Preliminary programme of the 2nd Workshop on "Remote sensing in oxygen absorption bands" 29–31 May 2024, KNMI, De Bilt, The Netherlands

Version date: 28 March 2024

Presentations are 15 minutes + 5 minutes for discussion.

Day 1: Wednesday 29 May 2024

12:00 - 13:30 Registration

13:30 - 13:40 Welcome & logistics

Session 1a

Chair: ...

15:20 - 15:40 Break

Session 1b

Chair: . . .

Day 2: Thursday 30 May 2024

Session 2a

Chair: . . .

Session 2b

<u>*Chair:*</u> ...

11:00 - 11:20	Cloud geometrical thickness's radiation pathlength account and retrieval using oxygen A band satellite measurements: past POLDER/PARASOL experience & future 3MI/EPS-SG *Nicolas Ferlay* (LOA, University of Lille)	page 13
11:20 - 11:40	Line intensity measurements and far-wing intensity redistribution in the 0.76 μm Oxygen band *Erin Adkins* (National Institute of Standards and Technology)	page 6
11:40 - 12:00	Cloud property retrieval based on DISAMAR: using Oxygen absorption band data from TROPOMI on Sentinel 5P *Xiaoyun Zhang* (KNMI)	page 41
12:00 - 12:20	Retrieval of aerosol layer height from Sentinel-3/OLCI observations *Gijsbert Tilstra* (KNMI)	page 36
12:20 - 12:30	Discussion	

12:30 - 13:40 *Lunch & Balloon launch & Group picture*

Session 3a

<u>*Chair:*</u> ...

13:40 - 14:00	Cloud top pressure retrieval from Sentinel-3 OLCI O2 A-band measurements *Rene Preusker* (Free University Berlin)	page 29
14:00 - 14:20	Retrieving XCO2, aerosols, and surface pressure from the CO2M mission *Sha Lu* (SRON)	page 24
14:20 - 14:40	Latest developments in Aerosol Layer Height retrievals from TROPOMI O2-A band measurements *Martin de Graaf* (KNMI)	page 12
14:40 - 15:00	Aerosol characterization using oxygen A-band measurements with application to CO2 retrievals *Vijay Natraj* (JPL, California Institute of Technology)	page 27
15:00 - 15:20	Proposal for intercomparison of radiative transfer simulations of the atmospheric O2 A- and B-bands *Piet Stammes* (KNMI)	page 33

15:20 - 15:40 *Break*

Session 3b

Chair: ...

17:00 - 17:20 Discussion

19:00 - ... *Dinner*

Day 3: Friday 31 May 2024

Session 4a

Chair: ...

10:40 - 11:00 *Break*

Session 4b

<u>*Chair:*</u> ...

12:20 - 12:30 Discussion

12:30 - 13:30 *Lunch*

Reception on the occasion of Piet Stammes' retirement

13:30 - 15:00 Talks by KNMI and international colleagues

15:00 - ... *Party*

Abstracts of oral & poster presentations

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

These are followed by the abstracts of the poster presentations:

Line intensity measurements and far-wing intensity redistribution in the 0.76 μm Oxygen band

Erin M. Adkins*, Ha Tran, Joseph T. Hodges

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Presenter: Erin Adkins

Abstract:

The well-known uniform atmospheric distribution of oxygen has led to frequent use of the near-infrared oxygen molecular absorption bands, centered at 0.76 μm and 1.27 μm, in remote sensing and satellite missions to measure the airmass of an atmospheric column. Fitting accurate parameterized spectroscopic models describing all relevant physics (and incorporating theoretical calculations) to laboratory measurements is critical to accurately retrieving the remote sensing target observables and uncertainties. In the Hartmann-Tran line profile, which is the recommended profile for high-resolution spectroscopy and can be reduced to the well-known Voigt profile[1], the spectrum is derived assuming that collisions occur instantaneously (impact approximation). When this approximation is not satisfied, the finite duration of collisions leads to a redistribution of the line intensity from the line cores to the far wings an effect that increases with the pressure [2-4]. While the line intensity is conserved over the line core and far-wing spectral regions, failure to account for this redistribution leads to observable depletion in the core line intensity as a function of pressure. Consequently, a spectroscopic model based on line intensities measured at low pressures would yield a biased concentration retrieval from observations acquired at higher pressures. This work reports cavity ring-down spectroscopy measurements of core line intensities and pressure-dependent line intensity redistribution in the 0.76 μm Oxygen band. The magnitude and rotational quantum number dependence of the core intensity depletion are compared to those predicted by renormalized classical molecular dynamics simulations. Additionally, we discuss how including these previously unaccounted-for physics might affect satellite and remote sensing retrievals.

1. Tennyson, J., et al., Pure and Applied Chemistry, 2014. 86(12): p. 1931-1943.
2. Reed, Z.D., et al., Phys Rev Lett, 2023. 130(14): p. 143001.
3. Tran, H., et al., J Chem Phys, 2023. 158(18).
4. Tran, H., et al., Phys Chem Chem Phys, 2023. 25(15): p. 10343-10352.

An original method to store and use LBL data in transmission form – Part I. Theory

Frederic Andre*, Rimboud Antoine, François Thieuleux, Céline Cornet, Philippe Dubuisson, Hervé Herbin

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Presenter: Frederic Andre

Abstract:

Line-by-Line data are usually stored at high spectral resolution and in an absorption coefficient form. Their application together with radiative transfer solvers based on a ray tracing approach requires evaluating transmissivities. The process is straightforward as it mostly consists of evaluating exponentials of the LBL absorption coefficients weighted by the path lengths encountered along the rays. However, in many application cases, encountered for example in remote sensing, we are not interested in the high-resolution values of transmissivities but only in spectrally averaged values. However, evaluating these averaged values directly from high resolution LBL data is computationally expensive, as it requires calculating numerous transmissivities at high spectral resolution before to compute their average.

We present in this work an original method to store and use LBL data directly in band / filter averaged transmission form (Andre, 2016). The method reduces the CPU cost required for the calculation of band / filter averaged transmissivities of uniform paths by several orders of magnitude compared to a LBL calculation, without any significant loss of accuracy. The main ideas to build and use the look-up tables will be first detailed. Then, several techniques to extend the method to non-uniform scenarios will be presented. The most recent one (Andre et al., 2023) combines the look-up table methodology to handle LBL data in transmission form with a statistical learning methodology to construct the model parameters directly from high resolution calculations over non-uniform paths. Results of the method will be illustrated in the case of the 02 A-band, for several distinct atmospheric profiles and imaging instruments of the EPS-SG mission (METimage, 3MI).

References

André, F., 2016. The L-distribution method for modeling non-gray absorption in uniform and non-uniform gaseous media. Journal of Quantitative Spectroscopy and Radiative Transfer 179, 19–32.

F. Andre, C. Delage, L. Guilmard, M. Galtier, C. Cornet (2023), Bridging physics and statistical learning methodologies for the accurate modeling of the radiative properties of non-uniform atmospheric paths. 299-306. 10.1615/RAD-23.460.

