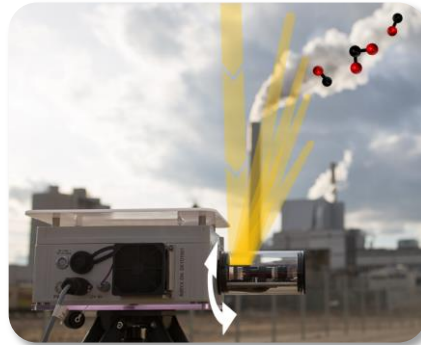


# SkySpec Instruments

PASSIVE REMOTE SENSING OF ATMOSPHERIC PARTICLES AND GASES



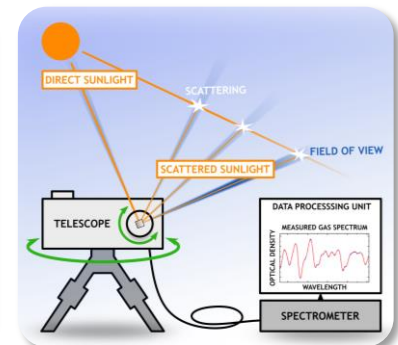
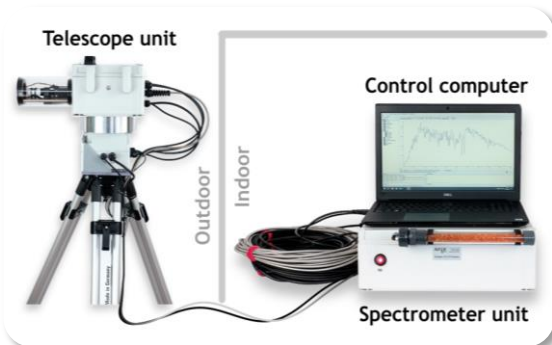
- Telescope-spectrometer systems for direct-sun and scattered skylight spectrum acquisition
- Optimized for DOAS (Differential optical absorption spectroscopy) observations; other spectroscopic applications are possible.
- Detectable gases: NO<sub>2</sub>, O<sub>3</sub>, SO<sub>2</sub>, HCHO, H<sub>2</sub>O, HONO, IO, BrO, Glyoxal, O<sub>4</sub>
- Default spectral range: ultraviolet & visible
- Modular systems with customizable configurations.
- Software packages for spectral analysis, post-processing and data visualization

## TELESCOPE FEATURES:

- Up to two motorized axes (elevation & azimuth)
- Fast and accurate pointing
- Automatic correction of telescope viewing elevation via accelerometer
- Narrow field of view
- Rugged and weather-proof design, minimum outside moving parts
- Integrated wide angle cameras for monitoring purposes

## SPECTROMETER FEATURES:

- Characterized and calibrated
- Active temperature stabilization
- Sub-nm spectral resolution
- High spectral sampling
- High optical sensitivity
- Homogeneous slit illumination

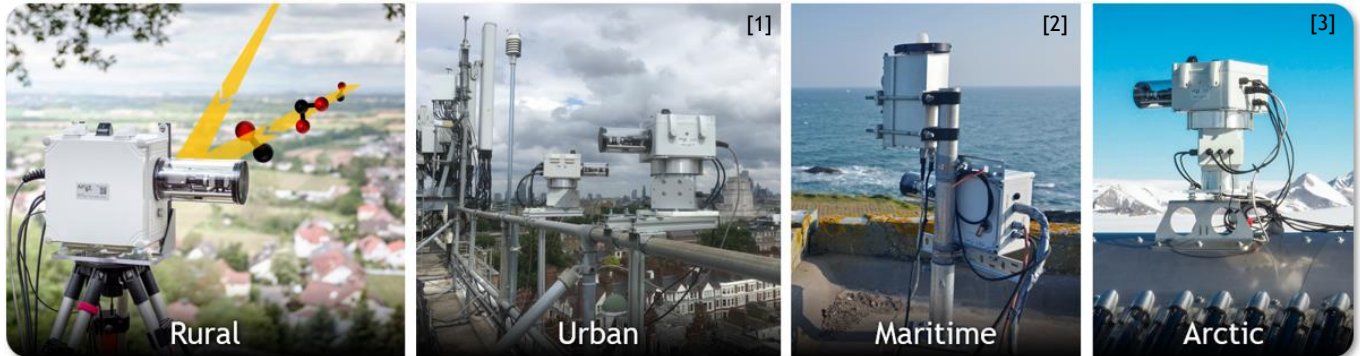


Typical system setups and measurement geometries

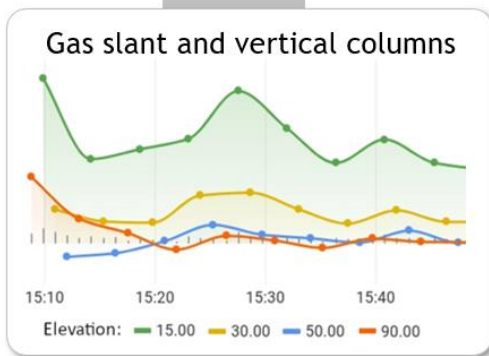
## APPLICATIONS

### GENERAL MONITORING

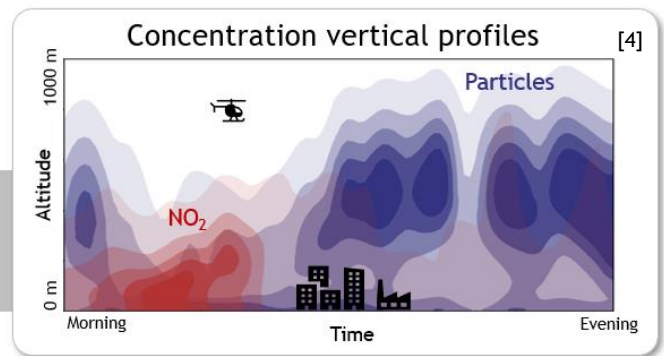
SkySpec observations provide trace gases and aerosol optical thicknesses averaged over horizontal distances of several kilometres; in many applications a great advantage over in-situ measurements which can be strongly affected by local events. SkySpec systems are therefore ideal to assess regional air quality; thanks to their high sensitivity also in very remote and clean environments. Airyx offers software packages to process the raw data into light path integrated gas abundancies (slant and vertical columns), and even vertical concentration profiles.



