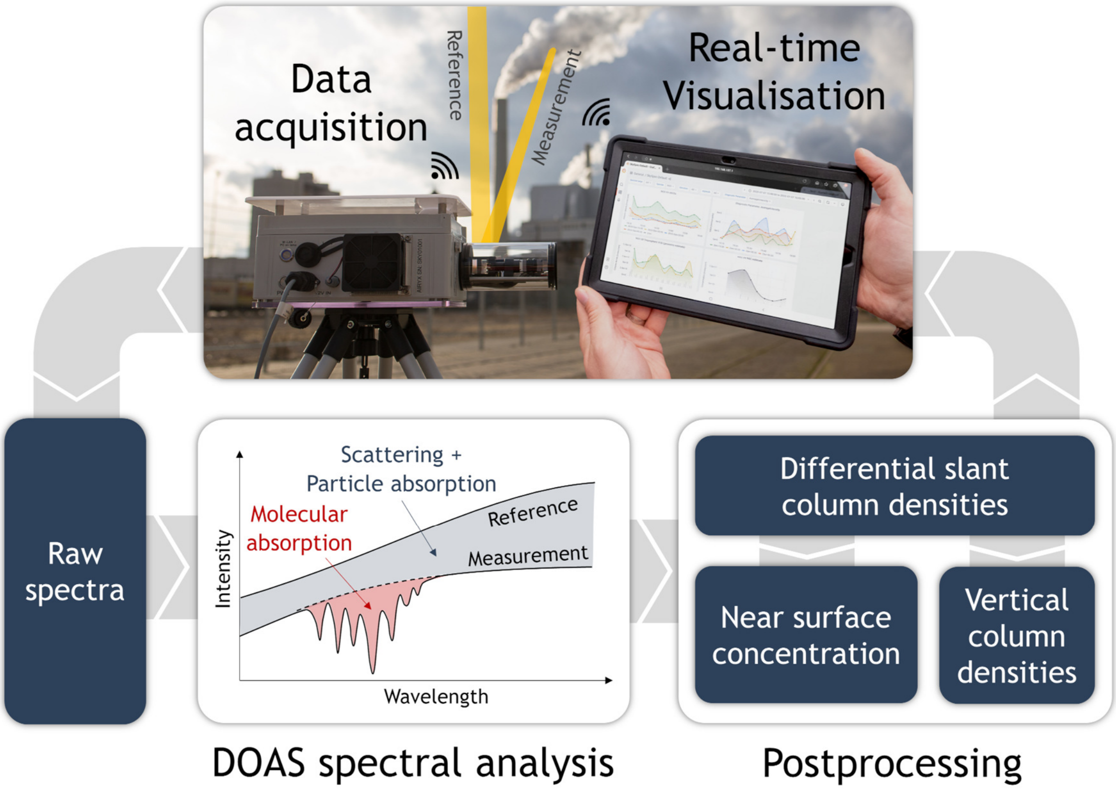
SkySpec Evaluation Software-Package

AUTOMATIC POST- AND REAL-TIME PROCESSING OF SKYSPEC SPECTRAL DATA



- **Automatic DOAS analysis**
- **Detectable gases: NO_2, SO_2, O_4, HCHO, BrO, H_2O, HONO, IO and CHOCHO**
- **Data products:**
  - Differential slant column densities (dSCD): gas amounts, integrated along the path of the detected light
  - Tropospheric vertical column density (VCD)
  - Near-surface concentration (NSC)
- **Results provided as CSV-files**
- **Web browser-based data visualisation**
- **Portability and flexible use:**
  - Runs on any Windows computer
  - (Re-)process already existing sets of spectra
  - Run on the control computer of your measuring SkySpec to obtain real-time results
- **Easy configuration:**
  - Choose the reference spectrum, depending on whether your focus is on stratospheric, tropospheric or locally emitted gases
  - Full control over DOAS fit settings
  - Add arbitrary species

