Universiteit Leiden
The Netherlands

Accessible remote sensing of water

Burggraaff, O.

Citation
Burggraaff, O. (2022, December 13). *Accessible remote sensing of water*. Retrieved from https://hdl.handle.net/1887/3497379

Version:	Publisher's Version
License:	Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden
Downloaded from:	https://hdl.handle.net/1887/3497379

Note: To cite this publication please use the final published version (if applicable).

6 | A universal smartphone add-on for portable spectroscopy and polarimetry: iSPEX 2

Adapted from

Olivier Burggraaff, Armand Perduijn, Robert van Hek, Norbert Schmidt,
Christoph Keller, Frans Snik

*Micro- and Nanotechnology Sensors, Systems, and Applications XII,
Proceedings of the SPIE 11389, 113892K (2020)*

doi:10.1117/12.2558562

Spectropolarimetry is a powerful technique for remote sensing of the environment. It enables the retrieval of particle shape and size distributions in air and water to an extent that traditional spectroscopy cannot. SPEX is an instrument concept for spectropolarimetry through spectral modulation, providing snapshot, and hence accurate, hyperspectral intensity and degree and angle of linear polarisation. Successful SPEX instruments have included groundSPEX and SPEX airborne, which both measure aerosol optical thickness with high precision, and soon SPEXone, which will fly on PACE. Here, we present a low-cost variant for consumer cameras, iSPEX 2, with universal smartphone support. Smartphones enable citizen science measurements which are significantly more scaleable, in space and time, than professional instruments. Universal smartphone support is achieved through a modular hardware design and SPECTACLE data processing. iSPEX 2 is manufactured through injection moulding and 3D printing. A smartphone app for data acquisition and processing is in active development. Production, calibration, and validation are ongoing, with promising initial results. Scientific applications will include citizen science measurements of aerosol optical thickness and surface water reflectance, as well as low-cost laboratory and portable spectroscopy.

6.1 Introduction

Spectropolarimetry, the characterisation of reflected or emitted light at different wavelengths and polarisation states, is a powerful technique for remote sensing of the environment [132, 238, 457]. Most prominently, the Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) satellite due for launch in 2024 will fly two spectropolarimetric instruments, namely HARP-2 and SPEXone [86, 111]. HARP-2 will observe linear polarisation (LP) in four spectral bands (440, 550, 670, 870 nm) at 10–60 angles with a polarimetric accuracy of <0.005 in Degree of Linear polarisation (DoLP) [86, 185]. Meanwhile, SPEXone will observe at five discrete angles (0°, ±20°, ±57°) with continuous spectral coverage from 385–770 nm and a DoLP accuracy of 0.0025 [184, 185]. Instruments observing circular polarisation are also under active development, such as the Life Signature Detection polarimeter (LSDpol) [458], but current efforts typically focus on linear polarimetry, as does this work.

Science cases for linear spectropolarimetry include the retrieval of aerosol and hydrosol particle properties, the beam attenuation and absorption coefficients (c, a) in water, and the study of vegetation covers. For aerosols, there is already a long history of multi-angle spectropolarimetric observations, from which parameters including particle size and shape distributions, spatial distributions, and chemical composition can be derived [132, 185]. More recently, this has been extended to oceanic hydrosols, where the bulk refractive index, particle size distribution, and c can be derived from DoLP [163]. This has been demonstrated for example by Gilerson et al. with a retrieval algorithm for c and a from multi-angular DoLP data [174]. Finally, spectropolarimetry of vegetation probes its physical characteristics, such as leaf orientation, and provides reflectance distribution functions, which are crucial for improving the accuracy of air- or space-based aerosol retrieval algorithms [459].

Combining spectral and polarimetric measurements can be done in multiple ways [170]. First, regular spectroradiometers can be fitted with rotating polarising filters, as was done in the aforementioned studies of water and vegetation [174, 459]. A second method is *channelled* spectropolarimetry, where polarisation information is encoded into the spectrum itself. One method for channelled linear spectropolarimetry is SPEX [175], the basis for SPEXone [184]. In SPEX, incoming light is modulated with a sine wave with an amplitude and phase depending on the DoLP and the Angle of Linear polarisation (AoLP), respectively [175]. This is further explained in Section 6.2.2.

6

The SPEX technique has been applied successfully in two high-end field-going instruments measuring aerosol optical thickness (AOT, sometimes termed aerosol optical depth, AOD), namely groundSPEX [125] and SPEX airborne [177]. GroundSPEX is a ground-based instrument based on a dual-channel fiber-optic spectrometer with SPEX optics on a moving mount, allowing sequential measurements at multiple angles. Its AOT measurements are well-correlated (Pearson $r = 0.932$) [125] with data from AERONET, the global network of photometers observing the solar almucantar and principal plane [134]. SPEX airborne, as the name implies, is an airborne instrument, simultaneously observing at nine fixed viewing angles. A 2017 campaign on a NASA ER-2 high-altitude aircraft demonstrated excellent agreement (RMS DoLP differences of 0.004–0.02) with coflying instruments [177].

