co-located in situ, ceilometer, and sun photometer observations.

Comparing ground-based MAX-DOAS measurements with airborne imaging DOAS measurements of ship emission plumes

André Seyler*, Andreas C. Meier, Folkard Wittrock, Lisa Kattner, Barbara Mathieu-Üffing, Enno Peters, Andreas Richter, Thomas Ruhtz, Anja Schönhardt, Andreas Weigelt, Stefan Schmolke, John P. Burrows

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Presenter: André Seyler

Abstract:

Simultaneous measurements and DOAS retrievals in the UV and visible spectral range can be used to probe air masses at different horizontal distances to the instrument to estimate two-dimensional pollutant distributions. Applying an "onion peeling" like approach to MAX-DOAS measurements of ship emissions on the island Neuwerk in the German Bight allows to investigate the strongly inhomogeneous NO₂ field over a shipping lane and provides the ability to derive the approximate plume positions in the observed area as well as to detect pollution several kilometers away from the instrument under wind directions unfavorable for in situ measurements. Airborne imaging DOAS measurements of ship emissions in the vicinity of the Neuwerk station have been performed during the NOSE (Nord-Ost-See Experiment) campaign 2013 in the framework of the MESMART project (see www.mesmart.de), a cooperation between the IUP Bremen and the German Federal Maritime and Hydrographic Agency (BSH). The measurements of the AirMAP (Airborne imaging Differential Optical Absorption Spectroscopy instrument for Measurements of Atmospheric Pollution) instrument on-board a Cessna 207 Turbo from the FU Berlin provide very detailed NO₂ maps of ship plumes, which at the same time have been probed by MAX-DOAS measurements. The direct comparison of both measurement techniques, with the MAX-DOAS instrument measuring horizontal transects of the plume having the possibility to scan the plume vertically by using different elevation angles and the AirMAP instrument measuring in nadir direction downward from the aircraft observing vertical transects of the plume provides mutual benefits: The MAX-DOAS measurements deliver horizontal columns or path averaged concentrations integrated over several kilometers, but contain no information about the fraction of the light path actually probing the plume, which the NO₂ maps of AirMAP can. The AirMAP measurements deliver vertical columns of NO₂ between ground and aircraft, but no information about the vertical location of the NO₂ inside the column, which the MAX-DOAS instrument's vertical scans can. It's the combination of both methods which makes it possible to derive in-plume NO₂ concentrations from each method, which agree quite well. For validation purposes, a simple Gaussian plume model was used to simulate the plumes' dispersion in lateral and vertical direction under the given weather conditions and to compare with the measurements.

MICRU effective cloud fractions for S-5P/TROPOMI

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

*) MPI for Chemistry, Mainz, Germany; holger.sihler@mpic.de

Presenter: Holger Sihler

Abstract:

We present results of effective cloud fractions retrieved from measurements of the Tropospheric Monitoring Instrument (TROPOMI) using the Mainz Iterative Cloud Retrieval Utilities (MICRU) algorithm. Cloud fraction (CF) data is used to study the distribution of clouds in general. Furthermore, CF is a crucial input parameter for retrievals of tropospheric trace gases from satellite measurements in the UV/vis spectral region because CF errors may even dominate vertical column density (VCD) retrieval errors of tropospheric trace gases. The MICRU algorithm has been specifically developed to retrieve small cloud fractions ($CF < 20\%$) at high accuracy in order to improve retrievals of tropospheric trace gases. Here, MICRU is applied to TROPOMI data offering a more than 100 times higher spatial resolution compared to GOME-2 (Global Ozone Monitoring Experiment-2), on which it was previously applied. Hence, MICRU CF can be used as an alternative to the operational CF product. The most important feature of MICRU is the derivation of the minimum reflectance map from the measurements themselves. The algorithm builds on the assumption that the surface is dark compared to clouds, and it is therefore limited to regions not permanently covered by clouds, ice or snow. In particular, the MICRU algorithm applies four parameters to constrain interferences with surface BRDF effects like sun glitter and shadowing. Our approach features a lower threshold map parameterised by time, viewing zenith angle, scattering angle, and reflection angle. We demonstrate that MICRU, compared to the operational cloud fraction algorithms OCRA and FRESCO, interferences less with viewing angle, solar glitter, and shore lines and, hence, significantly improves the determination of cloud fractions. Furthermore, CF features made visible by the unprecedented spatial resolution of TROPOMI are discussed.