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PERFORMANCE

MAIN DATA PRODUCTS

PRODUCT	DESCRIPTION	PREREQUISITES
Differential slant column density (dSCD)	DSCDs for the different trace gases are the direct output of the DOAS spectral analysis and the basis for the data products below. DSCDs represent the difference in integrated gas concentrations along two different slant light paths through the atmosphere (the “measurement” and the “reference” light path, respectively).	
Tropospheric vertical column density (VCD)	Vertically integrated gas concentration within boundary layer and lower troposphere. Based on trigonometric considerations assuming that photons pass the boundary layer along the instrument’s line of sight. Highest accuracy is achieved for dSCDs inferred at 15°< VEA* < 30°.	• Evaluation against current reference • Unobstructed view at: ○ 15° < VEA < 30° ○ VEA ≈ 90°
Near-surface concentration (NSC)	Average concentration in the lowest ≈ 100 m above ground. The NSC is obtained by scaling the target species dSCD at VEA = 1°with the corresponding O_4 dSCD (*see also Sinreich et al., DOI: 10.5194/amt-6-1521-2013*). Boundary layer height and resulting correction factors are inferred using dSCDs at VEA = 5° and parameterised radiative transport.	• Evaluation against current reference • Unobstructed view at: ○ VEA = 1° ○ VEA = 5° ○ VEA ≈ 90°

* VEA = viewing elevation angle

HIGHLIGHTS

BENEFITS	*PROPERTIES & INNOVATION*
State-of-the-art DOAS analysis	• *Full automatized spectral fitting of trace gas absorptions* • *Automatic spectral correction, including detector nonlinearity* • *DOAS fit accounts for inelastic scattering, spectrometer straylight and I_0-effects*
Real-time analysis	• *Works in parallel with the SkySpec measurement software to optimise real-time functionality.* • *Thanks to fast algorithms, dSCDs as well as VCD and NSC estimates for all trace gases are provided few seconds after spectrum acquisition* • *Automatic reinitialization after measurement computer reboot*
Data visualization	• *Web browser-based data visualization* • *accessible with any web compatible device (mobile, tablet, PC)* • *no third-party software required* • *Particularly useful for monitoring in the field e.g. with the SkySpec Compact*
Simple setup & data interpretation	• *Package preconfigured and optimised for your specific instrument to achieve best accuracy* • *Preinstalled and ready to run when ordered with a SkySpec control computer* • *Easy configuration provides high flexibility* • *Various data quality indicators for fast and reliable identification of problematic atmospheric conditions or instrumental issues* • *Results are provided in intuitive CSV files* • *Works hand-in-hand with the SkySpec measurement software to provide real-time*

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REFERENCE SPECTRUM OPTIONS

OPTION	*DESCRIPTION*
Current reference (default)	*Each spectrum is evaluated against the temporally closest spectrum recorded at a user defined reference elevation (typically zenith). Ideal for the evaluation of elevation scans at high temporal resolution, e.g. for tropospheric profile inversions or the investigation of point emission sources.*
Noon reference	*For each day of data, the spectrum recorded at a user defined reference elevation (typically zenith) closest to noon will be used as reference. "Noon" can be identified based on time or by minimum solar zenith angle. Ideal when focussing on stratospheric absorbers.*
Fixed reference	*User defines a fixed spectrum number to be used as reference spectrum. Flexible in application depending on the chosen spectrum and the applied post-processing.*

TYPICAL SPECIFICATIONS

Data based on MADCAT campaign data for an urban/rural measurement location (*see Lampel et al. 2015, doi:10.5194/amt-8-3767-2015*). Integration time: t_{exp} = 60 s (≈ 1000 scans). If not stated otherwise, values represent 1σ-deviations. Exact specifications depend on atmospheric and lighting conditions.