DOAS spectral analysis



Radiative transport inversion

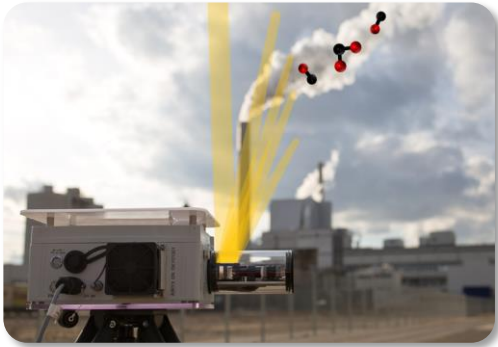


### GAS IMAGING

Sequential scanning and real-time data processing allow to visualize and quantify invisible gases in an intuitive way. The Airyx imaging package automatically produces overlays of integrated camera and slant column images.



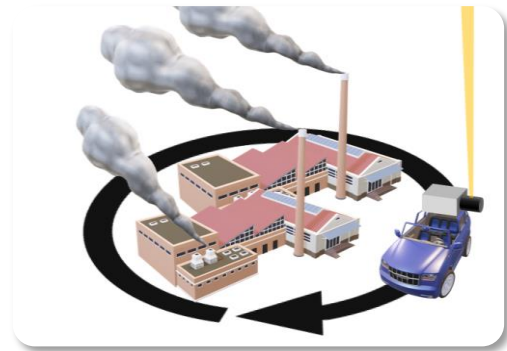
## POINT SOURCE MONITORING



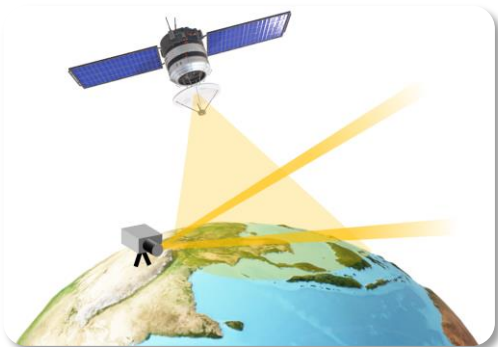
Targeted vertical scanning allows to determine the composition of point emission plumes (factories powerplants, volcanoes,...) at safe distance of up to several kilometres to potentially restricted or hazardous sources. Combine SkySpec observations with wind data to determine gas emission rates with high accuracy.

## MOBILE APPLICATIONS

The automated elevation angle correction and the compact design of SkySpecs are ideal for mobile application on cars, ships, or other moving platforms. E.g. driving around industrial parks or entire cities allows to determine the in- and outflow of pollutants and thus the emission rate of the encircled area.

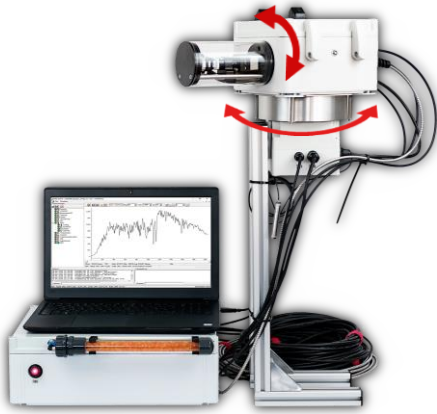


## SATELLITE VALIDATION



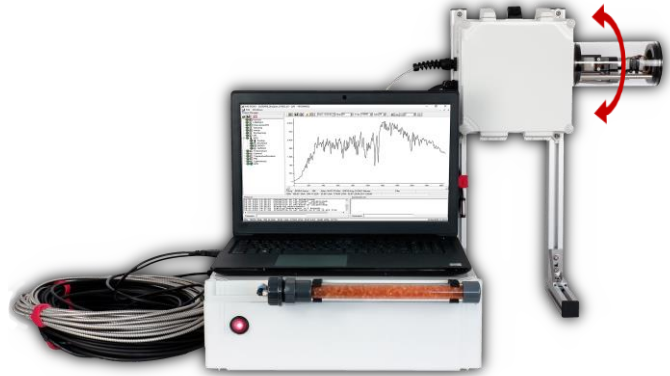
The spatial averaging interval of SkySpecs and the typical size of satellite ground pixels are of a similar order of magnitude. SkySpecs can therefore provide datasets of exceptional representativeness for the validation of satellite data.

## INSTRUMENT OVERVIEW



**SKYSPEC 2D**

- Separate outdoor telescope and indoor spectrometer unit.
- Two motorized axes for full sky hemisphere access
- Direct Sun and 2D imaging capability.