Cloud retrievals from the TROPOMI UV/VIS/NIR measurements with aerosol signature

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Presenter: Athina Argyrouli

Abstract:

TROPOMI on board of Sentinel-5 Precursor (S5P) provides continuous daily distribution of several cloud properties, which are required as input for trace-gas retrievals. The operational TROPOMI cloud retrieval involves the ROCINN (Retrieval of Cloud Information using Neural Networks) algorithm, which retrieves the cloud height, cloud optical thickness and cloud albedo from NIR radiance measurements in and around the oxygen A-band (758-771nm). Within the ROCINN algorithm two different models are applied: the Clouds-as-Reflecting-Boundaries (CRB), where the cloud is a simple Lambertian reflector, and the Clouds-as-Layers (CAL), where the cloud is a homogeneous layer of scattering liquid-water spherical particles. ROCINN requires the calculation of the sun-normalized radiances from a radiative transfer model (RTM) for simulating clear-sky and cloudy atmospheres. The contribution of atmospheric molecules in the measured NIR radiances is incorporated into the forward model through the Rayleigh scattering model. However, the contribution of larger atmospheric particles (i.e., aerosols) has not been yet considered in the RTM simulations. Some TROPOMI cloud retrievals appear as contaminated by aerosols. OCRA (Optical Cloud Recognition Algorithm), the synergistic algorithm working prior to ROCINN, which computes a radiometric cloud fraction using a broad-band UV/VIS color space approach, often derives an elevated radiometric cloud fraction corresponding to the given aerosol conditions. When OCRA retrieves a radiometric cloud fraction above a certain threshold (e.g., the threshold is 5% for TROPOMI), ROCINN is triggered and tries to further retrieve the two additional cloud parameters height and optical thickness/albedo. In heavy aerosol loads, OCRA might return falsely elevated cloud fractions. Those false alarms can usually be identified because ROCINN retrieves a cloud height close to the surface level in such cases. Nevertheless, there are cases in which ROCINN cloud outputs do not refer to the surface properties of the scene, but to aerosol layers present in the same TROPOMI footprint. In this work, we evaluated the signature of aerosols in the TROPOMI cloud retrievals with TropOMAER (TROPOMI aerosol algorithm), which derives aerosol information in cloud-free and above-cloud aerosol scenes. Validation of the aerosol layers is done via synergistic ground-based measurements from a PollyXT multiwavelength-Raman-polarization lidar and an AERONET sun-photometer.

Assessing the effects due to the sub-pixel heterogeneity in the O2 absorbing band of TROPOMI like measurements

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Presenter: Laurent C.-Labonnote

Abstract:

Modelling realistically and accurately interactions between solar radiation and atmospheric components is fundamental to assess radiative budget of the Earth and to correctly retrieve atmospheric components from remote sensing data. High spectral resolution measurements in absorbing bands such as the O2 A or B band are increasingly used for the retrieval of parameters such as the altitude or even the geometric thickness of scattering layers.

A good retrieval of these parameters nevertheless requires a detailed knowledge of the errors introduced by the forward modelling of the signal. These errors can be of different types and can result in particular from poor spectroscopic knowledge, poor representation of surface properties, poor representation of the optical properties of the scattering particles or their spatial distribution in the instrument FOV. Indeed, it is now well established that a miss-representation of the spatial heterogeneity of clouds can introduce important biases in the modelling of light reflected from them at pixel size, which highly depend on the degree of cloud heterogeneity.

In this study we use a 3D Monte-Carlo code (3DMCPOL) developed at the laboratoire d'optique atmosphérique (LOA) to quantify the sub-pixel heterogeneity effects that might be seen in the O2 absorbing bands measurements performed by the TROPOMI instrument. Different cloud configurations are analysed and a detailed study of the capabilities of the 1D approximation to reproduce 3D measurements in the A or B bands will be presented

On-going EUMETSAT developments based on the use of O2 absorption - Aerosol Layer Height (ALH) & Cloud Top Pressure (CTP) from Copernicus Sentinel-3/OLCI and EPS-SG/METimage sensors

Julien Chimot*, Loredana Spezzi, Alessio Bozzo, Rene Preusker, Martin de Graaf, Gijsbert Tilstra, Maarten Sneep, Olaf Tuinder, Ping Wang, Bertrand Fougnie

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Presenter: Julien Chimot

Abstract:

EUMETSAT is entrusted by the European Commission (EC) and its partners (ECMWF, CAMS, C3S, Met agencies) to develop a suit of Near Real Time (NRT) operational processors from Copernicus imagery O2-A sensors. As such, EUMETSAT has kicked-off two major developments: Cloud Top Pressure (CTP), and Aerosol Layer Height (ALH) from Copernicus Sentinel-3 (A and B units already flying, C unit intended for 2026), and Sentinel-3 New Generation Optical (S3-NGO), intended in the time frame of 2035.

These developments have well progressed with clear user requirements, and baseline specification (e.g. support to Atmospheric Motion Vector, further characterisation of aerosol vertical profiling). Two prototypes have been developed and further with KNMI and Berlin University partners. Evolution towards operational processors are under investigation for the next 3 years.

Moreover, in the timeframe 2025+, EUMETSAT will operate METimage, the multi-spectral high resolution imager (500m at Nadir) on board of the EUMETSAT Polar System Second Generation (EPS-SG). The METimage NRT processor suite includes the retrieval of CTP, cloud optical thickness (COT) and multi-layer flagging based on imagery in the O2-A band and surrounding VIS channels (0.6 to 1.38μm). The algorithm (named CTP-O2) has been developed for EUMETSAT by HYGEOS/University of Lille, and is based on an Optimal Estimation approach. The radiative transfer is parametrized in a Look Up Tables (LUT) as functions of surface type, COT and CTP and implicitly include parameterisations of cloud geometrical thickness and vertical water distribution. The algorithm performance has been validated on METimage synthetic data and MERIS proxy data.

In this presentation, EUMETSAT will present the lessons learned with ALH & CTP from Sentinel-3 O2-A sensors, the progress and validation, and plans for S3-NGO.

Likewise, the METimage CTP-O2 retrieval will be illustrated, together with the strategy to merge it with a classical visible / infrared cloud microphysics and bulk property retrieval algorithm.

Cloud and Aerosol Information Content in Pathlength Moments of Sunlight from O_2 Absorption Measurements

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Presenter: Anthony Davis

Abstract:

Satellite cloud/aerosol remote sensing end-users are interested in properties of the clouds and aerosols per se, a.k.a. "Level 2" products. Algorithm scientists translate "Level 1" radiances into said geophysical quantities. We argue that, in the case of O2 absorption observations, there is a "Level 1.5" product, namely, the distribution of pathlengths followed by sunlight inside the medium. These Level-1.5 products can also be the statistical moments of the pathlength distribution. We show that, unlike the Level-1 spectral (or multi-angle) radiances, the geophysical information content of successive pathlength moments is clear.

Conceptually, pathlength is tied to the time that measured light spent bouncing around inside the medium, which would normally call for a pulsed source and time-resolving sensors. However, one can also use gaseous absorption within the medium to characterize pathlengths, at least statistically. There is indeed an equivalency between pathlength distributions, in essence, "impulse responses" determined by single and multiple scattering, and their Laplace transforms, so-called "transfer functions" (TFs). The TF's independent variable is simply the absorption coefficient, assumed to be uniform. For a gas such as O2 with strong spectral variation across the absorption band, the TF is simply spectral radiances ordered by increasing absorption coefficient. Pathlength moments can be then derived from spectral data by using a short Taylor expansion of the TF.

We use numerically-validated analytical approximations applicable to aerosols and to clouds to show that:

- The 1st moment (mean pathlength) alone yields the "centroid" height of the scattering (cloud or aerosol) layer;
- Together, 1st and 2nd moments (pathlength mean and variance) yield both layer top and base heights (equivalently, the layer's top altitude and physical thickness);
- Adding the 3rd moment yields an estimate of the layer's optical thickness.

Since O2 absorption is based on spectral ratios, moments and ensuing geophysical properties can be obtained from sensors without absolute radiometric calibration. In the case of cloud optical thickness (COT) that contrasts sharply with the standard bi-spectral (Nakajima-King) technique for inferring COT and cloud-top effective particle size. Moreover, the standard technique saturates at COTs of a few tens while our O2-based 3-moment method is sensitive to arbitrarily high COTs.

Latest developments in Aerosol Layer Height retrievals from TROPOMI O2-A band measurements

Martin de Graaf*, Maarten Sneep, Mark Ter Linden, Gijsbert Tilstra, Pepijn Veefkind

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Presenter: Martin de Graaf

Abstract:

In 2019, the operational, global Aerosol Layer Height (ALH) product was released, retrieved from near-infrared measurements by TROPOMI on Sentinel-5P. The operational algorithm uses a machine learning technique in the forward model, to quickly and accurately resolve around 4000 spectral absorption lines in the O2-A band around 760 nm, and the inversion problem is solved iteratively using an optimal estimation routine, in order to have a proper error estimation.