EMI formaldehyde retrieval over China

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Presenter: Wenjing Su

Abstract:

We present formaldehyde (HCHO) retrieval for the Environmental trace gas Monitoring Instrument (EMI) which was launched on May 9, 2018 Onboard the Chinese GaoFen-5 (GF5) satellite. The slant column density (SCD) is retrieved using the basic optical differential spectroscopy (BOAS) technique, while air mass factor (AMF) is calculated with a priori HCHO profile from a higher resolution regional chemistry transport model. The retrieved EMI HCHO VCD is compared with TROPospheric Monitoring Instrument (TROPOMI) tropospheric HCHO VCD and with the ground based Multi-AXis Differential Optical Absorption Spectroscopy (MAX-DOAS) measurements in China. The results indicate EMI captures similar spatial patterns and amplitude of TROPOMI HCHO distribution. Good correlation is also found between pixel-to-pixel daily comparisons of EMI and TROPOMI HCHO observations over the North China Plain.

Assessment of the TROPOMI tropospheric NO₂ product based on airborne APEX observations

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Presenter: Frederik Tack

Abstract:

Sentinel-5 Precursor (S-5P), launched in October 2017, carrying the TROPospheric Monitoring Instrument (TROPOMI) nadir-viewing spectrometer, is the first mission of the Copernicus Programme dedicated to the monitoring of air quality, climate, and ozone. Its characteristics, such as the fine spatial resolution, introduce many new opportunities and challenges, requiring to carefully assess the quality and validity of the generated data products by comparison with independent reference measurements. In the presented study, the TROPOMI tropospheric nitrogen dioxide (NO₂) L2 product (3.5 x 7 km² at nadir observations) has been validated over strongly polluted urban regions by comparison with coincident high-resolution Airborne Prism EXperiment (APEX) remote sensing observations (~100 m²). Satellite products can be optimally assessed based on (APEX) airborne remote sensing observations as a large amount of satellite pixels can be fully mapped at high accuracy and in a relatively short time interval, reducing the impact of spatio-temporal mismatches. In the framework of the S5PVAL-BE campaign, the APEX imaging spectrometer has been deployed during four mapping flights (26-29 June 2019) over the two largest urban regions in Belgium, i.e. Brussels and Antwerp, in order to map the horizontal distribution of tropospheric NO₂. Per flight, 10 to 20 TROPOMI pixels were fully covered by approximately 2800 to 4000 APEX measurements within each TROPOMI pixel. The TROPOMI and APEX NO₂ vertical column density (VCD) retrieval schemes are similar in concept. L2 TROPOMI NO₂ VCDs are well correlated ($R > 0.9$) but biased low with respect to airborne APEX NO₂ retrievals. The bias is smaller ($-1.0\% \pm 12\%$ instead of $-14\% \pm 12\%$, on average) when compared to a custom NO₂ product, based on CAMS regional ENSEMBLE a priori profiles as it better captures the strong gradients in urbanised areas. However, both the standard and custom product are within the targeted bias of 25-50% for the tropospheric NO₂ product. The APEX data set allows as well to study the TROPOMI subpixel variability and impact of signal smoothing due to its finite satellite pixel size. The amount of underestimation of peak plume values and overestimation of urban background values in the TROPOMI data is in the order of 1-2 x 10¹⁵ molec cm⁻² on average, or 10% - 20%, depending on the amount of heterogeneity in the NO₂ field and assuming a TROPOMI pixel size of 25 km².