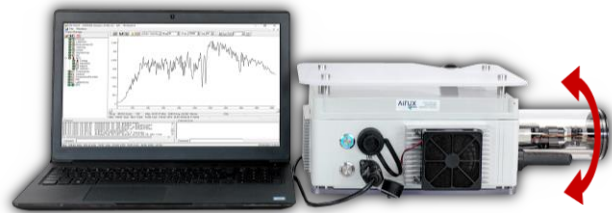
**SKYSPEC 1D**

- Separate outdoor telescope and indoor spectrometer unit.
- Motorized elevation axis, fixed azimuth



**SKYSPEC COMPACT**

- Telescope, spectrometer and embedded computer in a single box
- Motorized elevation axis, fixed azimuth



**SKYSPEC MINI**

- Telescope and spectrometer in a single box. External control computer.
- Motorized elevation axis, fixed azimuth



**SEPARATE UNITS**

- Customizable telescopes and spectrometers as separate units.
- For integration in custom measurement systems for various spectroscopic applications

## HIGHLIGHTS



**BENEFITS**

**INNOVATION**

**High measurement accuracy**

- Low spectrometer stray-light (< 0.1%) due to optimized optical bench and color filters
- Individual spectrometer fine adjustment to achieve best spectral resolution at high light throughput and sufficient spectral sampling (min. 5 Pixel over FWHM of line function).
- Detector nonlinearity correction included
- Temperature stabilized spectrometers (precision better than 0.02 °C), assures stable spectral properties.
- Optimized optical fiber bundle setup (cross-sectional converter) for high light throughput, at still small field of view and high spectral resolution.
- Built-in mercury (HG) lamp systems available for automatized wavelength calibration.
- Continuous monitoring and fast active correction of telescope elevation angle allow measurements at changing environments and on moving platforms (ships, cars, bicycles).
- Prism telescope guarantees best spectral light deflection, avoiding varying spectral reflection properties for different light polarizations (as occurring e.g. for mirrors).
- The small vertical field of view (< 0.3°) is optimal for further data processing involving radiative transfer calculations (e.g. vertical profile retrievals)
- Diffusor plate system assures high spectral quality of direct-sun data (2D-model only)

**Simple setup & maintenance**

- Automatic, fast and accurate telescope elevation position due to built-in inclination sensor including temperature correction
- Fast instrument power-up
- Simple telescope cleaning, low optic contamination, low levels of light intensity from other viewing directions
- Prism telescope rotates in a closed quartz glass tubing without any outside moving parts to avoid mechanical problems and failure of the telescope resulting in long lifetime and operation in harsh environmental conditions (strong wind and snow).
- Integrated telescope heating (activates below 5 °C), allows operation at low temperatures by melting snow and ice and operation even in polar regions (down to -30 °C).
- Telescope and spectrometer units are sealed air tight and include desiccant to avoid water condensation on the optics and inside the spectrometer. Spectrometer unit indoor installation (1D / 2D systems) are equipped with an additional desiccant system which dries the air diffusing to the inside of the spectrometer unit. This allows easy maintenance of the desiccant.
- 1D & 2D telescopes can also be used stand-alone and connected to arbitrary spectrometers.
- Weather proof IP64 housings.
- Easily adaptable measurement routine provides high flexibility



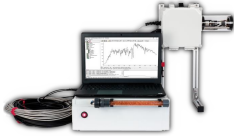

**Custom Configuration**

- Individual spectrometer configurations for the customer needs (spectral range, spectral resolution)
- Optimizing spectrometer configuration for optimal measurement quality, avoiding spectral under-sampling (an often-underestimated problem)
- Different fibre and cable lengths are available
- Optical systems for optimised direct-sun and automatic wavelength calibration
- Components separately available

**Low power consumption**

- Typical power consumption of 20 to 30 W for low operation costs
- Allow simple, mobile operation
- 12V supply voltage allows battery for operation as uninterrupted power supply solution.

## SPECIFICATIONS

Model				
	MINI	COMPACT	1D	2D
Measurement PC	External	Embedded	External	External
Direct sun mode available	No	No	No	Yes
Data communication	USB	LAN / WiFi	USB	USB
Azimuth angle range and accuracy	Fixed	Fixed	Fixed	-5° to 185°, ± 2° <sup>15</sup>
Camera options <sup>*1</sup>	None or single	None or single	None, single or dual	None, single or dual
Weight	≈ 7 kg	≈ 7 kg	≈ 13 kg	≈ 14 kg
Size of telescope unit (WxDxH)	Box <sup>*8</sup> : 30 x 20 x 13.2 cm <sup>3</sup> Quartz tube length: 16 cm	Box <sup>*8</sup> : 30 x 20 x 13.2 cm <sup>3</sup> Quartz tube length: 16 cm	Box <sup>*8</sup> : 20 x 20 x 13.2 cm <sup>3</sup> Quartz tube: 16 cm	Boxes <sup>*8</sup> : 20 x 20 x 29 cm <sup>3</sup> Quartz tube: 16 cm
Telescope stand-alone possible	No	No	Yes <sup>*6</sup>	Yes <sup>*6</sup>
Size of spectrometer unit (WxDxH)	Embedded in telescope	Embedded in telescope	Box <sup>*8</sup> : 40 x 30 x 13.2 cm <sup>3</sup>	Box <sup>*8</sup> : 40 x 30 x 13.2 cm <sup>3</sup>
Operation temperature	-10°C to 40°C	-10°C to 40°C	-30°C to 50°C (telescope unit)	-30°C to 50°C (telescope unit)
GPS option	Yes	Yes	No	No
Calibration lamp options <sup>*2</sup>	External handheld lamp <sup>*3</sup>	External handheld lamp <sup>*3</sup>	Integrated and/or external handheld lamp <sup>*3</sup>	Integrated and/or external handheld lamp <sup>*3</sup>
Spectrometers	Single	Single	Single or dual (UV and Vis) <sup>*7</sup>	Single or dual (UV and Vis) <sup>*7</sup>
Typical spectral range	300-460 nm <sup>*4</sup>	300-460 nm <sup>*4</sup>	300-405 nm (UV) and 420-565 nm (Vis) <sup>*4</sup>	300-405 nm (UV) and 420-565 nm (Vis) <sup>*4</sup>
Typical spectral resolution (FWHM)	0.6 nm <sup>*4</sup>	0.6 nm <sup>*4</sup>	UV: 0.45 nm and 0.6 nm (Vis) <sup>*4</sup>	UV: 0.45 nm and 0.6 nm (Vis) <sup>*4</sup>
Available detectors	back-thinned CCD or CMOS (back-thinned CCD highly recommended for UV)			
Elevation angle range and accuracy	-10° to 190°, ± 0.2° (automatic adjustment with inclination sensor)			
Field of view FWHM, Vertical x Horizontal	Scattered skylight: 0.3° x 1°, direct sunlight (SkySpec2D with diffusor system only): 10° x 10°			
Tripod & Adapter	Adapter for telescope and outdoor tripod <sup>*3</sup>			
Power consumption	avg. <30 W (100 W max.), supply voltage 9-15 V, 110 - 220V AC power supply incl., operation with battery battery <sup>*1</sup> possible			
Housing material	Polycarbonate (IP64), UV resistant			
Additional sensors	Ambient temperature, pressure, humidity in spectrometer housing, temperature on electronic board			