Since its release, many important improvement have been implemented. First focused on single, selected layers of absorbing aerosols, the processor now provides the ALH for all cloud-free scenes, including scattering aerosol layers. The algorithm performed well over oceans (within the 1 km accuracy requirement) but not over land surfaces. The surface albedo is an important error source, especially over bright surfaces and for thin aerosol layers. In order to improve the retrieval over land, a surface albedo fitting routine was implemented, yielding highly improved results. For the operational processor this required the retraining of the neural network, since the derivatives to the fit parameters are needed in the optimal estimation routine. Therefore, the derivatives to surface albedo at two wavelengths in the continuum (outside the O2-A band) were added to the algorithm forward model. The result is an improved ALH accuracy over land and a large increase in the number of successful retrievals. The latest version of the S5P/TROPOMI ALH (version 2.6.0, including all these improvements and the surface fit) was released in November 2023.

The latest validation results will be presented, including ALH estimates from various instruments in space and from ground-based lidar networks. Active instruments, such as the lidars on Caliop and Aeolus have provided important insight in the vertical distribution of aerosols, but these missions had a small spatial coverage and have now ended. EarthCare will provide an important replacements for these instruments, but the daily, global coverage provided by passive instruments, such as TROPOMI, remains essential. The height of aerosols is important for many applications, such as the Earth's radiation budget, transport of aerosols, aviation, retrieval of aerosol optical thickness and the atmospheric correction.

Cloud geometrical thickness's radiation pathlength account and retrieval using oxygen A band satellite measurements: past POLDER/PARASOL experience and future 3MI/EPS-SG

Nicolas Ferlay*, Nicolas Henriot, Anthony B. Davis, Laurent C-Labonnote, Frédéric Parol, Jérôme Riédi, François Thieuleux

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Presenter: Nicolas Ferlay

Abstract:

The exploitation of measurements in the absorption band of oxygen offers a conceptually simple approach to infer from the ratio of solar backscattered radiations an effective pressure's level of scattering medium like clouds. However, an important drawback of this inference, recognized very early, in order to retrieve with accuracy cloud macrophysical parameters of clouds from such spectral measurements, is the fact that the "absorption along the scattering paths within clouds must be considered" (Yamamoto et Wark, 1961) and that "we must determine how this extra average path or this extra absorption within the clouds depends on cloud parameters" (Saiedy et al, 1965).

The exploitation of POLDER coarse-resolution oxygen A band measurements on the PARASOL plateform and its multi-year coincidence with measurements from the active sensors CALIOP and CloudSat within the A Train from 2006 to 2013 has offered a fantastic opportunity to study this additional radiation path from satellite measurements and to tackle the understanding of its dependence on the cloud geometrical thickness.

We remind here how the particular multiangular property of POLDER-like measurements permit the retrieval of the cloud geometrical thickness and to target unbiased estimate of cloud boundaries. We present the performance of the updated version of the CLOud VErtical Structure (CLOVES) PARASOL product and how we turn our objectives to the future measurements of 3MI, POLDER heritage, on EPS-SG (expected launched at the end of 2025).

Cloud top height retrieval from O2 A-band measurements: from early airborne to MERIS applications

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Presenter: Jürgen Fischer

Abstract:

Based on radiative transfer simulations a potential cloud top (pressure) height retrieval has been defined by Fischer and Grassl (1987, published in 1991), considering perturbation effects, such as varying cloud properties, sun elevation and surface albedo, which all modulate the penetration depth of the backscattered solar radiation in the O2 A band. In a first airborne campaign in 1988 the applicability of such an algorithm could be demonstrated, when cloud top heights, estimated from hyper spectral photometer, covering the O2 A-band and lidar measurements (Fischer et al, 1991). During the 'European Lidar Airborne Campaign' (ELAC) in 1990 the back-scattered sunlight in the region of the 02A-band was measured with a spectral resolution of 0.42 nm above various clouds. The analysis of this study has led to the definition of the MERIS O2 Band and its reference channel, as well latter to the three OLCI O2 A-band channels.

First satellite applications could be realized with MOS (1998, published in 2007). The cloud top pressure retrieval was based on small artificial neural networks, trained with radiative transfer simulations. Sensitivity studies have shown that an overall accuracy of 30 hPa (rmse) could be achieved for single layer clouds. The accuracy depends primarily on the optical thickness of the cloud and the reflectivity of the underlying surface.

Intensities of all rovibrational electric quadrupole absorption lines in $O_2(X^3\Sigma_g^-)$ calculated using a new quadrupole moment curve for O_2

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Presenter: Maciej Gancewski

Abstract:

There are no electric dipole components in the absorption spectrum of isolated $^{16}O_2$, since the molecule is homonuclear. The magnetic dipole and electric quadrupole transitions do occur in O_2, however, and their mutual contribution to the observed line intensity cannot always be clearly separated. In this regard, theoretical predictions concerning the intensities of absorption lines may play a decisive role in guiding the experiment and in unraveling the contribution of different multipoles to the recorded spectra. Such *ab initio* inquiries become even more important when the analyzed spectrum cannot be described simply as a product of the vibrational Franck-Condon factors and the squared modulus of some permanent molecular multipole moment. Such is the case of the electric quadrupole (E2) absorption in $^{16}O_2(X^3\Sigma_g^-)$, where the dependence of the quadrupole moment on the bond length ought to be taken into account when calculating the spectral line intensities. Furthermore, the electronic spin-spin interaction in ground-state O_2 needs to be included, leading to additional absorption lines which are absent when using the pure Hund's case$\sim$(*b*).

Here, we report the results of our *ab initio* calculations of the intensities of all rovibrational E2 transitions in $^{16}O_2(X^3\Sigma_g^-)$ corresponding to the values of the vibrational quantum number $v \leq 35$ and the total angular momentum quantum number $J \leq 40$ (these include both the vibrational overtones and hot bands). In the calculations, we use a newly computed quadrupole moment curve for the ground state of O_2 and we take into account the mixing of rotational states induced by the electronic spin-spin interaction in the effective Hamiltonian. We compare our calculated line intensities with those available in the HITRAN database which, at present, includes only the (1,0) vibrational band of the E2 absorption in $^{16}O_2(X^3\Sigma_g^-)$. Since a good agreement is observed, we recommend incorporating into HITRAN the *ab initio* line intensities for the other vibrational bands reported here.

Pressure broadening and shift of the 118 GHz line and the P1 P1 *A*-band line in O_2 perturbed by N_2 from *ab initio* calculations

Maciej Gancewski*, Hubert Jóźwiak, ikodem Stolarczyk, Ernesto Quintas-Sánchez, Rirchard Dawes, Erin Adkins, Joseph T. Hodges, Piotr Wcisło

*) Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Toruń, Poland; ganc@doktorant.umk.pl

Presenter: Maciej Gancewski

Abstract:

The absorption spectrum of atmospheric O_2 is by no means due to isolated molecules. On the contrary, interactions of O_2 with other species, such as N_2 – the most abundant ($\sim 78\%$) atmospheric constituent – impact the shape of the oxygen spectral lines, influencing their half-widths and shifts of the absorption frequencies. A detailed knowledge of such collisional effects in O_2 spectra, resulting from extensive experimental and theoretical studies, is thus required for the calibration of the remote-sensing instruments (such as the OCO-2 satellite mission) and the correct interpretation of the retrieved atmospheric spectra.