An automated dynamic chamber system combining IB-BCEAS to measure HONO flux and NO₂ flux in farmland

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Presenter: Ke Tang

Abstract:

A HONO flux and NO₂ flux measurement system was developed for continuous field measurement by using an IB-BCEAS combined with an automated dynamic chamber. The air cylinder is used to control the opening and closing of the lid of the dynamic chamber to ensure that the material energy inside and outside the chamber can be exchanged in time. During the brief closing of the lid, the concentrations of HONO and NO₂ in the dynamic chamber are measured by IB-BCEAS. The uniformity of gas mixing in the dynamic chamber was verified by measuring the concentration of HONO at different sampling heights. The diurnal variation of HONO flux before and after rainfall showed two different trends. Before rainfall and later stage after rainfall (FR), the maximum of HONO flux appeared in the morning, then decreased gradually. At the early stage after rainfall (BR), HONO flux gradually increased in the morning, and reached the maximum in the afternoon, the maximum of HONO flux was 7.69 ng N m⁻² s⁻¹. There was no significant correlation between HONO flux and temperature in FR period, but the correlation coefficient (R²) between HONO flux and temperature reached 0.78 in BR period, and the correlation coefficient between NO flux and HONO flux reached more than 0.6 in FR period and BR period. the HONO flux of fresh soil samples was the same order of magnitude as that of field observation. NO₂ shows negative emission in most time periods, and soil is the sink of NO₂. The correlation coefficient (R²) between ambient NO₂ concentration and NO₂ flux is 0.79, and the compensation point of NO₂ is 5ppb.

Implications for deriving absolute effective O3 temperature

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Presenter: Martin Tiefengraber

Abstract:

Accurate O3 column retrievals from direct or scattered sunlight depend on the knowledge of the absolute effective O3 temperature (O3temp), a measure for the O3 weighted atmospheric temperature. O3temp is used to scale the strongly temperature dependent O3 absorption cross sections, but already an error of 1 K translates to about 1 DU slant column error for total column measurements. Since common DOAS like O3 retrievals usually apply a fixed O3temp, a resulting seasonal bias e.g. lessens the usability for satellite validation.

In BlickP, the operational processor for Pandora data, the temperature dependency of gas absorption is accounted for by parameterizing the cross sections. This allows for the direct retrieval of the O3temp as part of the spectral fitting procedure and therefore avoids a temperature error in the O3 columns.

Beside the calibration, the accurate knowledge of the wavelength registration of the Fraunhofer reference spectrum plays a crucial role in the accuracy of the retrieved O3temp. This aspect, and possible consequences for the wavelength registration of O3 cross sections are discussed in this presentation. Further, implications for the retrieval of columnar SO2 are considered.

Spatiotemporal variations of NO_2 over Fukuoka Japan, observed by multiple MAX-DOAS and 3-D coherent Doppler lidar

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Presenter: Hironobu Ueki

Abstract:

To clarify spatiotemporal variations and transport processes in nitrogen dioxide (NO_2) over Fukuoka, an urban area in Japan, continuous NO_2 profile observations using Multi Axis Differential Optical Absorption Spectroscopy (MAX-DOAS) with high temporal resolution of four minutes have been conducted since October 2018 at three observatories: Yakuin (33.580°N, 130.396°E), Sohara (33.580°N, 130.356°E) and Fukuoka University (33.550°N, 130.364°E).

We first performed case studies at particular days and observed enhanced NO_2 contents above the city center on some days. In the case of 29 November 2018, high NO_2 concentrations were observed near the ground in the morning (around 7:00–10:30 am). Higher contents of NO_2 appeared gradually at higher altitudes over the urban area, and disappeared at around 13:30–14:00 pm. We investigated a three-dimensional (3-D) wind field observed using a 3-D coherent Doppler lidar installed at Fukuoka University. The NO_2 variations were consistent with the wind variation: the air mass with high NO_2 concentration was transported upward from near the ground over an urban area; it advected southward (landward) because of a sea breeze in the afternoon.

We also validated the tropospheric NO_2 vertical column density (VCD) using the Sentinel-5P/TROPospheric Ozone Monitoring Instrument (TROPOMI) satellite with MAX-DOAS observations. Results showed that the satellite data are underestimates, as shown in earlier studies (e.g., Kanaya et al., 2014), but large variations exist from 34% to 154%. These results suggest that underestimation can be attributable not only to the shield effect by aerosols near the ground but also to inhomogeneity and transport processes of the NO_2 air mass over urban areas.