Parameter	**Quantity / unit**	**NO_2**	**SO_2**	**HCHO**	**BrO**	**H_2O**	**O_4**	**HONO**	**IO**	**Glyoxal**
Typical observed values	DSCD [molec/cm^2]	2e17	4e15	1e16	1e13	3e23	3e43 *1	2e15	5e12	5e14
	VCD [molec/cm^2]	2e16	4e14	1e15	1e12	3e22	-	2e14	5e11	5e13
	NSC [molec/cm^3]	2e11	4e9	1e10	1e7	3e17	-	2e9	5e6	5e8
	NSC [pptv] *3	8000	160	400	0.4	1.2 *5	-	80	0.2	20
Detection limit (2σ)	DSCD [molec/cm^2] *2	8e14	8e15	6e15	2e13	1e22	1e41 *1	4e14	1e13	4e14
	VCD [molec/cm^2]	8e14	8e15	6e15	2e13	1e22	-	4e14	1e13	4e14
	NSC [molec/cm^3]	1e9	8e9	6e9	2e7	1e16	-	4e8	1e7	4e8
	NSC [pptv] *3	40	320	240	0.8	0.04 *5	-	16	0.4	16
Sensitivity error	DSCD [%]	≤ 5 % (systematic uncertainty in literature absorption cross-sections → time invariant)								
	VCD [%]	15 % (simplified radiative transport → variable over time)								
	NSC [%]	15 % (simplified radiative transport → variable over time)								
Accuracy for typical observed values	DSCD [molec/cm^2]	1e16	4e15	3e15	1e13	1.5e22	2e42 *1	2e14	5e12	2e14
	VCD [molec/cm^2]	3e15	4e15	3e15	1e13	6.5e21	-	2e14	5e12	2e14
	NSC [molec/cm^3]	4e10	4e9	3.5e9	1e7	6e16	-	4.5e8	5e6	2e8
	NSC [pptv] *3	2000	160	140	0.4	0.25 *5	-	18	0.2	9
Signal-to-noise ratio (SNR)	DSCD *6	500	1	3.5	1	60	600	10	1	0.25
	VCD	7	0.1	3.5	0.1	4.5	-	1	0.1	2.5
	NSC *3	5	1	2.5	1	5	-	4.5	1	2
Max. temporal resolution	DSCD	t_{exp} (per viewing direction; reference spectrum acquisition time not considered)								
	VCD	2 x t_{exp} (requires two spectra, see algorithm description above)								
	NSC	3 x t_{exp} (requires three spectra, see algorithm description above)								

**1 in units of molec^2 cm^{-5}*
**2 Fit coefficient error x 2*
**3 Conversion to ppt assumes standard pressure and temperature*
**4 Systematics error in literature absorption cross-section*
**5 volume mixing ratio in %*
**6 constant sensitivity error not considered*

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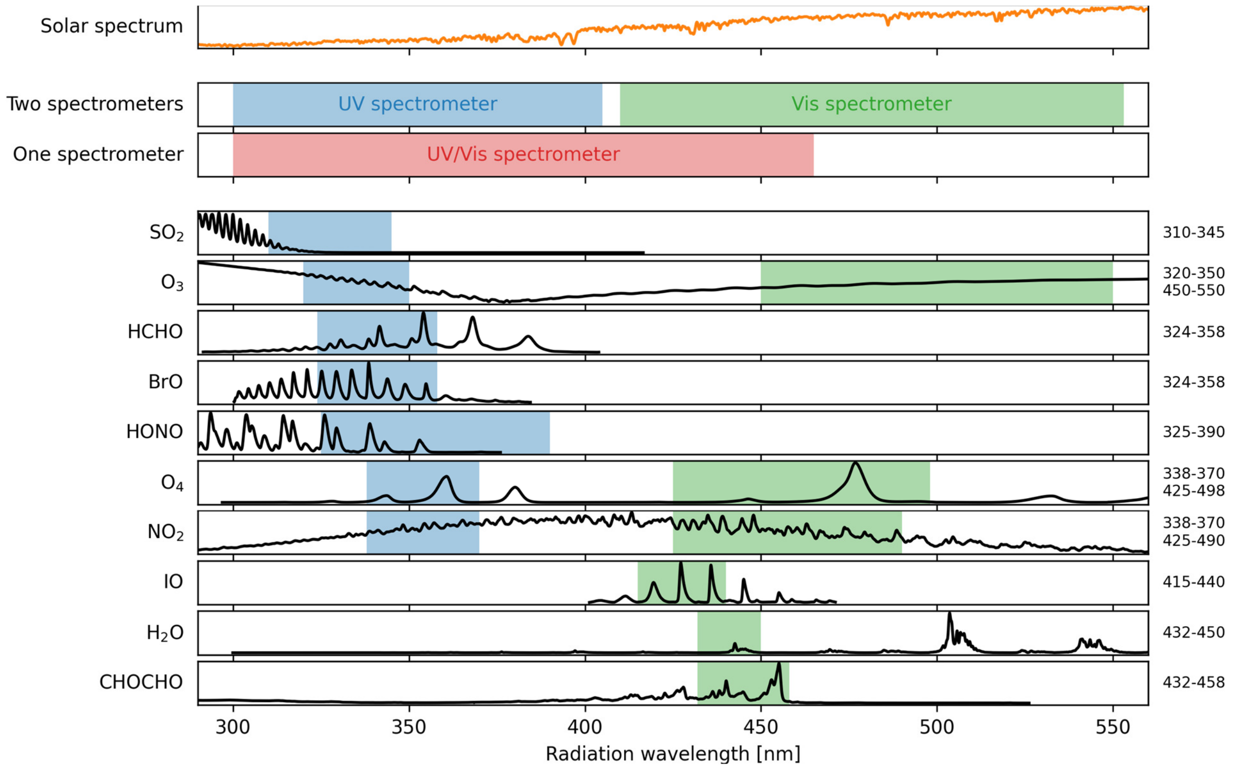
TYPICAL FIT RANGES



Target species absorption cross sections (black lines), typical fit ranges (coloured areas) and typical SkySpec spectral coverages.