Here, we report the results of our fully quantum calculations of the N_2-induced collisional line-shape parameters of atmospheric O_2. Starting from the *ab initio* O_2-N_2 potential energy surfaces, with O_2 in the $X^3\Sigma_g^-$ and $b^1\Sigma_g^+$ electronic states, we perform close-coupling quantum scattering calculations and determine the pressure broadening and shift parameters of the fine-structure 118 GHz line in $O_2(X^3\Sigma_g^-)$ and of the P1 P1 line in the oxygen *A*-band (which involves the electronic $X^3\Sigma_g^- \rightarrow b^1\Sigma_g^+$ transition). We include the non-zero electron spin of the ground-state O_2 in our calculations. The results for the P1 P1 *A*-band line reported here are the first *ab initio* calculation of the electronic transition in a diatomic molecule perturbed by another diatomic molecule. We compare the *A*-band results with accurate experimental spectra measured using the CRDS technique.

Molecular Oxygen in HITRAN2024

Iouli E. Gordon*

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Presenter: Iouli Gordon

Abstract:

The line list of molecular oxygen was added to HITRAN (www.hitran.org) right at its inception half a century ago [1]. Since then, every quadrennial edition of the database (the most recent is HITRAN2020 [2]) featured important updates and expansions. The HITRAN2024 database (expected to be publicly released in late 2024 or early 2025) will make use of very substantial advances in oxygen spectroscopy that were reported in the last four years in all parts of the spectra from MW to UV. In recent editions, the relational structure of the database allows the provision of additional parameters that were not previously available in the traditional ".par" format. This includes the non-Voigt line shape parameters, line-mixing representations, and broadening by gases other than "self" and "air" (for instance, broadening by water vapor [3]). Collision-induced data for collision systems involving molecular oxygen will also be updated in different spectral regions. A summary of the planned updates will be provided.

[1] Rothman, L. S. 2021, Nat Rev Phys, 3, 302, http://dx.doi.org/10.1038/s42254-021-00309-2

[2] Gordon, I. E., Rothman, L. S., Hargreaves, R. J., et al. 2022, J Quant Spectrosc Radiat Transf, 277, 107949, https://doi.org/10.1016/j.jqsrt.2021.107949

[3] Tan, Y., Kochanov, R. V., Rothman, L. S., & Gordon, I. E. 2019, J Geophys Res Atmos, 33, 2019JD030929, https://onlinelibrary.wiley.com/doi/abs/10.1029/2

Estimation of Aerosol Layer Height from OLCI Measurements in the O2A-Absorption Band over Oceans

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Presenter: Lena Jänicke

Abstract:

The aerosol layer height (ALH) is an important parameter that characterizes aerosol interaction with the environment. An estimation of the vertical distribution of aerosol is necessary for studies of those interactions, their effect on radiance and for aerosol transport models. ALH can be retrieved from satellite-based radiance measurements within the oxygen absorption band between 760 and 770nm (O2A band). The oxygen absorption is reduced when light is scattered by an elevated aerosol layer. The Ocean and Land Colour Imager (OLCI) has three bands within the oxygen absorption band. We show a congruent sensitivity study with respect to ALH for dust and smoke cases over oceans. Furthermore, we developed a retrieval of the ALH for those cases and an uncertainty estimation by applying linear uncertainty propagation and a bootstrap method. The sensitivity study and the uncertainty estimation are based on radiative transfer simulations. The impact of ALH, aerosol optical thickness (AOT), the surface roughness (wind speed) and the central wavelength on the top of atmosphere (TOA) radiance is discussed. The OLCI bands are sufficiently sensitive to ALH for cases with AOTs larger than 0.5 under the assumption of a known aerosol type. With an accurate spectral characterization of the OLCI O2A bands better than 0.1nm, ALH can be retrieved with an uncertainty of a few hundred meters. The retrieval of ALH was applied successfully on an OLCI dust and smoke scene. The found ALH is similar to parallel measurements by the Tropospheric Monitoring Instrument (TROPOMI). OLCI's high spatial resolution and coverage allow a detailed overview of the vertical aerosol distribution over oceans.

15-year O2 A band dataset with TANSO-FTS onboard GOSAT

Akihiko Kuze*

*) Japan Aerospace Exploration Agency (JAXA); kuze.akihiko@jaxa.jp

Presenter: Akihiko Kuze

Abstract:

Since 2009, Thermal And Near infrared Sensor for carbon Observation Fourier-Transform Spectrometer (TANSO-FTS) onboard the Greenhouse gases Observing SATellite (GOSAT) has been providing long-term high-resolution radiance spectra with the oxygen (O2) A band to correct light path modification induced by thin clouds and aerosol scatterings. The single FTS with a common field of view provides solar scattered light at 0.76, 1.6 and 2.0μm with two orthogonal linear polarization and thermal emission, simultaneously. Together with nadir looking measurement data, we have acquired solar spectra with 0.2 cm-1 spectral resolution. In 2018, GOSAT-2 with TNASO-FTS-2 was launched. NASA OCO-2, OCO-3, and ESA TROPOMI also provide high spectral O2 A band data. JAXA and ANA Holdings have started the Greenhouse gas Observations of Biospheric and Local Emissions from the Upper sky (GOBLEU) project using passenger aircrafts by carrying imaging spectrometer suites for O2 A, solar-induced chlorophyll-fluorescence (SIF), and nitrogen dioxide (NO2). We will present long term instrument characterization and calibration of GOSAT and intercomparison between multiple sensors.

Determination of oxygen dimer cross-sections for different temperatures under ambient conditions from long-term long-path DOAS observations in the Antarctic

Bianca Lauster*, Udo Frieß, Thomas Wagner

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Presenter: Bianca Lauster

Abstract:

The atmospheric absorption of the oxygen dimer $(O_2)_2$ – in the following referred to as O_4 – can be used to derive properties of aerosols and clouds from remote sensing observations. In recent years, inconsistencies between the measured atmospheric O_4 absorption and radiative transfer simulations were found for Multi-AXis Differential Optical Absorption Spectroscopy (MAX-DOAS) measurements.

In the presented study, over two years of observations from a long-path (LP-)DOAS instrument deployed at the German research station Neumayer, Antarctica, are analysed. While MAX-DOAS instruments measure spectra of scattered sunlight at different elevation angles, LP-DOAS belongs to the active DOAS applications utilising an artificial light source and providing a fixed (and well-defined) light path. Further, the pristine measurement location allows to investigate the relation between measured and modelled O_4 over a large range of temperatures (-45°C to +5°C). The retrieved O_4 cross-sections are higher than those measured in the laboratory by about 5 to 10%. Thus, if applied to MAX-DOAS observations, they would even further increase the overestimation of the retrieved O_4 column densities compared to model simulations. This holds for the typically used O_4 absorption cross-sections of Thalman and Volkamer (2013) as well as the new cross-sections of Finkenzeller and Volkamer (2022). Further investigations are needed to understand these new findings.

Impact on the accuracy of aerosol and cloud properties derived from the oxygen bands by ignoring rotational Raman scattering

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Presenter: Luca Lelli

Abstract:

In a special issue of the Indian Journal of Physics of 31 March 1928, and in a letter to Nature, C. V. Raman presented results on an anomalous radiation from light scattered by transparent liquids at wavelengths shifted from the incident one. The same effect in crystal lattices was reported in the Soviet Union by Landsberg and Mandelstam. Inelastic Raman scattering is now commonly used to describe both observed effects.

Raman scattering can be thought of as an inelastic two-photon process. Lower or higher energy transitions are observed together with elastically scattered Rayleigh radiation at the excitation wavelength. Depending on the energy states involved, electronic, vibrational and rotational Raman transitions can be distinguished. Each is characterised by intensity, phase function and cross-section. The cross-section of the rotational component is 2-to-3 orders of magnitude larger than that of the others and it is also observed on air molecules. This affects only molecules with asymmetric polarisability (H_2, N_2, O_2), as reported by Shefov in 1959 and by Grainger and Ring. They provide the trans-spectral photons that fill telluric absorption bands as solar Fraunhofer lines of stellar bodies and gaseous bands (oxygen B- and A-band), thereby reducing their absorption strength.

