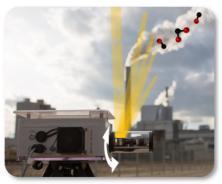


# SkySpec Instruments

# PASSIVE REMOTE SENSING OF ATMOSPHERIC PARTICLES AND GASES







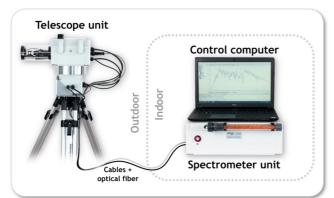
- Telescope-spectrometer systems for direct-sun and scattered skylight spectrum acquisition
- Optimized for UV/Vis aerosol and trace gas remote sensing with the DOAS method
- Other applications are possible
- Detectable gases: NO<sub>2</sub>, O<sub>3</sub>, SO<sub>2</sub>, HCHO, H<sub>2</sub>O, HONO, IO, BrO, Glyoxal, O<sub>4</sub>
- Modular and customizable to meet your specific requirements
- Software packages for spectral analysis, post-processing and data visualization

#### **TELESCOPE:**

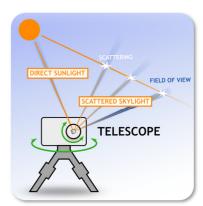
- Up to two motorized axes (elevation & azimuth)
- Fast and accurate pointing
- Automatic correction of telescope viewing elevation via inclination sensor
- · Narrow field of view
- Rugged and weather-proof design, minimum outside moving parts
- Integrated wide angle cameras for monitoring purposes

#### SPECTROMETER:

- Grating spectrometer in compact and rugged enclosure
- Characterized and calibrated
- Active temperature stabilization
- Low straylight design
- Sub-nm spectral resolution
- High spectral sampling
- Homogenized 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\*1.

Recommended systems:

SkySpec 1D or 2D for long-term monitoring Compact or Mini for short-term monitoring

**Recommended software:** SkySpec evaluation package



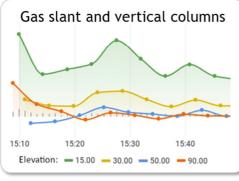




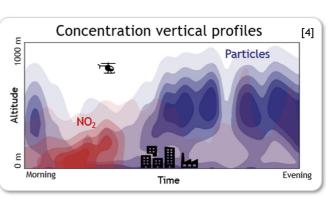
SkySpec imaging evaluation package



DOAS spectral analysis







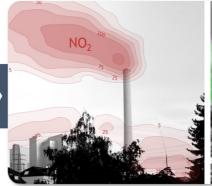
<sup>\*1</sup> Software for full radiative transfer profile inversions is not yet available from Airyx GmbH

#### **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.

Required software:

Required system: SkySpec 2D







#### 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.

Recommended system: SkySpec Compact

Recommended software: SkySpec evaluation package

#### 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.

Recommended system: SkySpec Compact

Recommended software: SkySpec evaluation package



#### 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.

Recommended systems: SkySpec 1D or 2D

Recommended software: SkySpec evaluation package

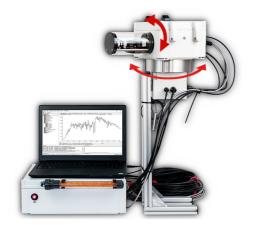
#### **FURTHER APPLICATIONS**

As SkySpec systems are highly modular and customizable, they can be applied for various other spectroscopic applications comprising for example:

- Remote measurements of surface reflection properties
- Biomedical spectroscopy
- Remote measurements of solar induced plant fluorescence
- Material science



# **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**

# Measurement accuracy

- Individual in-house spectrometer fine adjustment to optimize spectral properties
- Spectrometer characterization included: wavelength calibration, offset and dark current spectra, detector non-linearity function
- Active spectrometer temperature stabilization ensures stable properties
- High spectral sampling prevents quantization errors
- Low noise and high precision in narrow-band optical density
- Color filters and optical bench design minimize spectrometer stray-light
- Cross-section converting fiber bundle for maximum light throughput and homogeneous spectrometer illumination
- Real-time correction of telescope elevation via inclination sensor, ideal for measurements on moving platforms (ships, cars) or in changing environments
- Prism deflector and optical fiber setup prevent polarization induced biases
- Small vertical field of view optimized for vertical profiling applications