<sup>\*1</sup> Wide field of view (≈90° vertical) cameras on telescope housing e.g. for monitoring of cloud conditions

<sup>\*2</sup> Mercury (HG) gas lamp for spectrometer wavelength calibration check. Re-calibration typically not necessary due to stable in-house calibration.

<sup>\*3</sup> Available accessory

<sup>\*4</sup> Customizable, contact Airyx for more information.

<sup>\*5</sup> Accuracy applies if azimuth is automatically calibrated from sun position

<sup>\*6</sup> Control over RS232, enables switching between devices and connection to arbitrary spectrometers

<sup>\*7</sup> Two spectrometers improve spectral coverage without loss of spectral quality.

<sup>\*8</sup> Size of cuboid main enclosure. Outsticking components like connectors, optical tube, coolers, cameras, etc. are not considered.

## TYPICAL SENSITIVITIES

Data based on MADCAT campaign data (see Lampel et al. 2015, doi:10.5194/amt-8-3767-2015). Integration time: 60 s (≈ 1000 scans), Saturation: 60 %, volume mixing ratios assume 10 km light path.

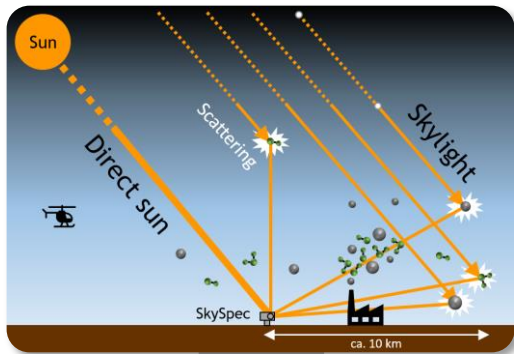
Parameter	Quantity / unit	NO <sub>2</sub>	SO <sub>2</sub>	HCHO	BrO	H <sub>2</sub> O	O <sub>4</sub>	HONO	IO	Glyoxal
Limit of detection	Slant column / molec cm <sup>-2</sup>	7e14	7e15	5e15	2e13	1e22	1e41 <sup>*1</sup>	4e14	1e13	3e14
	Volume mixing ratio / pptv	30	300	200	0.7	0.05 <sup>*2</sup>	-	15	0.6	20
Measured SNR (urban)	Signal-to-noise ratio	285	< 0.6	2	0.5	30	300	5	< 0.5	< 2.5
	Assumed slant column / molec cm <sup>-2</sup>	2e17	4e15	1e16	1e13	3e23	3e43 <sup>*1</sup>	2e15	5e12	5e14

<sup>\*1</sup> in units of molec<sup>2</sup> cm<sup>-5</sup>

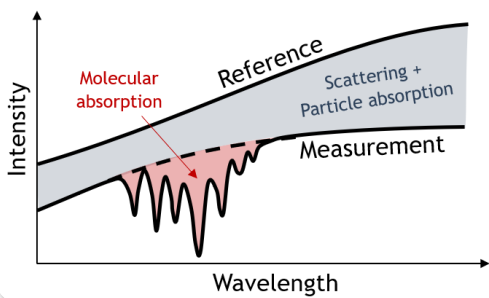
<sup>\*2</sup> in units of %

## MEASUREMENT PRINCIPLE

Passive Differential Optical Absorption Spectroscopy (DOAS) is a manifold technique. The basis shall be outlined here. for more details, please refer to the comprehensive book by Platt and Stutz (2008).

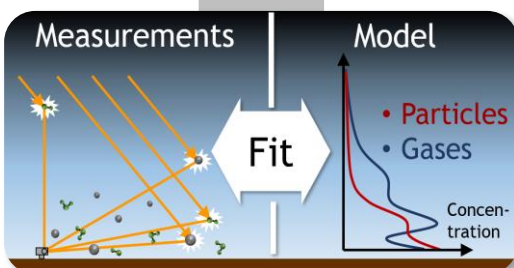


Raw spectra



Differential slant  
column densities

for each viewing direction and gas



Vertical columns  
Concentration profiles

### SPECTRA ACQUISITION

SkySpec systems are designed to acquire UV/Vis-spectra of direct sunlight and scattered skylight coming from distinct directions. Common viewing configurations are direct sun and zenith sky measurements as well as elevation scans (multiple observations at different viewing elevation angles).

Depending on the direction, the detected light's path through the atmosphere differs, as does the amount of gas encountered along the way (see figure on the left). It shall be noted, that the light path also depends on the current visibility conditions, hence, the abundance and properties of atmospheric particles, including fog and clouds.

Each gas absorbs characteristic wavelengths of light, leaving its characteristic trace in the spectrum. The absorption effects are typically small. For many gases, attenuations < 0.1 % have to be resolved to achieve useful detection limits.

### DOAS SPECTRAL ANALYSIS

In the DOAS spectral analysis, always two spectra are compared:

1. **Reference** spectrum: preferably recorded in a direction where little light-gas-interaction is expected (e.g. zenith)
2. **Measurement** spectrum: acquired in the direction of interest, e.g. pointing through an exhaust plume.