REAL-TIME VISUALIZATION

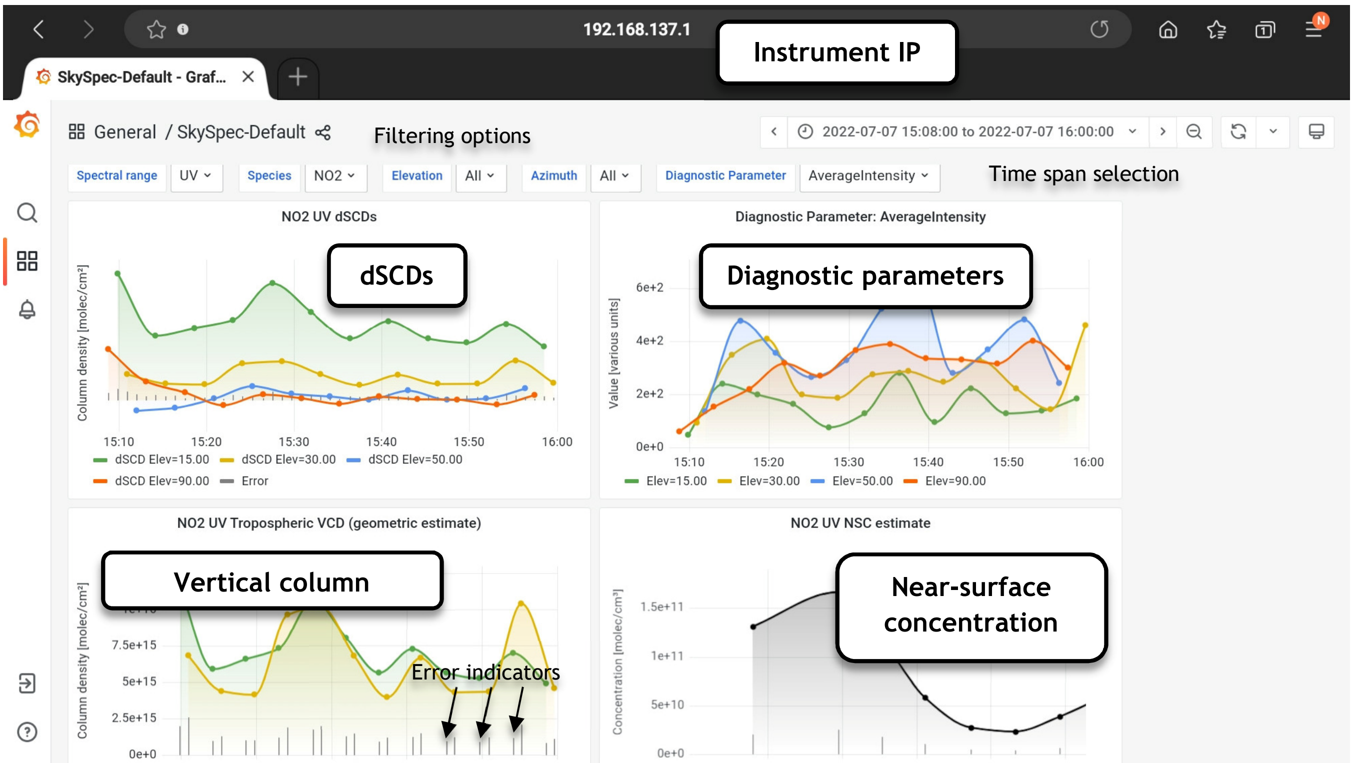


Figure 1: Screenshot of the web-browser based visualisation of the evaluation results. It can be accessed with any web compatible device (in this example with a tablet computer).