# Setup, lifetime • & maintenance

- Quartz glass enclosure minimizes outside moving parts for:
  - long lifetime even under in harsh environmental conditions
  - simple cleaning
- Integrated telescope heating (activates at < 5°C) prevents:
  - freezing of mechanical components
  - water condensation, snow and ice and on quartz cylinder and other optics
- Weather proof and UV resistant IP64 housings
- 12V/DC power supply with low consumption, ideal for mobile operation via battery or car-cigarette-lighter
- Easily adaptable measurement routines
- Fast instrument power-up

#### Customization

- Individual spectrometer configurations to best meet your spectral requirements
- Various optical fiber configurations
- Different fiber and cable lengths available
- Integrable opto-mechanical components for direct-sun observations and calibration monitoring purposes
- Stand-alone operation of separate spectrometer and telescope units for integration in arbitrary spectroscopic measurement system



# **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°, $\pm$ 2° *5				
Camera options*1	None or	· single	None, single or dual	None, single or dual				
Weight	≈ 7	kg	≈13 kg	≈ 14 kg				
Size of telescope unit (WxDxH)	Box *8: 30 x 20 Quartz tube le		Box *8: 20 x 20 x 13.2 cm <sup>3</sup> Quartz tube: 16 cm	Boxes *8: 20 x 20 x 29 cm <sup>3</sup> Quartz tube: 16 cm				
Telescope stand-alone possibility	No		Yes *6					
Size of spectrometer unit (WxDxH)	Embedded in	n telescope	Box *8: $40 \times 30 \times 13.2 \text{ cm}^3$					
Operation temperature	-10°C to	o 40°C	-30°C to 50°C (telescope unit)					
GPS option	Ye	es	No					
Calibration lamp options*2	External hand	lheld lamp *3	Integrated and/or external handheld lamp *3					
Spectrometers	Sing	gle	Single or dual (UV and Vis) *7					
Typical spectral range	300-460	) nm *4	300-405 nm (UV) and 410-553 nm (Vis) *4					
Typical spectral resolution (FWHM)	< 0.7	nm *4	UV: < 0.5 nm and < 0.6 nm (Vis) *4					
Spectral sampling	> 5 sampling points over spectrometer slit function FWHM							
Available detectors	back-thinned CCD or CMOS (back-thinned CCD highly recommended for UV)							
Elevation angle range and accuracy	-10° to 190°, automatic adjustment with inclination sensor to < 0.1° accuracy (1 $\sigma$ )							
Field of view FWHM, vertical x horizontal	Scattered skylight: < $0.3^{\circ}x\ 1^{\circ}$ , direct sunlight (SkySpec 2D with diffusor system): $10^{\circ}\ x\ 10^{\circ}$							
Tripod & adapter	Adapter for telescope and outdoor tripod *3							
Power consumption	Average < 30 W (100 W max.), supply voltage 9-15 V, 110-220 V AC power supply incl., operation with battery *1 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 ( $^{\sim}90^{\circ}$  vertical) cameras on telescope housing e.g. for monitoring of cloud conditions

arbitrary spectrometers 
'7 Two spectrometers improve spectral coverage without loss of spectral

#### TYPICAL SENSITIVITIES

Integration time: 60 s (≈ 1000 scans), volume mixing ratios assume 10 km light path.