Since RRS is proportional to optical path lengths and sensor spectral resolutions, it is expected that as the capabilities of space-based spectrometers improve, RRS will play an increasingly important role in those applications using gaseous absorption signature to diagnose properties of tropospheric components.

In this study, we aim to characterise the errors introduced in the retrieval of optical and physical properties of scatterers when RRS is not included in the forward problem. We do this by generating measurements of the Sentinel-4 mission. It aims to provide hourly measurements over Europe of trace gases, aerosols and clouds. The latter are a key input for the former, which are retrieved in the UV-Vis at 0.5 nm resolution. In this case the RRS signature is flattened and it can be neglected. However, the retrieval of aerosol and clouds' properties use the oxygen B- and A-band at 0.12 nm, for which the filling is no longer negligible. As the RRS is an additive component, a practical application is its inclusion as a spectral correction in cases where the retrieved parameters' accuracy is not within the nominal mission requirements.

Cloud retrieval for the CO2M NO_2 algorithm using the O_2-O_2 absorption band

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Presenter: Benjamin Leune

Abstract:

The future Copernicus Anthropogenic CO2 Monitoring Mission (CO2M) will provide CO_2 data at a high resolution of 2x2 km^2 with unprecedented accuracy and precision. In addition to bands in the near- infrared and shortwave infrared, the CO2I spectrometer on board of CO2M also contains a visible band for the retrieval of NO_2 tropospheric columns. NO_2 observations will be performed to aid the detection and identification of CO_2 emission plumes, as NO_2 is co-emitted during combustion processes and acts as a tracer of CO_2.

The onboard cloud imager instrument (CLIM) provides co- registered cloud information to aid the greenhouse gas and NO_2 retrievals. From the measured O_2-O_2 absorption bands effective cloud/aerosol parameters can be retrieved by using DOAS in combination with a scattering layer model with Henyey-Greenstein phase functions. The scattering layer method provides the NO_2 retrieval with more realistic air-mass factors for the vertical column calculation compared to the Lambertian cloud approach from the OMI O_2-O_2 cloud algorithm.

An unique data-set from S5P/TROPOMI with increased spatial sampling of 2x2 km^2, in combination with co- located cloud information from NPP-VIIRS. provide a good test bed for the CO2M NO_2 algorithm.

Geometrical thickness of single-layer liquid cloud retrieved from OCO-2 hyperspectral oxygen A-band over both land and ocean

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Presenter: Siwei Li

Abstract:

The retrieval of Cloud Geometrical Thickness (CGT) from satellite observations is crucial for understanding cloud microphysics and radiative balance. However, the retrieval of CGT over land remains challenging due to incomplete knowledge of land surface reflection, resulting in limited passive remote sensing algorithms available. We propose a novel algorithm to retrieve CGT in single-layer liquid clouds, applicable to both land and ocean. The method utilizes hyper-spectral observations from the Orbiting Carbon Observatory-2 (OCO-2) at the oxygen A-band (O2A) and employs an O2A white-sky albedo estimation method to correct land disturbances. The retrieval is achieved in near real-time using a fast radiative transfer approximation scheme, while maintaining accuracy comparable to that of a full radiative transfer model. The comparison with satellite-based lidar-radar products shows a correlation coefficient of 0.619, a mean bias of 5 hPa (46 m), and a root-mean-square error of 40 hPa (393 m). Uncertainties arise from inaccurate inputs and references, as well as non-negligible biases due to cloud vertical inhomogeneity and three-dimensional radiative transfer effects at cloud edges.

Retrieving XCO2, aerosols, and surface pressure from the CO2M mission

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Presenter: Sha Lu

Abstract:

In support of the Copernicus Anthropogenic Carbon Dioxide Monitoring (CO2M) mission, SRON Netherlands Institute for Space Research developed the Remote sensing of Trace gas and Aerosol Product (RemoTAP) algorithm. RemoTAP is able to perform simultaneous retrieval of trace gases and aerosol using measurements from the Multi-Angle Polarimeter (MAP) and CO2I Imager aboard the CO2M mission. At the same time, it has the capability to perform the retrieval of trace gas columns from only CO2I measurements.

To compute the column-averaged dry air mole fraction of CO2 (XCO2), the column of dry air is needed. In our baseline setup, we compute the column of dry air from the surface pressure provided by meteorological re-analysis data. Obviously, the error of the XCO2 retrieval is correlated with the error in surface pressure, e.g. an overestimation of surface pressure leads to an underestimation of XCO2 retrieval.

This study investigates the capability to retrieve surface pressure from the O2 A-band measurements of CO2I itself, making it less dependent on the accuracy of the re-analysis surface pressure. We evaluate the effect of a priori surface pressure on XCO2 retrieval in our baseline setup and investigate under which conditions XCO2 retrievals can be improved by fitting surface pressure from the CO2I observations in the O2 A-band. We base our evaluation on synthetic CO2M measurements simulated for realistic atmospheric, surface and geometry conditions. The study shows that fitting surface pressure from the O2 A-band can help increase the number of successful retrievals, reduce systematic bias and significantly improve the precision of XCO2 retrievals, if errors on the re-analysis surface pressure are larger than about 2 hPa. In addition, the MAP-CO2I retrieval method is able to reduce the aerosol-induced retrieval error compared to CO2I-only retrieval, and makes the XCO2 retrieval meet the mission requirements (precision$<$0.7 ppm and bias$<$0.5 ppm).

Deep space observations of oxygen absorption bands

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Presenter: Alexander Marshak

Abstract:

Earth Polychromatic Imaging Camera (EPIC) on the Deep Space Climate Observatory (DSCOVR) provides 10 narrow band spectral images of the entire sunlit face of Earth at 10 km resolution. Two of these bands are the A and B oxygen absorption bands at 764 and 688 nm, respectively. Using these bands cloud and aerosol height are retrieved. In this presentation I will focus on different retrievals of these products, their correlation and daytime variability.

Effect of using fixed input parameters on the retrieval of cloud properties in the oxygen bands: Case study with synthetic EPIC/DSCOVR measurements

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Presenter: Víctor Molina García

Abstract:

Radiance measurements in the oxygen bands have been widely used by UV/VIS/NIR remote sensing missions to estimate cloud macrophysical properties, including GOME on board ERS-2, GOME-2 on board MetOp-A/B/C, TROPOMI on board Sentinel-5 Precursor, and EPIC on board DSCOVR. The upcoming atmospheric Copernicus missions Sentinel-4 and Sentinel-5 will also offer the possibility to retrieve these cloud properties in the UV/VIS/NIR spectral region, which is crucial for the precise retrieval of trace- and greenhouse gases.

Simpler cloud models make the assumption that clouds can be modelled as Lambertian reflectors (CRB, cloud-as-reflective-boundaries), for which the cloud-centroid height and the cloud albedo are estimated. More sophisticated cloud models treat clouds as a single layer of scattering particles (CAL, cloud-as-layers), for which the cloud-top height and the cloud optical thickness are estimated. However, additional cloud parameters cannot be retrieved in the oxygen bands due to the ill-posedness of the optimisation problem. Under such conditions, the remaining cloud parameters are obtained from external sources, such as retrieval algorithms in other spectral bands, climatological databases and long-term satellite observations. These cloud parameters are usually introduced as fixed constant values which are not allowed to vary within the cloud retrieval algorithm.

In this work, we use the EPIC instrument on board the DSCOVR mission as the example sensor to investigate the effect of using fixed input parameters on the retrieval of cloud properties. In particular, by using EPIC synthetic measurements in the oxygen A- and B- bands, we analyse the errors induced to the retrieved cloud-top height and cloud optical thickness from fixing the cloud geometrical thickness and the cloud effective particle size for a well-covered set of cloud parameters in the input space.