The **DOAS fit** is used to identify and separate the trace gas characteristic absorption patterns in the intensity differences between the spectra. The patterns' magnitudes are direct measures of the so-called **Differential slant column density (dSCD)**, breaking down as follows:

- „Column density“: the integrated trace gas concentration encountered along the light's path.
- „Slant“: the light's path through the atmosphere is slant. Counterpart are the so-called „vertical“ column densities.
- „Differential“: the dSCD represents the slant column density **difference** between the measurement the reference light path, not an absolute amount of gas.

DSCDs are provided for each gas and each viewing direction with significant absorption in the investigated spectral range.

### POST-PROCESSING

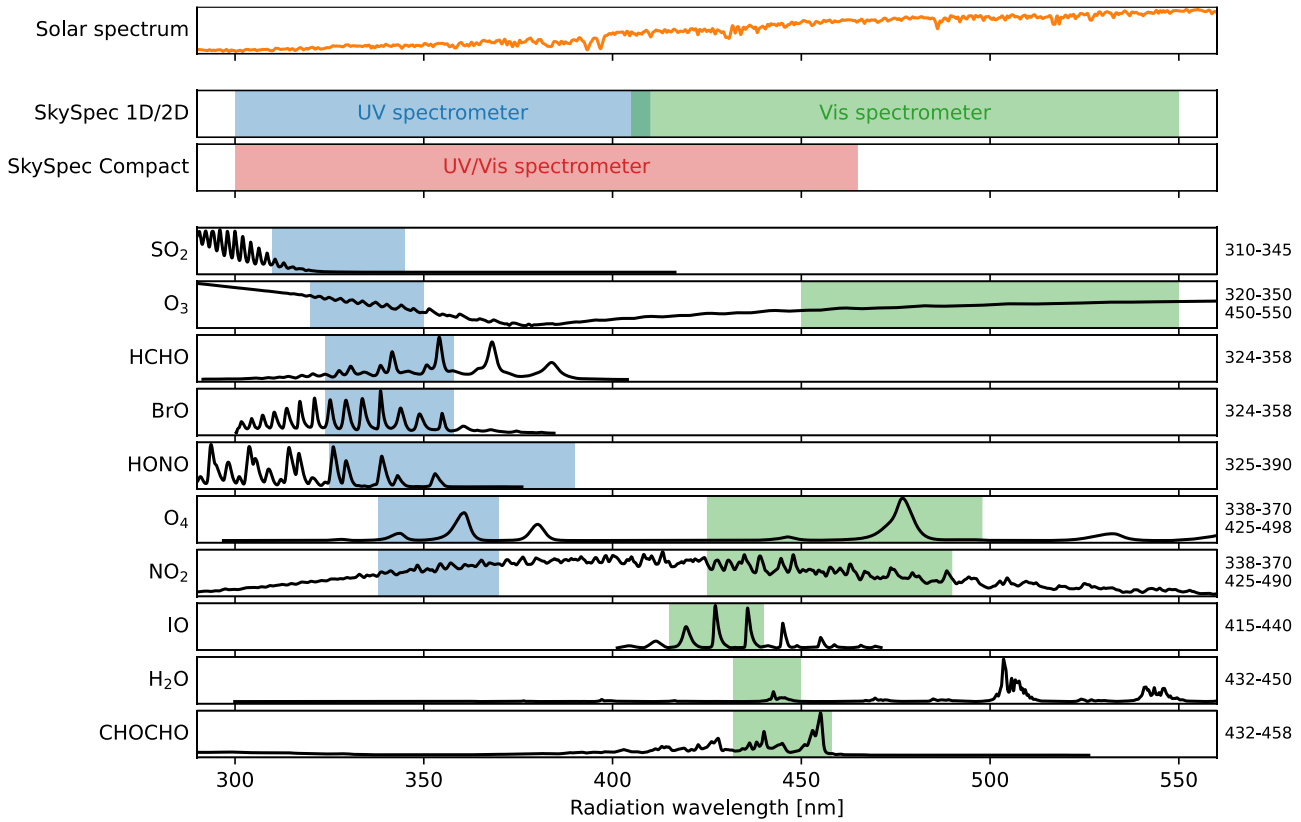
DSCDs can be extremely useful e.g. to determine the integrated emission of local sources. For many applications however, e.g. regional air-quality assessment, vertical column densities or even concentrations are desirable.

Good estimates for vertical columns and concentrations close to the ground can be derived by approximating the light paths geometrically.

Better results can be achieved with **profile retrieval algorithms**, which fit an atmospheric model (considering the physics of photons and the measurement geometry) to the observed dSCDs along various light paths to derive concentrations at multiple altitudes. For simplicity, this approach might be perceived as “atmospheric tomography”. The proxy gas O<sub>4</sub> can even be used to infer particle concentration (see e.g. Frieß, 2004)