Parameter	Quantity / unit	NO <sub>2</sub>	SO <sub>2</sub>	нсно	BrO	H <sub>2</sub> O	O <sub>4</sub>	HONO	10	Glyoxal
Limit of detection (1σ)	Slant column / molec cm <sup>-2</sup>	4e14	4e15	3e15	1e13	5e21	1e41 *1	2e14	5e12	2e14
	Volume mixing ratio / pptv	16	160	120	0.4	0.02 *2	-	8	0.2	8
Measured SNR (urban)	Signal-to-noise ratio	500	1	3	1	60	600	10	1	2.5
	Assumed slant column / molec cm <sup>-2</sup>	2e17	4e15	1e16	1e13	3e23	3e43 *1	2e15	5e12	5e14

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

 $<sup>^{*2}</sup>$  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.

 $<sup>^{\</sup>circ 5}$  Accuracy applies if azimuth is automatically calibrated from sun position \*6 Control over RS232, enables switching between devices and connection to

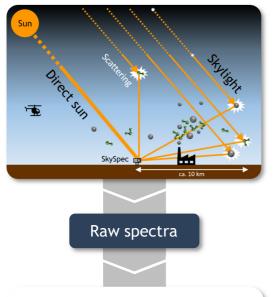
quality.
\*\* Size of cuboid main enclosure. Outsticking components like connectors,

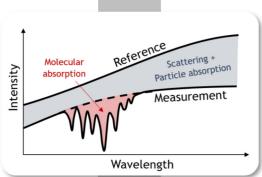
optical tube, coolers, cameras, etc. are not considered.



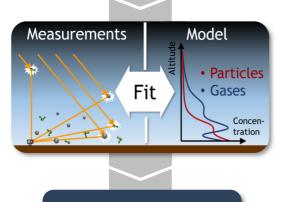
# MEASUREMENT PRINCIPLE

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).









Vertical columns and 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 distinct 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:

- Reference spectrum: preferably recorded in a direction where little light-gas-interaction is expected (e.g. zenith)
- 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 viewing direction and each gas 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

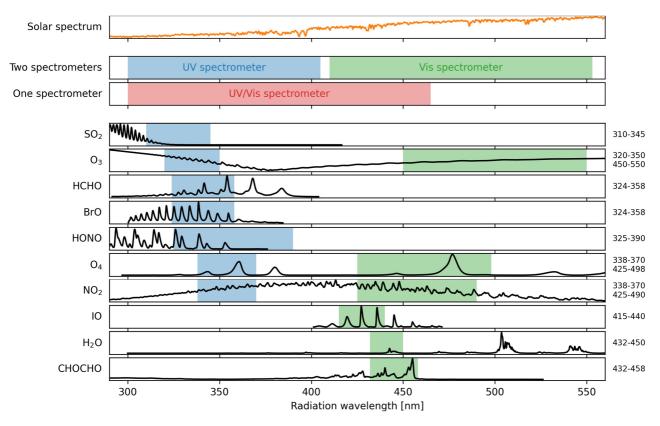
Good estimates for vertical columns and concentrations close to the ground can be derived by approximating the light paths geometrically.

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  $O_4$  can even be used to infer particle concentration (see e.g. Frieß, 2004)



#### GAS SPECTRAL ABSORPTION PATTERNS

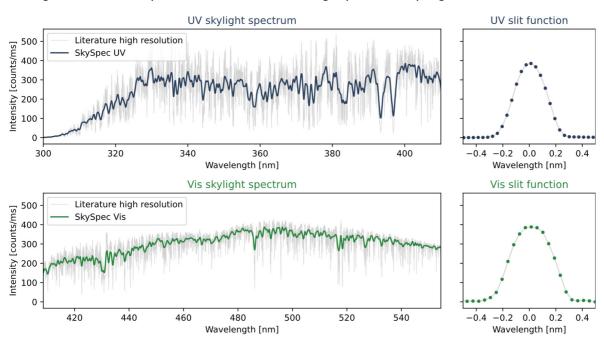
Default SkySpec spectral coverages and absorption cross-sections of typical detectable gases. Shadings indicate the standard ranges considered for the DOAS fit.