Aerosol Characterization Using Oxygen A-band Measurements With Application to CO2 Retrievals

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Presenter: Vijay Natraj

Abstract:

Atmospheric aerosols represent a significant part of the anthropogenic forcing responsible for climate change. They also affect greenhouse gas remote sensing by altering the path length of solar radiation. However, aerosol effects are difficult to quantify because of the large spatiotemporal variability in their composition, loading, and vertical distribution.

Spectrally resolved measurements of oxygen absorption contain information about the vertical distribution of aerosols. We use a machine learning approach to retrieve aerosol optical depth and layer height from Orbiting Carbon Observatory-2 (OCO-2) O2 A-band measurements. A case study over the Saudi Arabian desert shows retrievals that compare well with collocated lidar measurements. We also demonstrate the impact of improved aerosol priors from the machine learning approach on CO2 retrievals.

Uncertainty of GEMS AEH products caused by AOD and surface reflectance

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Presenter: Sang Seo Park

Abstract:

From the previous studies (e.g., Chimot et al., 2017; Park et al., 2016; Sanders et al., 2015; Sanghavi et al., 2012), the oxygen-related absorption bands can be used to retrieve the aerosol/cloud vertical information by identifying the optical path length change. The Geostationary Environment Monitoring Spectometer (GEMS) also retrieve the aerosol properties and the oxygen-related absorption bands were adopted to retrieve the aerosol vertical information. Because the GEMS have spectral range of 300-500 nm with spectral resolution of 0.6 nm, the O2-O2 absorption band at 477 nm has been solely used to retrieve the aerosol height information. From Park et al. (2016), the aerosol height parameter (aerosol effective height; AEH) has uncertainty due to the error of aerosol optical properties and surface reflectance.

After launching the GEMS, the scientific products have been stably retrieved. The AEH product from GEMS is also retrieved after estimating the aerosol optical properties and surface reflectance. The AEH retrieval used to the GEMS aerosol and surface products as input parameters. However, these retrieval results include the uncertainty, thus, the AEH also includes the uncertainty.

In this study, we identified the uncertainty of AEH retrieval results based on the empirical results from GEMS observation. During the retrieval, we also estimated the sensitivity of AEH retrieval for the aerosol optical depth (AOD) and surface reflectance.

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Cloud Top Pressure Retrieval from Sentinel-3 OLCI O2 A-Band Measurements

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Presenter: Rene Preusker

Abstract:

We present a noval cloud top pressure (CTP) retrieval, based on Sentinel-3 OLCI top-of-the-atmosphere (TOA) solar radiances, measured in the near-infrared spectral bands, which includes all three O2 A-band channels at 760nm. The major problem of the O2 A-band CTP retrieval is the photon penetration depth, which depends mainly on the vertical distribution of cloud properties. This is treated by introducing two additional state variables describing the vertical structure of the cloud extinction: the cloud geometrical thickness (CGT) and the 'centre of gravity' (CoG, the vertical position of the maximum scattering extinction). The output of the retrieval process are CTP, CGT and CoG. The look-up tables, used in the retrieval, have been built on line-by-line and multiple-scattering simulations which have been extended to consider the O2 A-band continuum absorption and variable cloud profiles. The quality of the new algorithm will be demonstrated based on comparisons with Lidar cloud-top heights, taken during the EURC4A campaign in 2020. Further comparisons with one year of Radar / Lidar measurements at the Climate Research Facility of the US Department of Energy ARM in Oklahoma will be presented.

An original method to store and use LBL data in transmission form – Part II. Application to radiative transfer in the O2 A-Band

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Presenter: Antoine Rimboud

Abstract:

This work is devoted to a comparison of various techniques to treat gaseous absorption in realistic scattering atmospheres. Several models and methods to approximate the radiative properties of non-uniform atmospheric paths are considered and compared in cloudy atmospheres.

For this purpose, 4 models of gaseous absorption were implemented inside the 3DMCPOL code (Cornet et al., 2010) that allows to solve the radiative transfer equation with the Monte-Carlo method. This reference code (Emde et al, 2018) is widely used in the remote sensing community to simulate the radiative effects of heterogeneous clouds in a three-dimensional atmosphere. The gaseous models considered are the CKD model for various numbers of gray gases (16, 64 and 256), the standard L-distribution method, the mixture L-distribution approach and the most recent Augmented L-distribution technique (Andre et al., 2023). These methods are assessed against reference LBL calculations over a set of scattering atmospheres of increasing complexity: 1/ pure molecular scattering, 2/ two configurations with a single layer of cloud, 3/ one configuration with two cloud layers with distinct optical thicknesses. The methods are evaluated against LBL calculations both in terms of accuracy and CPU cost. The results of the comparisons in the O2 A-band indicate that the so-called Augmented L-distribution approach provides the highest accuracy (much lower than 0.1% in all the cases considered) of all approximate methods at the smallest CPU cost. In terms of computational efficiency, it outperforms a CKD model with 16 gray gases by nearly 6 times in pure molecular scattering scenarios and by 2.5 times in situations involving cloud layers. The Augmented L-distribution approach can be considered as a relevant candidate for applications that requires a large number of evaluations of non-uniform paths transmissivities, as encountered in many remote sensing applications.

Cloud top pressure retrievals from the O_2 A-band for the NASA PACE OCI sensor

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Presenter: Andrew Sayer

Abstract:

We introduce the Cloud Height Retrieval from O_2 Molecular Absorption (CHROMA) algorithm, designed for the Ocean Color Instrument (OCI). OCI is the primary payload on the NASA Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) mission which should be in operation by the time of this workshop. OCI has a horizontal pixel size of approximately 1.2 km at the sub-satellite point and a 2,700 km swath width. It has continuous sampling at a 2.5 nm step size and 5 nm FWHM bandwidth from the UV to the NIR (and 1.25 nm step size in the O_2 A and B bands), plus seven discrete SWIR bands.

CHROMA is a Bayesian approach which uses measurements in the O_2 A-band to simultaneously retrieve cloud optical thickness (COT), cloud top pressure/height (CTP/CTH), and (with a significant prior constraint) surface albedo. Simulated retrievals suggest that the sensor and algorithm should be able to meet the PACE mission goal for CTP error, which is ± 60 mb for 65 % of opaque (COT$\geq$ 3) single-layer clouds on global average. CHROMA will provide pixel-level uncertainty estimates, which are demonstrated to have skill at telling low-error situations from high-error ones. CTP uncertainty estimates are well-calibrated in magnitude, although COT uncertainty is overestimated relative to observed errors. CTP error is only weakly sensitive to correct cloud phase identification or assumed ice crystal habit/roughness. As with other similar algorithms, for simulated retrievals of multi-layer systems consisting of optically thin cirrus clouds above liquid clouds, retrieved height tends to be underestimated because the satellite signal is dominated by the optically-thicker lower layer. Total (liquid plus ice) COT also becomes underestimated in these situations. However, retrieved CTP becomes closer to that of the upper ice layer for ice COT$\approx$3 or higher.

Prior to PACE launch, we have also applied CHROMA to the Ocean Land Colour Instrument (OLCI) currently flying on the Sentinel 3 satellites, and we show example retrievals and validation results from that sensor.

See also Sayer *et al.* (2023), The CHROMA cloud-top pressure retrieval algorithm for the Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) satellite mission, *Atmos. Meas. Tech.*, 16, https://doi.org/10.5194/amt-16-969-2023.