## GAS SPECTRAL ABSORPTION PATTERNS

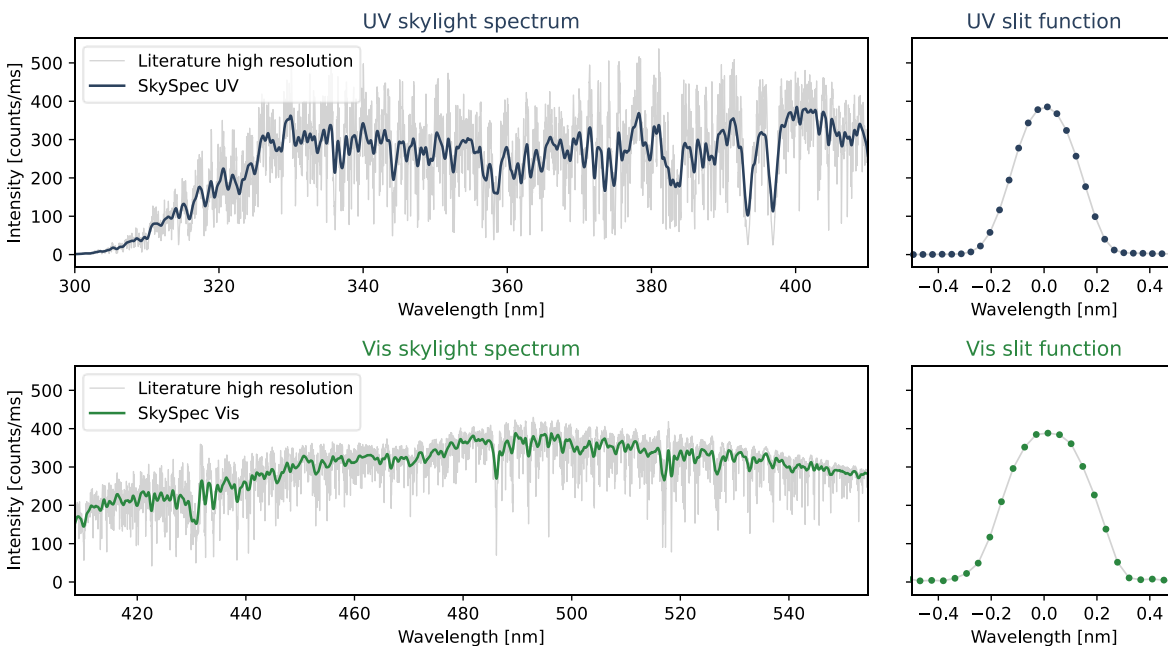
Default SkySpec spectral coverages and absorption cross-sections of typical detectable gases. Shadings indicate the standard ranges considered for the DOAS fit.



## EXAMPLE DATA

### SPECTRA

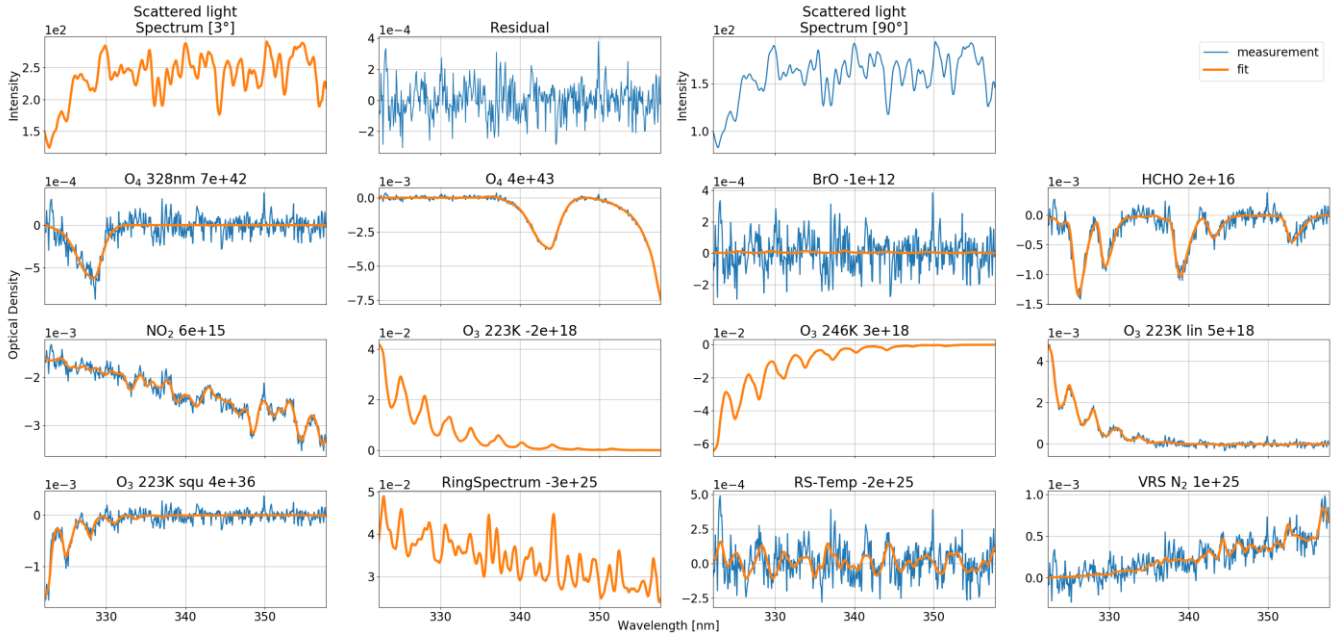
Example blue sky zenith spectra recorded with a SkySpec 2D system. By default, the spectrometer unit contains two spectrometers dedicated to the UV and Vis spectral range, respectively. The instrumental slit functions on the right demonstrate spectral resolution and the high spectral sampling.