A third successful SPEX variant was iSPEX, a smartphone-based version [94, 256]. Developed as a low-cost citizen science (CS) tool for AOT measurements, in 2013 iSPEX was used in CS campaigns yielding ~10 000 observations in the Netherlands. iSPEX data agreed well with AERONET reference data, showing typical standard errors and offsets in AOT of <0.1, while the typical absolute DoLP uncertainties were ~0.03 [94]. However, the original iSPEX add-on, app, and data had several limitations. First and foremost, the add-on was tailored to the iPhone 4 and 5 and did not work on later iPhone models (bar the iPhone SE) or any Android devices, limiting its reach and future compatibility. Second, at the time iOS only offered very limited camera controls for third-party applications, meaning iSPEX spectra were gathered at very coarse resolution, in the highly non-linear JPEG format, and with varying and uncontrollable exposure settings [281]. Thus, iSPEX data were only reliable when averaged over at least 50 individual measurements. Finally, iSPEX had a single-beam SPEX implementation, meaning the polarisation modulation could not be distinguished from inherent spectral features [94].

We present iSPEX 2, an upgraded version of iSPEX, solving the problems faced by its predecessor. First, the iSPEX 2 hardware is designed to universally support all smartphones. Second, using our SPECTACLE method and database for camera calibration, smartphone cameras offer data similar in quality to professional radiometers [281]. Third, a dual-beam SPEX implementation facilitates distinguishing between spectral and polarimetric signals. This improves the polarimetric accuracy and enables pure spectroscopy for uniform targets.

iSPEX 2 was developed specifically for aerosol and ocean colour measurements. Like its predecessor, it can be used for large CS campaigns to measure AOT [94], with higher quality data, but also for individual AOT measurements like other SPEX variants [125, 177], though with a coarser spectral resolution. These can be used to fill in temporal and spatial gaps in AOT coverage for satellite atmospheric correction algorithms. The AOT data may be further improved through aureole, almucantar, and near-horizon measurements [134, 460, 461]. Ocean colour measurements will include unpolarised remote sensing reflectance (R_{rs}), similar to the HydroColor app [121] but hyperspectral, and polarised reflectance as discussed above [174, 238]. These too can be used to provide coverage in scenarios without coverage by high-end sensors, but also to validate satellite measurements. Finally, iSPEX 2 can be used as a low-cost instrument for portable or laboratory spectroscopy [98, 143].

The working principle of SPEX and its implementation in iSPEX 2 are described in Section 6.2. The physical design of the add-on is described in Section 6.3. Section 6.4 describes the production process. The current and planned data acquisition and processing pipeline are given in Section 6.5. Finally, Section 6.6 contains current progress on and future plans for calibration, validation, and scientific applications of iSPEX 2.

6.2 Working principle

6.2.1 Definitions

Spectral polarisation states are most easily described using a wavelength-dependent Stokes vector $\vec{S}(\lambda)$, defined in Equation (6.1). Here $I(\lambda)$ is the total spectral radiance, $Q(\lambda)$ and $U(\lambda)$ the linear polarisation state, and $V(\lambda)$ the circular polarisation state. Here, we define $+Q$ as horizontal and $-Q$ as vertical polarisation, $+U$ and $-U$ as $+45°$ and $-45°$ from the horizontal, and $+V$ and $-V$ as right- and left-handed circular polarisation, respectively. Lowercase q, u, v are the fractional polarisation, normalised by $I(\lambda)$. I, Q, U, V are sometimes referred to as S_0, S_1, S_2, S_3 respectively [457]. In this work, circular polarisation in incoming light will be neglected as typically $v \lesssim 10^{-3}$ in nature [458].

$$\vec{S}(\lambda) = \begin{bmatrix} I(\lambda) \\ Q(\lambda) \\ U(\lambda) \\ V(\lambda) \end{bmatrix} = I(\lambda) \begin{bmatrix} 1 \\ q(\lambda) \\ u(\lambda) \\ v(\lambda) \end{bmatrix} = \begin{bmatrix} I_0(\lambda) + I_{90}(\lambda) \\ I_0(\lambda) - I_{90}(\lambda) \\ I_{45}(\lambda) - I_{-45}(\lambda) \\ I_R(\lambda) - I_L(\lambda) \end{bmatrix} \tag{6.1}$$

The state of linear polarisation is also described by the degree and angle of linear polarisation, DoLP or $P_L(\lambda)$ and AoLP or $\phi_L(\lambda)$ respectively. These are defined in Equations (6.2) and (6.3) [175]. In practice, the arctan2 operator is used in Equation (6.3).

$$P_L(\lambda) = \frac{\sqrt{Q(\lambda)^2 + U(\lambda)^2}}{I(\lambda)} = \sqrt{q(\lambda)^2 + u(\lambda)^2} \tag{6.2}$$

$$\phi_L(\lambda) = \frac{1}{2} \arctan\left(\frac{U(\lambda)}{Q(\lambda)}\right) = \frac{1}{2} \arctan\left(\frac{u(\lambda)}{q(\lambda)}\right) \tag{6.3}$$

Finally, optical elements are described through their 4×4 Mueller matrix M, describing how the element modifies the incident $\vec{S}(\lambda)$. Each element of M can have its own wavelength dependence. Passing through an element X modifies $\vec{S}(\lambda)$ to be $M_X\vec{S}(\lambda)$. The Mueller matrix of a chain of elements X, Y, Z is simply the product of their individual Mueller matrices $M_Z M_Y M_X$.