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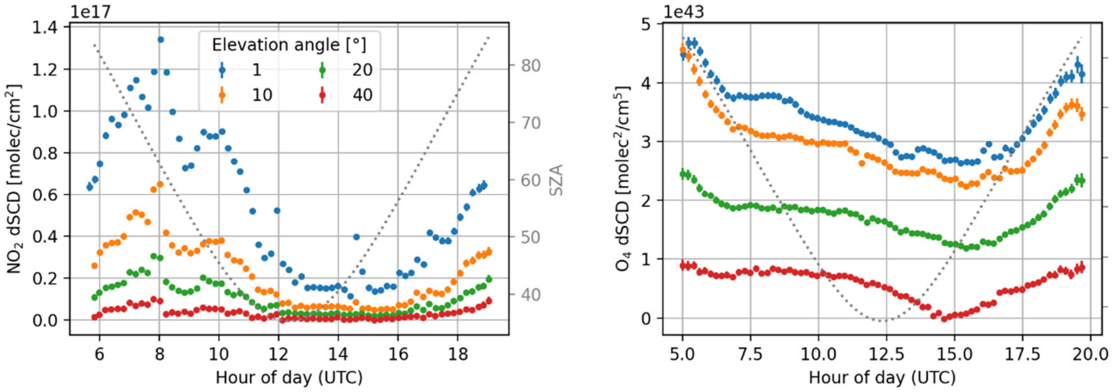
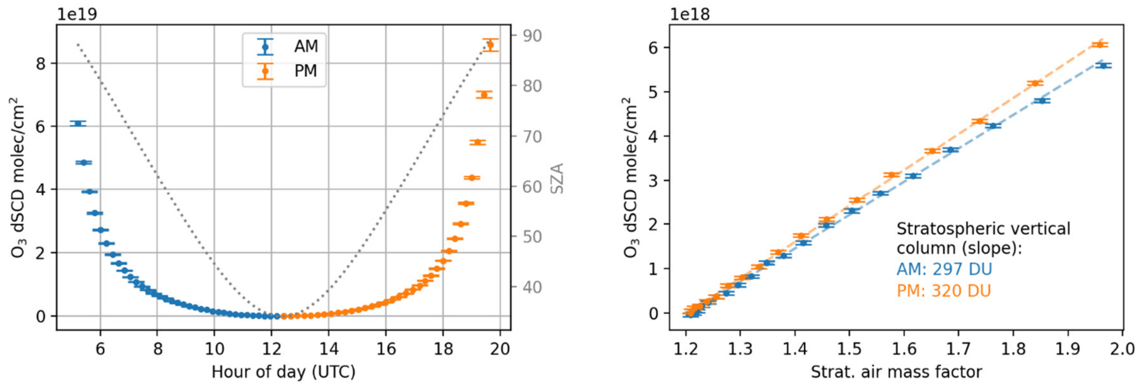
EXAMPLE RESULTS

The software to create the following figures is not included in the package!

EXAMPLE DSCDS

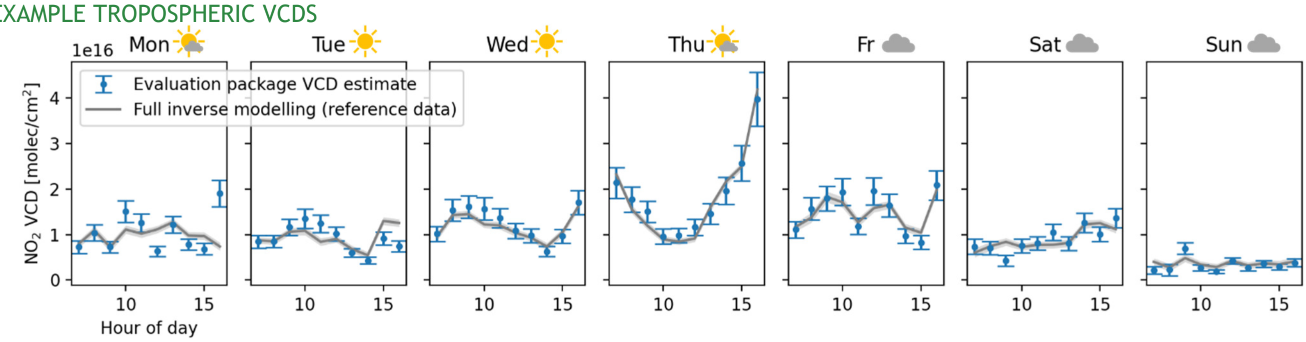


Timeseries of dSCDs for NO_2 and O_4, evaluated against the closest zenith reference spectrum. Data was recorded during a clear-sky summer day using a stationary 1D SkySpec instrument (see also J. Lampel et al., DOI:10.5194/acp-18-1671-2018, 1 minute exposure time, recorded near Plymouth, England).