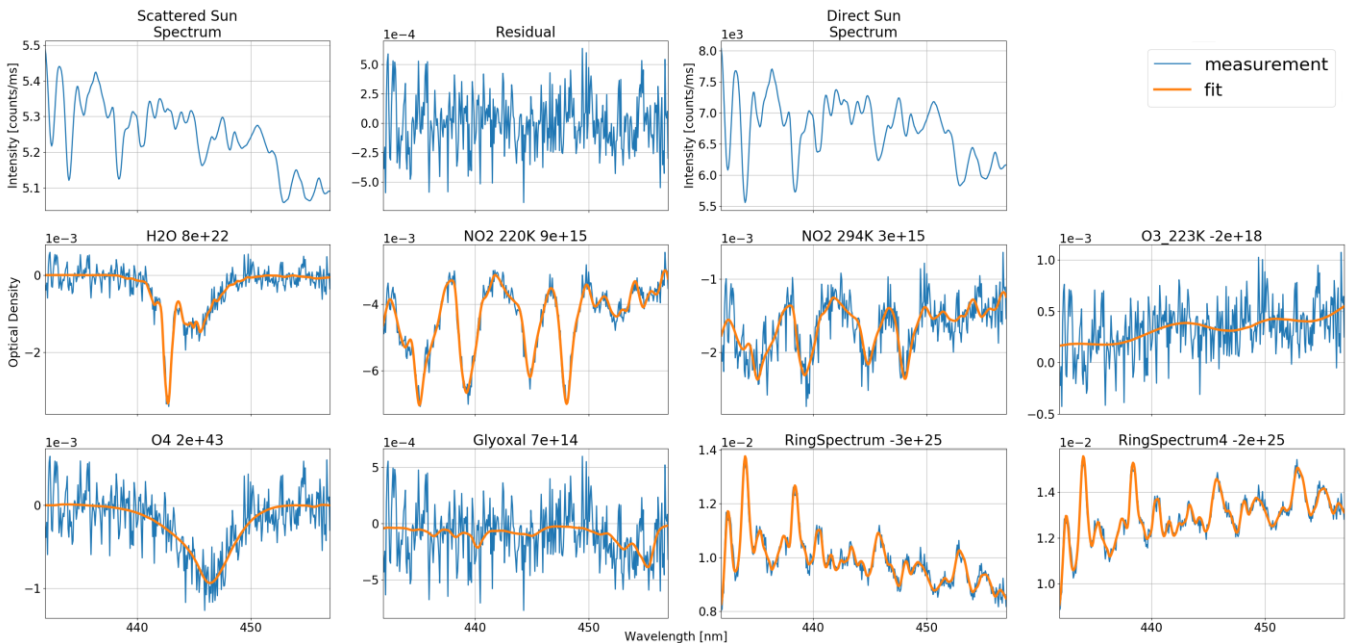


## DOAS FIT RESULTS

Optimized for trace gas detection with DOAS, SkySpecs are designed to achieve exceptional precision in narrow-band optical density. The high spectral quality can best be demonstrated on DOAS fit results. The residual magnitude indicates a precision of few  $10^{-4}$ . Its near-statistical nature indicates that it can even be further improved by extending the exposure times.

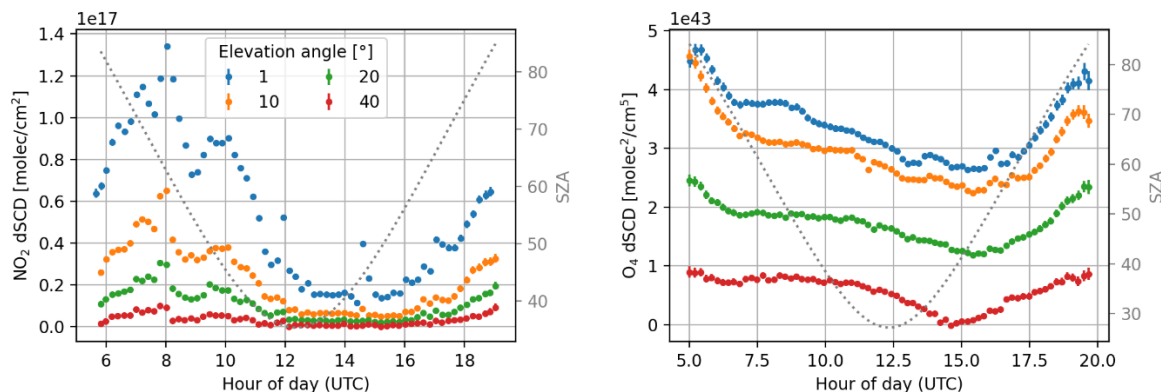


Example fit of the optical density between two skylight spectra, recorded with a 1D SkySpec instrument (from Lampel et al., 2018, 4 minute exposure time, recorded near Plymouth, England).



Example fit of the optical density between a direct sun and a skylight spectrum, recorded with a stationary 2D SkySpec instrument (1 min exposure time). The light diffuser system for direct sun measurements guarantees an optimal spectral mixing avoiding systematic spectral residual structures.

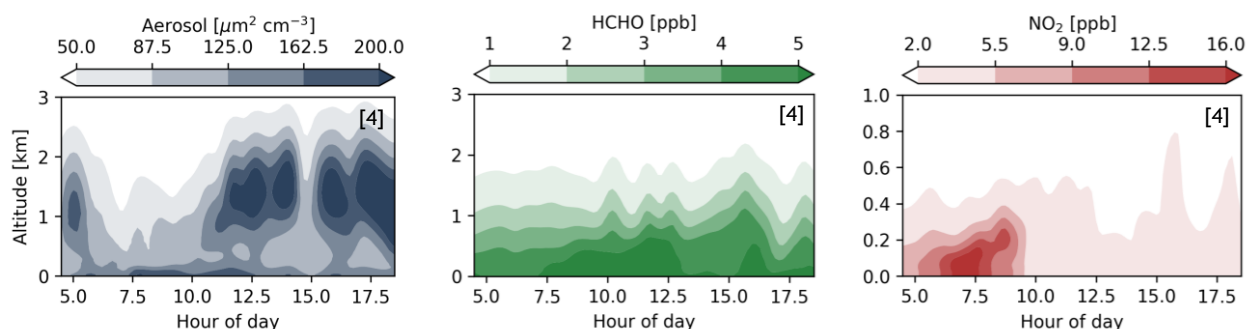
## DIFFERENTIAL SLANT COLUMNS



Timeseries of differential slant columns for  $\text{NO}_2$  and  $\text{O}_4$ , evaluated against the closest zenith reference spectrum. Data was recorded during a clear-sky summer day using a stationary 1D SkySpec instrument (Lampel et al., 2018, 1 minute exposure time, recorded near Plymouth, England).

## VERTICAL PROFILES

As described in more detail in the “PASSIVE DOAS MEASUREMENT PRINCIPLE” section, differential slant column densities can be processed to vertical concentration profiles of particles and trace gases applying radiative transfer inversion algorithms.



Vertical profiles measured with a SkySpec 2D on a summer day in London.