TROPOMI SO₂ column retrievals: validation, inter-comparison with other satellite data sets and algorithm evolution

Nicolas Theys*, C. Li, N. Krotkov, I. De Smedt, C. Lerot, H. Yu, J. Vlietinck, V. Fioletov, P. Hedelt, D. Loyola, T. Wagner, M. Van Roozendael

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Presenter: Michel Van Roozendael

Abstract:

Since nearly two years, the operational SO₂ product from the TROPOspheric Monitoring Instrument (TROPOMI) onboard Sentinel-5 Precursor (S5P) platform has provided important information on volcanic and anthropogenic SO₂ emissions, with an unprecedented level of details. In this presentation, we critically discuss the advantages and disadvantages of the current operational algorithm in light of the validation results obtained so far, and present how the retrieval scheme could evolve in the future. In the first part, we briefly present the main algorithm features and an overview of the SO₂ product validation. One challenge in this respect is the current lack of ground-based SO₂ measurements for anthropogenic source regions. We therefore rely largely on comparisons with other satellite datasets (e.g., OMI and OMPS). The main lesson learnt is that satellite SO₂ retrievals generally agree very well for large SO₂ columns (mostly volcanic) while persisting differences exist for low columns when different algorithms are compared. This motivates the second part of the presentation which aims at extensively comparing the results from existing S5P SO₂ operational and scientific algorithms, notably DOAS and PCA retrievals (or other alternative approaches). Here, all configuration settings and auxiliary data (e.g. absorption cross-sections) are aligned in order to better understand the differences through sensitivity tests. This effort is not only important to improve the TROPOMI SO₂ results but it is also particularly relevant in the context of the forthcoming Sentinel-4 mission that will mainly probe weak anthropogenic SO₂ sources. The last part of the presentation gives a general overview of new features planned for the next versions of the operational SO₂ algorithm.

Spatial and temporal changes of SO₂ regimes over China in recent decade and the driving mechanism

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Presenter: Ting Wang

Abstract:

The spatial and temporal changes of SO₂ regimes over China during 2005 to 2016 and their associated driving mechanism are investigated based on a state-of-the-art retrieval dataset. Climatological SO₂ exhibits pronounced seasonal and regional variations, with higher loadings in wintertime and two prominent maxima centered in the North China Plain and the Cheng-Yu District. In the last decade, overall SO₂ decreasing trends have been reported nationwide, with spatially varying downward rates according to a general rule—the higher the SO₂ loading, the more significant the decrease. However, such decline is in fact not monotonic, but instead four distinct temporal regimes can be identified by empirical orthogonal function analysis. After an initial rise at the beginning, SO₂ in China undergoes two sharp drops in the periods 2007–2008 and 2014–2016, amid which 5-year moderate rebounding is sustained. Despite spatial coherent behaviors, different mechanisms are tied to North China and South China. In North China, the same four regimes are detected in the time series of emission that is expected to drive the regime of atmospheric SO₂, with a percentage of explained variance amounting to 81%. In contrast to North China, SO₂ emissions in South China exhibit a continuous descending tendency, due to the coordinated cuts of industrial and household emissions. As a result, the role of emissions only makes up about 45% of the SO₂ variation, primarily owing to the decoupled pathways of emission and atmospheric content during 2009 to 2013 when the emissions continue to decline but atmospheric content witnesses a rebound. Unfavorable meteorological conditions, including deficient precipitation, weaker wind speed and increased static stability, outweigh the effect of decreasing emissions and thus give rise to the rebound of SO₂ during 2009 to 2013.