Overview of the FRESCO cloud retrieval algorithm for satellite spectrometers

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Presenter: Piet Stammes

Abstract:

FRESCO is a fast algorithm for cloud retrievals from the O2 A-band, of which the development started more than 20 years ago at KNMI (Koelemeijer et al., JGR, 2001). The FRESCO algorithm determines cloud fraction and cloud height to enable a cloud correction of trace gas retrievals, e.g. ozone and NO2. The FRESCO algorithm assumes that a cloud is a Lambertian reflector with a fixed albedo of 0.8. Oxygen absorption is simulated line-by-line along the path from sun-to-cloud and from cloud-to-satellite; in addition single Rayleigh scattering may occur along this path (Wang et al., ACP, 2008). In FRESCO only three 1-nm wide parts of the O2 A-band are used: the continuum at 758-759 nm, the strongest absorption part at 760-761 nm, and the weaker absorption part at 765-766 nm. From simulation and validation we find that the retrieved cloud height is close to the optical mid-level of the cloud. The FRESCO algorithm has been and is being used for a series of European satellite spectrometers measuring atmospheric composition: GOME on ERS-2 (1995-2003), SCIAMACHY on Envisat (2002-2012), GOME-2 on Metop-A (2006-2021), and on the currently flying GOME-2 on Metop-B/C. An adapted version, called FRESCO-S, has been developed for TROPOMI, which makes use of more spectral information in the O2 A-band to have more sensitivity to low clouds. This version of FRESCO will also be applied to Sentinel-5 and CO2M data. In this presentation we will discuss the important development steps of FRESCO and its results.

Proposal for intercomparison of radiative transfer simulations of the atmospheric O2 A- and B-bands

Piet Stammes*, Ping Wang, Nicolas Ferlay, René Preusker, Jürgen Fischer, et al.

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Presenter: Piet Stammes

Abstract:

A correct simulation of the atmospheric oxygen bands in the red and near-infrared region (A- and B-bands) is important for several reasons, but especially for satellite retrievals of surface pressure, cloud and aerosol height, and CO2 light path correction.

There are many radiative transfer (RT) models around to simulate the O2 bands. However, to our knowledge there has not yet been an intercomparison of O2 A- and B-band simulations. A correct simulation of the A- and B-bands, which have hundreds of strong and weak lines, combined with atmospheric scattering and surface reflection, is a challenge. Many choices on physics and model settings have to be made.

Our proposal is to provide a benchmark on the basis of several RT models at high spectral resolution. In this intercomparison we may identify several phases, for example: (1) clear sky case with everything prescribed; (2) clear sky, with operational settings per RT model, convoluted for specific satellite instrument channels, e.g. TROPOMI, MetImage; (3) all sky comparison with real measurement data.

The aim is to achieve a benchmark simulation of the O2 bands. We invite others to collaborate.

From oxygen to carbon dioxide and back – an A-band journey

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Presenter: Graeme Stephens

Abstract:

Today, applications abound in the use of the measurements of the absorption of sunlight by oxygen in the spectral regions of the A-band. One of the earliest proposed uses of such measurements (e.g. Wark, 1965) was to estimate the pressures of reflecting surfaces in the atmosphere including the surface pressure of Earth. These early concepts were based on moderate to coarse spectral measurements and many studies today report on use of satellite measurements of cloud top pressure. This concept, applied to surface pressure retrieval, was eventually matured in the studies of O'Brien in the early part of the 1990's. Those studies clearly demonstrated the need for hyperspectral resolution measurements to account for atmospheric scattering at a level needed to retrieve surface pressure at sub-hPa resolutions and, in an analogous way, column CO2 to better than 1 ppmv. Rather than focus on the retrieval of the column amount of oxygen, which is generally known to a few parts in 1000 from present-day operational weather analysis, the studies of Stephens proposed that measurements could be used instead to infer properties of the scatterers, including their vertical distributions. This notion, and the synergy it offered, led to the proposals of including A-band hyperspectral measurements with both the lidar and radar observations of CALIPSO and CloudSat. The spectrometers originally proposed where subsequently descoped due to cost and the CloudSat concept ultimately morphed into the definition of the OCO mission which today makes these hyperspectral A-band measurements as a way of making atmospheric corrections in support of the CO2 absorption measurements. This talk will briefly describe the journey outlined above and how hyper-spectral A-band measurements of OCO are now used to deduce cloud profile information.

Cloud altitudes and optical thicknesses retrieved by O2A-band spectropolarimetry of Earthshine

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Presenter: Michael Sterzik

Abstract:

Observations of Earthshine allow to measure reflected light integrated of whole Earth from ground. The scattered light is polarized and contains characteristic information about the Earth's atmosphere and its reflecting surfaces. For more than 20 years we have collected a wealth of linear polarization spectra of Earthshine with the ESO Very Large Telescope in Chile in the visible wavelength domain, under distinct and varying viewing geometries. The observed spectra compare very well with simulations of Earth in full spherical geometry applying the MYSTIC Monte-Carlo model. Our spectra, in particular the depth of the O2A line as compared to the adjacent continuum, are sensitive on cloud top heights and optical thicknesses, and we have studied their dependencies on the phase angle. We find that the information content in the phase curve and in the O2A line are complementary. Moreover we exploit twilight polarisation spectra and can discern and characterize tropospheric and stratospheric aerosol above the Observatory. The methodology that we develop may in the future be applied to Earth-like exoplanets, and could be useful to constrain their cloud parameters.

Retrieval of aerosol layer height from Sentinel-3/OLCI observations

Gijsbert Tilstra*, Martin de Graaf, Maarten Sneep, Ping Wang, Olaf Tuinder, Pepijn Veefkind, Piet Stammes

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Presenter: Gijsbert Tilstra

Abstract:

We have developed an aerosol layer height (ALH) retrieval for the OLCI instrument onboard the Sentinel-3 satellites. The retrieval algorithm is based on the TROPOMI ALH retrieval algorithm, but then adapted to the OLCI instrument. The retrieval makes use of five OLCI wavelength bands covering the Oxygen-A absorption band. It is based on optimal estimation, in which aerosol optical depth (AOD), ALH and surface albedo are all fitted. For reasons of speed, the algorithm uses a Neural Network (NN) approach to calculate the simulated reflectance in each step, instead of having the (much slower) radiative transfer code do this each time. We will briefly explain the retrieval algorithm, present results for a selection of case studies, and show first validation results.

Calculating the vertical column density of O_4 during daytime from surface values of pressure, temperature and relative humidity

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Presenter: Thomas Wagner

Abstract:

We present a formalism that relates the vertical column density (VCD) of the oxygen collision complex O_2-O_2 (denoted as O_4 below) to surface values of temperature and pressure, based on physical laws. In addition, we propose an empirical modification which also accounts for surface relative humidity (RH). This allows for simple and quick calculation of the O_4 VCD without the need for constructing full vertical profiles. The parameterization reproduces the true O_4 VCD, as derived from vertically integrated profiles, within -0.7% ± 1.2% (mean±SD) for WRF simulations around Germany, 0.2% ± 1.8% for global reanalysis data (ERA5), and -0.3% ± 1.4% for GRUAN radiosonde measurements around the world. When applied to measured surface values, uncertainties of 1 K, 1 hPa, and 16% for temperature, pressure, and RH correspond to relative uncertainties of the O_4 VCD of 0.3%, 0.2%, and 1%, respectively. The proposed parameterization thus provides a simple and accurate formula for the calculation of the O_4 VCD which is expected to be useful in particular for MAX-DOAS applications.

Aerosol Optical Centroid Height (AOCH) retrieval from oxygen absorption bands: recent advances and next steps

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Presenter: Jun Wang

Abstract:

Here we will provide our recent advances of using O2 A and B bands from EPIC/DSCOVR, TROPOMI, and TMEPO satellite to retrieve aerosol centroid layer height (AOCH) over both ocean and land. Inter-comparison of AOCH retrievals with lidar and other observation will be shown together with the application of AOCH data for surface air quality estimate. We will also discuss the emerging opportunities of using multiple angle measurements of polarization in oxygen A and B bands to derive AOCH and possibly aerosol vertical profile near the surface.