Left: timeseries of zenith O_3 dSCDs, evaluated against noon zenith reference spectrum. Right: Langley extrapolation from the same data (SZA < 60°) to infer the stratospheric vertical column (not included in the package, for demonstration only). Data was recorded during a clear-sky summer day using a stationary 1D SkySpec instrument (see also J. Lampel et al., DOI:10.5194/acp-18-1671-2018, 1 min exposure time, recorded near Plymouth, England).

EXAMPLE TROPOSPHERIC VCDS



One week of tropospheric NO_2 VCD estimates. For validation, underlying dSCDs were also fed to inverse modelling algorithms applying full radiative transport calculations. See also J.-L. Tirpitz et al. (DOI: 10.5194/amt-14-1-2021) and K. Kreher et al. (DOI: 10.5194/amt-13-2169-2020), 1 min exposure time, data recorded in Cabauw, Netherlands.

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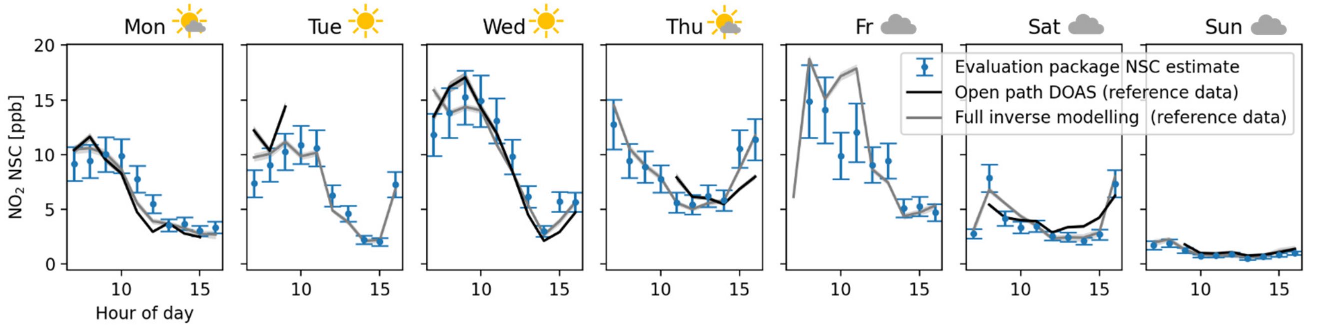
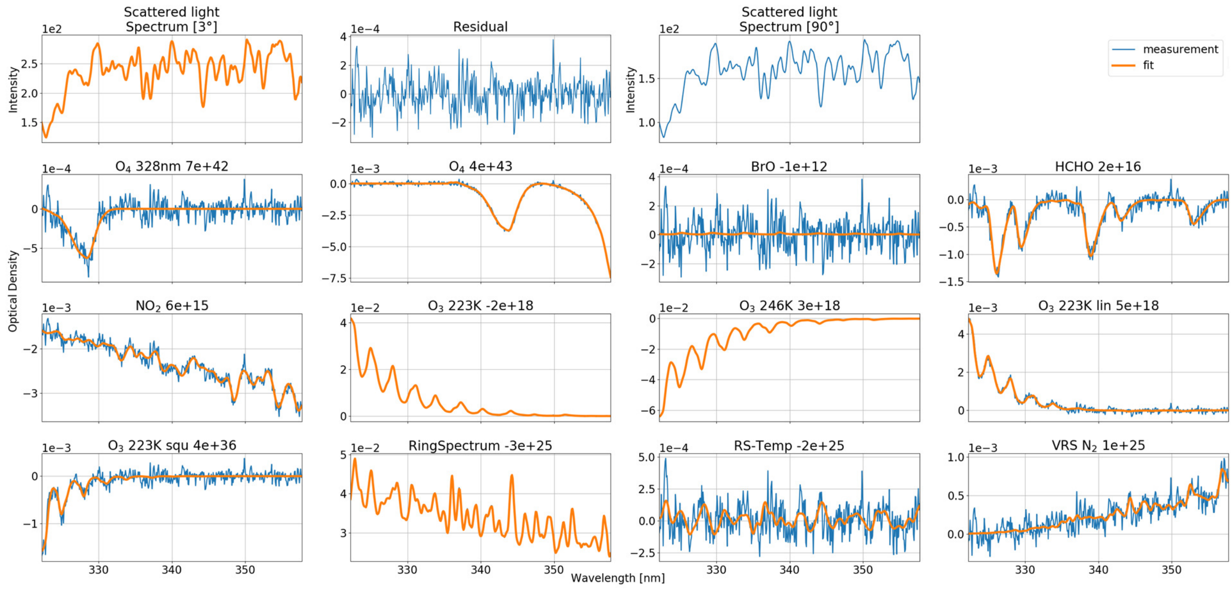
EXAMPLE NEAR-SURFACE CONCENTRATIONS