Soil and anthropogenic source of nitrous acid observed by MAX- DOAS operated in the North China Plain

Yang Wang*, Steffen Dörner, Sebastian Donner, Russell R. Dickerson, Zhanqing Li, Xinrong Ren, Yuying Wang, Thomas Wagner

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Presenter: Yang Wang

Abstract:

Nitrous acid (HONO) can considerably contribute to tropospheric OH radicals, which impact oxidation of trace gas pollutants to form fine particles. Unexpected high concentrations of HONO during the daytime have been reported by some observations all over the world. We operated a Multi Axis (MAX-) DOAS instrument in the rural area of Xingtai, which is one of the most polluted cities in China and is located on the western edge of the large industrial zone of the North China plain, in the period from May to June 2016. Vertical profiles of HONO, together with NO₂, SO₂, HCHO, and aerosols, are retrieved from the MAX-DOAS instrument. Meteorology conditions, including winds, temperatures, humidity, and precipitations, were also measured during the campaign. Meanwhile effects of regional transports on pollutants can be analyzed based on HYSPLIT trajectories. MAX-DOAS observed that high amounts of HONO were often observed for air masses from the southern industrialized areas. The phenomenon indicates that anthropogenic emissions can significantly contribute to morning HONO amounts in an area far away from the source by up to 50 km. In addition, MAX-DOAS observed high HONO concentrations (up to 1ppb near the ground), but low NO₂ concentrations around noon on some days. Since the phenomenon can not be explained by the well-known reaction of NO with OH, missing HONO source is expected and its emission rate is estimated as up to 250 ng m⁻² s⁻¹. Soil emissions of HONO could explain the phenomenon, because the measurement station was dominantly surrounded by wheat and cotton fields, which has been proved to emit a substantial amount of HONO under the appropriate soil temperature and water content based on studies in laboratories. The appropriate soil condition was reached at the time when the large HONO amount was observed by the MAX-DOAS instrument around noon.

A MAX-DOAS aerosol profile retrieval algorithm based on look-up table method: application to high-altitude measurements at Schneefernerhaus (UFS), Germany

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Presenter: Zhuoru Wang

Abstract:

We developed a MAX-DOAS aerosol extinction profile retrieval algorithm based on the look-up table (LUT) method. It is applied to retrieve aerosol profiles from the long-term measurements at a high altitude site — the Environmental Research Station Schneefernerhaus (UFS), Germany, located near the summit of Zugspitze at an altitude of 2650 m.

Aerosol profiles are parameterized as aerosol extinctions in 3 layers (0–0.5, 0.5–1 and 1–2 km). A profiles set consists of 7553 profiles is defined, which is assumed to cover all possible profiles under clear-sky. In the retrieval, simulated O_4 DSCDs for all the profiles in the profile set are derived from the LUT. The cost functions are calculated for each profile based on the simulated O_4 DSCDs, the O_4 DSCD observations as well as the measurement uncertainties. Valid profiles are selected from all the possible profiles according to the cost function, and the optimal solution is defined as the weighted mean of all the valid profiles. A comprehensive error analysis is performed to better estimate the total uncertainty. Based on the assumption that the profile set covers all possible profiles, we determined a set of O_4 DSCD scaling factors for different elevation angles and wavelengths. The profiles retrieved from synthetic measurement data can reproduce the synthetic profile. The result also shows that the retrieval is insensitive to measurement noise, indicating the retrieval is robust and stable. The aerosol optical depths (AODs) retrieved from the long-term measurements were compared to coinciding and co-located sun photometer observations. High correlation coefficients (R) of 0.733 and 0.798 are found for measurements at 360 and 477 nm, respectively. The MAX-DOAS measurements also indicate that the aerosol extinction decreases with increasing altitude during all seasons, which agrees with the co-located ceilometer measurements. Our results also show maximum AOD and maximum Ångström exponent in summer, which is consistent with observations at an AERONET station located ~ 43 km from the UFS.