Line-shape parameters and their temperature dependency for the air-broadened oxygen B-band lines

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Presenter: Szymon Wojtewicz

Abstract:

The molecular oxygen B band used together with other O_2 bands can reduce the uncertainties in the pressure and temperature profiles determined across the atmosphere or improve the accuracy of aerosol layer height retrieval over vegetated surfaces. Despite growing importance for the remote sensing of the B band (e.g. EPIC-DISCOVR [1], GOME-2 and SCIAMACHY [2] missions), its line-shape parameters for the air-broadening were not known accurately. Here we present the first set of high-quality measurements of the air-broadened O_2 B band. The measurements were performed with the frequency-stabilized cavity ring-down spectroscopy (FS-CRDS) technique referenced to the optical frequency comb (OFC) [3]. The line-shape analysis was performed with the speed-dependent Nelkin-Ghatak profile (SDNGP) [4], which is a limiting case of the recommended Hatrtmann-Tran profile (HTP) [5]. This approach made it possible to take into account the mechanisms of line narrowing and line asymmetry.

We determined the temperature dependency of the collisional broadening and the collisional shift, while no significant temperature dependency of the speed-dependent parameters and the Dicke narrowing was observed [6]. We demonstrated that the temperature dependency of the collisional broadening can be estimated based on its speed dependence. We also present corrected values of the line intensities. Moreover, the pressure broadening as well as its temperature dependence are very similar for A and B bands [7], whereas the pressure shift for the B band is up to 100% larger.

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Harmonized OMI and TROPOMI cloud datasets using the O2-O2 absorption band at 477nm

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Presenter: Huan Yu

Abstract:

We present scientific approach at BIRA-IASB for deriving effective cloud fraction and effective cloud pressure from OMI and TROPOMI measurements, based on the O2-O2 absorption band near 477 nm. The aim of this work is to derive consistent cloud parameters to be used as input of algorithms to retrieve atmospheric trace gases from multi-decadal satellite observations, and to mitigate the influence of clouds. The cloud retrieval consists of two main steps: initially, a spectral fitting is conducted within the spectral range of 440 to 490 nm to determine the O2-O2 slant column and the reflectance at 465 nm. Subsequently, these parameters are converted into cloud fraction and cloud pressure using radiative transfer simulations. This retrieval algorithm builds on the OMI O2-O2 operational cloud algorithm (OMCLDO2), incorporating several improvements. The fitting procedure employs a broader fitting window, including two O2-O2 absorption bands (446 and 477 nm), to precisely derive O2-O2 slant column densities. Additionally, a de-striping correction is implemented to address across-track variability, while an offset is introduced for OMI to correct the O2-O2 SCD bias relative to TROPOMI. The OMCLDO2 algorithm introduces a temperature correction on the O2-O2 slant columns, while the new retrieval approach has improved upon this correction factor by further considering the temperature dependence of the O2-O2 absorption cross- section. Both OMI and TROPOMI retrievals are based on the surface albedo from the $0.125° \times 0.125°$ TROPOMI directionally dependent Lambertian-equivalent reflectivity (DLER) climatology version 2.1. Finally, we compare the new O2-O2 cloud parameters with the OMCLDO2 cloud products. The cloud pressures derived from BIRA-IASB consistently show higher values than those of OMCLDO2 for OMI and lower values for TROPOMI, especially in scenes with nearly cloud-free conditions (cloud fraction < 0.2). However, the BIRA-ISAB O2-O2 cloud parameters derived from both OMI and TROPOMI demonstrate good agreement, particularly regarding cloud pressure. Nevertheless, the cloud fraction retrievals consistently display a bias of approximately 0.05, which is likely linked to a calibration error in the L1 data between OMI and TROPOMI.

Cloud property retrieval based on DISAMAR: using Oxygen absorption band data from TROPOMI on Sentinel 5P

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Presenter: Xiaoyun Zhang

Abstract:

DISAMAR (determining instrument specifications and analysing methods for atmospheric retrieval) is a computer model developed to simulate the retrieval of properties of atmospheric trace gases, aerosols, clouds and the surface from passive remote sensing observations in the wavelength range 270-2400 nm. It is used for the TROPOMI/Sentinel-5P and Sentinel-4/5 missions to derive Level 1b product specifications. It is also used in some research to obtain aerosol and trace gas properties, but its application to the retrieval of cloud properties is limited. This study presents the retrieval of cloud pressure and cloud optical thickness, as well as cloud-free surface pressure, based on TROPOMI Oxygen-A (Band 6) and Oxygen-B (Band 5) band measurements, and compares the results with FRESCO and NPP-Suomi Level 2 cloud property data. Several cross-sectional datasets including JPL2008, HITRAN 2008 and HITRAN2020 are also tested in this study. In conclusion, for surface pressure retrieval, using O2-A band gives more reliable results than O2-B band and is easier to converge in the calculation, especially over the land surface. But while over the sea surface, using O2-B band in retrieval performs better than O2-A band. Secondly, the retrieval based on the JPL2008 cross section file shows better results when using O2-A band, but HITRAN2020 gives better results when using O2-B band. Thirdly, setting an appropriate a-priority value in DISAMAR and removing some of the wavelengths with high residual simulated reflectivity can significantly improve the results, both in terms of convergence and reduction of validation error. The cloud pressure correlation coefficient between the retrieval and NPP or FRESCO data is 0.85 and 0.99 respectively, while the cloud optical thickness has a correlation coefficient of 0.77 between the retrieval and NPP COT data sets.

Retrieving SIF from tall towers with the O2-Band Shape Fitting method

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Presenter: Christiaan Van der Tol

Abstract:

Retrieving SIF from tall towers with the O2-Band Shape Fitting method We carried out hyperspectral measurements of downwelling and upwelling radiance at the Cabauw measurement tower to test techniques for Solar Induced Fluorescence (SIF) retrieval, including techniques that extract information about SIF from O2 bands. When measurements are carried out close to the ground, then the O2A and O2B bands of the upwelling radiance are shallower than that of the downwelling radiance due to SIF infilling, and this feature is often used to detect SIF. When the instruments are placed far from the vegetation, then the path of the radiance from the sun to the sensor of the reflected (upwelling) radiance is longer than that of the downwelling radiance, resulting in deeper O2 bands in the upwelling radiance. It is then necessary to differentiate fluorescence infilling from the additional deepening by oxygen. We developed and tested the Band Shape Fitting (BSF) method for this purpose. Rather than modelling the transmittance with a detailed radiative transfer model, we used log-linear extrapolation of the downwelling radiance and retrieved SIF and the optical path length simultaneously by minimizing a cost function. This extrapolation is valid for short paths and for monochromatic radiation, such that a correction depending on the spectral response of the instrument was necessary. We tested the method with three Fluorescence Box (FLOX) systems placed at 16, 100 and 200 m above grassland, where the footprints of the two higher sensors overlapped. Intercomparison of methods, sensitivity analysis, comparisons of retrievals from three heights and to SCOPE modelled SIF (after tuning SCOPE to the measured reflectance in the 400-900 nm range) showed that BSF enables the successful retrieval of SIF from observations up to at least 200 m height. Further tests on airborne data to explore the applicability of the technique are ongoing. However, the underlying assumptions make the method unsuitable for spaceborne retrievals.

Comparison between RTTOV and DISAMAR for GOME-2

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Presenter: Jerome Vidot

Abstract:

An intercomparison exercise between 2 radiative transfer models (RTTOV and DISAMAR) was proposed in 2022 as NWPSAF visiting scientist program in order to evaluate the capability of RTTOV to simulate hyperspectral instrument in the UV-VIS-NIR spectral domain. The benchmark simulations were performed for the GOME-2 instrument, both on clear-sky and aerosols situations, and for different angular and surface configurations. The primary objective was to evaluate ozone bands and window channels for aerosols. We found that RTTOV performs very well compared with the reference model DISAMAR with absolute difference of around 1-2% in reflectance. However, this intercomparison highlights also large discrepancies between the two models in the O2-A band (up to 30% in relative difference). In this poster we will present results of this intercomparison and discuss further improvement that is needed to improve RTTOV simulations for the O2-A band.