# **EXAMPLE DATA**

#### **SPECTRA**

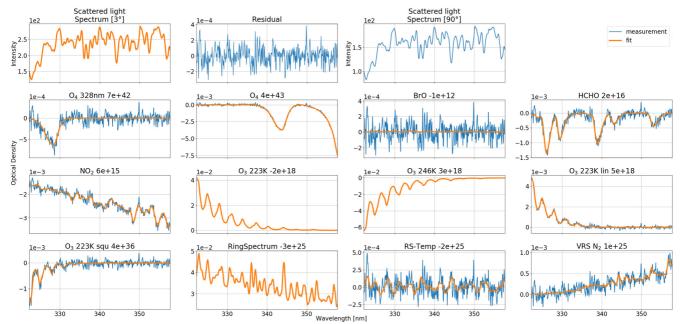
Example blue sky zenith spectra recorded with a SkySpec 2D system. By default, the spectrometer unit contains two spectrometers dedicated to the UV and Vis spectral range, respectively. The instrumental slit functions on the right demonstrate spectral resolution and the high spectral sampling.



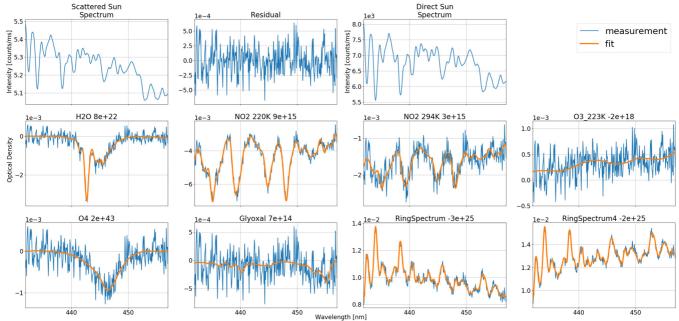


#### DOAS FIT RESULTS

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<sup>-4</sup>. Its near-statistical nature indicates that it can even be further improved by extending the exposure times.



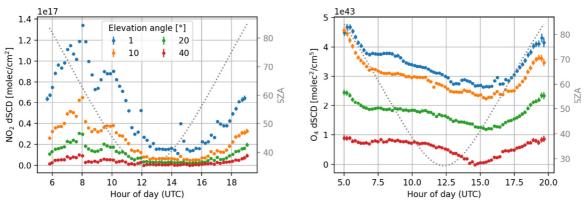
Example fit of the optical density between two skylight spectra, recorded with a 1D SkySpec instrument (from Lampel et al., 2018, 4 minute exposure time, recorded near Plymouth, England).



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.



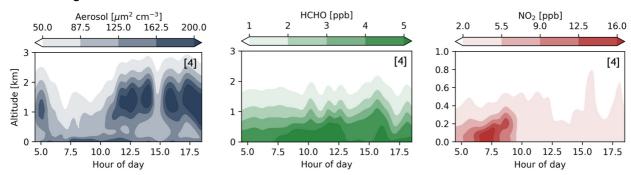
#### **DIFFERENTIAL SLANT COLUMNS**



Timeseries of differential slant columns for  $NO_2$  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 (Lampel et al., 2018, 1 minute exposure time, recorded near Plymouth, England).

#### **VERTICAL PROFILES**

As described in more detail in the "Measurement principle" section on page 7, 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.

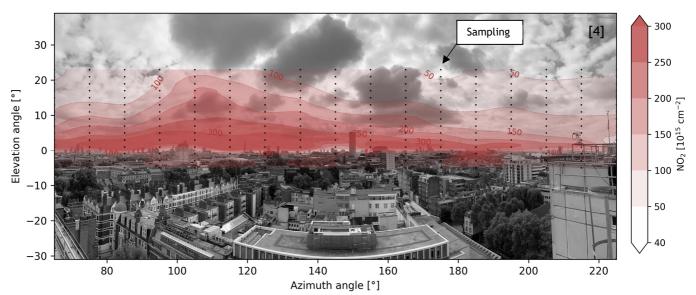


Image representation of  $NO_2$  differential slant columns above the London skyline.



# 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 at 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 O₄ 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