Wintertime aerosol, NO₂ and HONO distributions from MAX-DOAS observations in Sichuan, southwest China

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Presenter: Chengzhi Xing

Abstract:

Ground-based multi-axis differential optical absorption spectroscopy (MAX-DOAS) observations were operated from 02 to 21 December 2018 in Leshan, southwest China, to measure HONO, NO₂ and aerosol extinction vertical distributions, and these were the first MAX-DOAS measurement results in Sichuan Basin. During the measurement period, characteristic ranges for surface concentration were found to be 0.26 to 4.58 km⁻¹ and averaged at 0.93 km⁻¹ for aerosol extinction, 0.49 to 35.2 ppb and averaged at 4.57 ppb for NO₂ and 0.03 to 7.38 ppb and averaged at 1.05 ppb for HONO. Moreover, vertical profiles of aerosol, NO₂ and HONO were retrieved from MAX-DOAS measurements using the Heidelberg Profile (HEIPRO) algorithm. By analysing the vertical gradients of pollutants and meteorological information, we found that aerosol and HONO are strongly localised, while NO₂ is mainly transmitted from the north direction (city center direction). Nitrogen oxides such as HONO and NO₂ are important for the production of hydroxyl radical (OH) and oxidative capacity in the troposphere. In this study, the maximum value of OH production rate from HONO is about 0.63 ppb h⁻¹, and maximum value of ratio between OH production from HONO and from (HONO+O₃) is up to 75% during 10:00-11:00 in Leshan. In addition, combustion emission contributes to 26% for the source of HONO in Leshan, and we found that more NO₂ being converted to HONO under the conditions with high aerosol extinction coefficient and high relative humidity is also a dominant factors for the secondary produce of HONO. The soil emission might also be an important source of HONO based on the soil water content (SWC) being 15%-27% in this area.

Observation of two-dimension distribution of NO₂, SO₂ and HCHO from plumes using imaging DOAS technology

Jin Xu*, Pinhua Xie, Ang Li, Qiang zhang, Zhaokun Hu, Xin Tian, Yeyuan Huang, Wenqing Liu

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Presenter: Jin Xu

Abstract:

In recent years, frequent pollution accidents have seriously affected human health and industrial and agricultural production. It is very important for pollution control to quickly master the temporal and spatial distribution, diffusion situation and emission flux of pollution plume. Here we developed an imaging spectroscopy remote-measuring system to carry out the two-dimensional distribution measurement study of atmospheric pollutants, using passive Imaging Differential Optical Absorption Spectroscopy (IDOAS) technology and image optimization algorithms. It covers the wave range of 290 to 450nm with the resolution of 0.3nm. It takes 1 to 5 minutes to finish one scanning procedure. In order to obtain accurately matched two-dimensional distribution information of pollutants, a dual-channel system combining ultraviolet spectrum and visualized images was developed to filter and process the data matching. Aiming at the data processing of pollutants under complex backgrounds, especially the problem of missing data under the conditions of dense smoke and obstacles, the concentration information was optimized combining the smoke plume diffusion model and the curved cubic spline interpolation algorithm. We carried out remote measurements aiming at factory chimneys, ship emissions, the two-dimensional distribution information of pollutants (NO₂, SO₂, HCHO) is obtained, the emission flux of the chimneys was estimated.

First observation of tropospheric nitrogen dioxide from the Environmental Trace Gases Monitoring Instrument onboard the GaoFen-5 satellite

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Presenter: Chengxin Zhang

Abstract:

The Environmental Trace Gases Monitoring Instrument (EMI) is the first Chinese satellite-borne UV-Vis spectrometer aiming to measure the distribution of atmospheric trace gases on a global scale. The EMI instrument onboard the GaoFen-5 satellite was launched on 9 May 2018. In this paper, we present the tropospheric nitrogen dioxide (NO₂) vertical column density (VCD) retrieval algorithm dedicated to EMI measurement. We report the first successful retrieval of tropospheric NO₂ VCD from the EMI instrument. Our retrieval improved the original EMI NO₂ prototype algorithm by modifying the settings of the spectral fit and air mass factor calculations to account for the on-orbit instrumental performance changes. The retrieved EMI NO₂ VCDs generally show good spatiotemporal agreement with the satellite-borne Ozone Monitoring Instrument and TROPOspheric Monitoring Instrument (correlation coefficient R of ~ 0.9 , bias below 50 Differential Optical Absorption Spectroscopy) observations also shows good correlation with an R of 0.82. The results indicate that the EMI NO₂ retrieval algorithm derives reliable and precise results, and this algorithm can feasibly produce stable operational products that can contribute to global air pollution monitoring.