## GAS IMAGING

Airyx provides software to automatically produce overlays of the SkySpec’s integrated camera and slant columns recorded at high angular resolution.

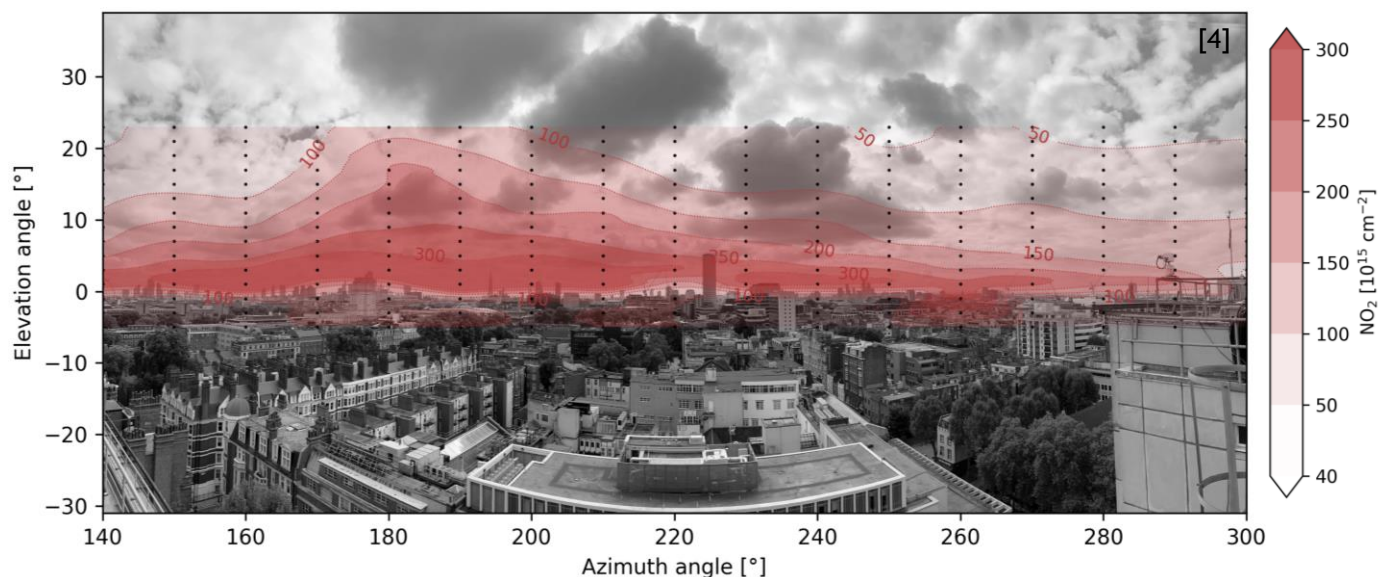


Image representation of  $\text{NO}_2$  differential slant columns above the London skyline.

## PUBLICATIONS AND REFERENCES

### SELECTED PUBLICATIONS CONTAINING RESULTS FROM SKYSPEC MEASUREMENTS

- Tirpitz et al.: Intercomparison of MAX-DOAS vertical profile retrieval algorithms: studies on field data from the CINDI-2 campaign, Atmos. Meas. DOI: 10.5194/amt-2019-456, 2021.
- Kreher et al.: Intercomparison of NO<sub>2</sub>, O<sub>4</sub>, O<sub>3</sub> and HCHO slant column measurements by MAX-DOAS and zenith-sky UV-Visible spectrometers during the CINDI-2 campaign, Atmos. Meas. Tech., DOI: 10.5194/amt-2019-157, 2020.
- Wang et al.: Inter-comparison of MAX-DOAS measurements of tropospheric HONO slant column densities and vertical profiles during the CINDI-2 Campaign, Atmos. Meas. Tech., DOI: 10.5194/amt-2019-464, 2020.
- Ryan et al.: G., Silver, J. D., Querel, R., Smale, D., Rhodes, S., Tully, M., Jones, N., and Schofield, R.: Comparison of formaldehyde tropospheric columns in Australia and New Zealand using MAX-DOAS, FTIR and TROPOMI, Atmos. Meas. Tech., 13, 6501-6519, DOI: 10.5194/amt-13-6501-2020, 2020.
- Wang et al.: Shipborne MAX-DOAS measurements for validation of TROPOMI NO<sub>2</sub> products, Atmos. Meas. Tech., 13, 1413-1426, DOI: 10.5194/amt-13-1413-2020, 2020.
- Lampel et al.: Detection of O<sub>4</sub> absorption around 328 and 419 nm in measured atmospheric absorption spectra, Atmos. Chem. Phys., 18, 1671-1683, DOI: 10.5194/acp-18-1671-2018, 2018.
- Lampel et al.: The tilt effect in DOAS observations, Atmos. Meas. Tech., 10, 4819-4831, DOI: 10.5194/amt-10-4819-2017, 2017.

### FURTHER READING

- Platt and Stutz: Differential Optical Absorption Spectroscopy, vol. 1, Springer Berlin Heidelberg, DOI: 10.1007/978-3-540-75776-4, 2008
- Frieß et al.: A new technique to derive information on atmospheric aerosols: 2. Modeling studies, Journal of Geophysical Research: Atmospheres 111, No. D14, 2006.

## CREDITS

### WE GRATEFULLY ACKNOWLEDGE THE FOLLOWING CONTRIBUTIONS

- [1] Image by Robert Ryan, Department of Geography, University College London
- [2] Image by Ming Xi Yang, Plymouth Marine Laboratory
- [3] Image by Alexis Merlaud, Belgian Institute for Space Aeronomy, Brussels
- [4] Data recorded and evaluated by Robert Ryan, Eloise Marais, University College London
- [5] Measurements performed in cooperation with Robert Ryan, Eleanor Smith, Karn Vohra and Eloise Marais, Department of Geography, University College London

October 2022

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