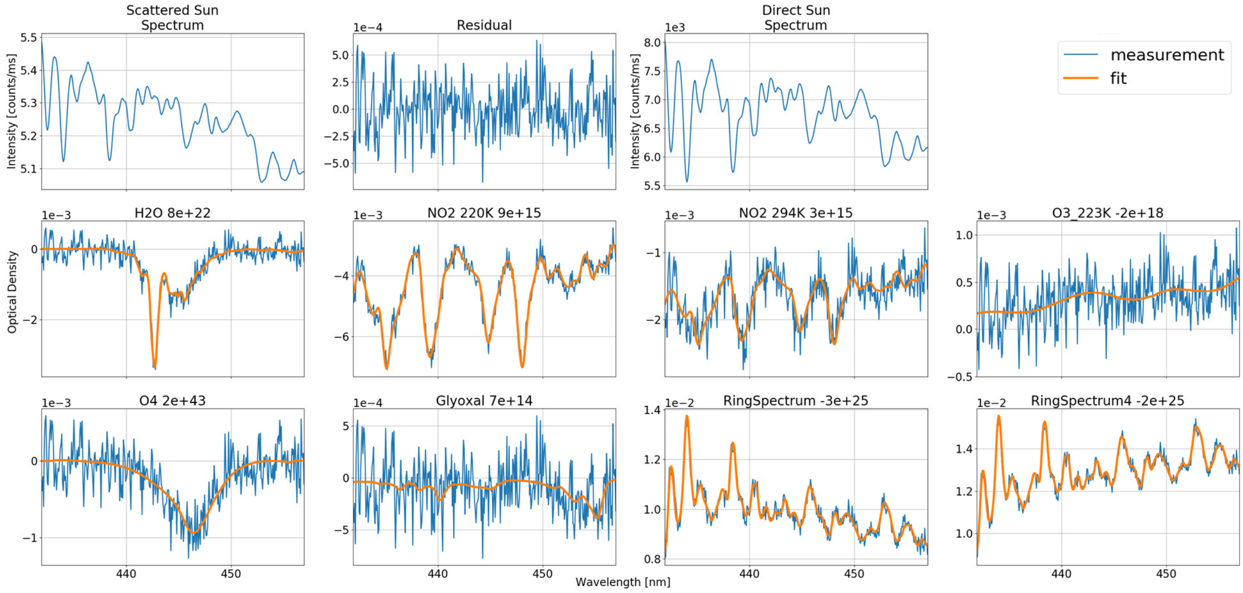


One week of NO_2 NSC. Data from a near-surface open path system is shown for comparison. Furthermore, a reference set of NSCs was derived by feeding the underlying dSCDs to inverse modelling algorithms applying full radiative transport calculations. For further details, see J.-L. Tirpitz et al. (DOI: 10.5194/amt-14-1-2021) and K. Kreher et al. (DOI: 10.5194/amt-13-2169-2020), 1 min exposure time, data recorded in Cabauw, Netherlands.

EXAMPLE DOAS FIT RESULTS



Example spectral fit result for scattered sun light using a stationary 1D SkySpec instrument (from Lampel et al., DOI:10.5194/acp-18-1671-2018, 4 minute exposure time, recorded near Plymouth, England).



Example spectral fit direct sun light using a stationary 2D SkySpec instrument. The light diffuser system for direct sun measurements guarantees an optimal spectral mixing avoiding systematic spectral residual structures. Here, a direct sun spectrum recorded at a Solar Azimuth Angle (SZA) of 54° is chosen as reference spectrum and evaluated against a scattered light spectrum recorded at an SZA of 47° at an elevation of 40°, each for 1 min total exposure time.

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