6.2.2 SPEX polarisation modulation optics

The SPEX polarisation modulation optics (PMO) consist of three elements, namely a quarter-wave plate (QWP), multi-order retarder (MOR), and analysing linear polariser (ALP) [175]. Their orientations and function are as follows:

- *Quarter-wave plate*: The QWP has its fast axis at 0° ($+Q$, horizontal). It should be highly achromatic and interchanges the Stokes U and V components, making the instrument insensitive to circular polarisation. Residual chromaticity from misalignment, deviations in retardance $\delta_{QWP}(\lambda)$, and other effects must be calibrated [125]. In iSPEX 2, an Edmund Optics WP140HE (#88-253) $\lambda/4$ polymer retarder foil is used.

- *Multi-order retarder*: The MOR has its fast axis at +45° from horizontal ($+U$). Its retardance $\delta_{MOR}(\lambda)$ is highly chromatic, exchanging the incoming Q and V components by a fraction depending on the wavelength. As with the QWP, the performance of the MOR requires extensive calibration [125]. The first iSPEX 2 units contain a stack of two Meadowlark B4 polymer retarder foils [462], with a nominal retardance of 4λ each at 560 nm. For the future, alternatives are being investigated, as described in Section 6.4.1.

- *Analysing linear polariser*: The ALP imprints the modulation onto the exiting spectrum in Stokes I, and can be implemented in several ways. The single-beam approach uses a single linear polariser, parallel or orthogonal to the slit, as in the original iSPEX [94]. This approach does not allow for full linear spectropolarimetry, as the modulation and inherent spectral properties cannot be fully distinguished. This is possible in the dual-beam approach, where both directions are measured. A polarising beamsplitter is used in groundSPEX [125], SPEX airborne [177], and SPEXone [184]. In iSPEX 2, a pair of Polarization.com PFSC NA foils is used, oriented parallel or orthogonal to the two slits (Section 6.3.1).

6

Together, the PMO induce a modulation in the outgoing Stokes I radiance $I_\pm(\lambda)$ (where the sign ± corresponds to the two ALP orientations) that depends only on the incoming radiance $I_{in}(\lambda)$, $P_L(\lambda)$, $\phi_L(\lambda)$, λ, and $\delta_{MOR}(\lambda)$. This is described in Equation (6.4). The modulation is a sine wave on the radiance spectrum, quasi-periodic in $1/\lambda$, its amplitude and phase corresponding to the DoLP (P_L) and AoLP (ϕ_L), respectively [175]. These parameters are retrieved by fitting Equation (6.4).

$$I_\pm(\lambda) = \frac{I_{in}(\lambda)}{2}\left[1 \pm P_L(\lambda)\cos\left(\frac{2\pi\delta_{MOR}(\lambda)}{\lambda} + 2\phi_L(\lambda)\right)\right] \tag{6.4}$$

In dual-beam mode, the modulations in $I_+(\lambda)$ and $I_-(\lambda)$ are exactly opposite for a uniform target, so the total radiance and modulation can be disentangled as shown in Equations (6.5) and (6.6). However, this is complicated in practice due to imperfections in the optical elements, misalignments, differences in transmission between the two beams, and nonnormal incidence [125, 177].

$$I_+(\lambda) + I_-(\lambda) = I_{in}(\lambda) \tag{6.5}$$

$$\frac{I_+(\lambda) - I_-(\lambda)}{I_+(\lambda) + I_-(\lambda)} = P_L(\lambda)\cos\left(\frac{2\pi\delta_{MOR}(\lambda)}{\lambda} + 2\phi_L(\lambda)\right) \tag{6.6}$$

6.3 Add-on design

The iSPEX 2 add-on is a whole divided into three parts, as shown in Figure 6.1. These are a tube containing the PMO and other optics (Section 6.3.1), a clip to clamp onto a smartphone (Section 6.3.2) and a backplate for aligning the tube with the smartphone camera (Section 6.3.3). A cross-section is shown in Figure 6.2. The tube can be used on any camera, including smartphones but also UAVs and webcams. The clip can be used with nearly all smartphones, as most models have a similar form factor [281]. Finally, the backplate is unique to each smartphone model.

6.3.1 Optical tube

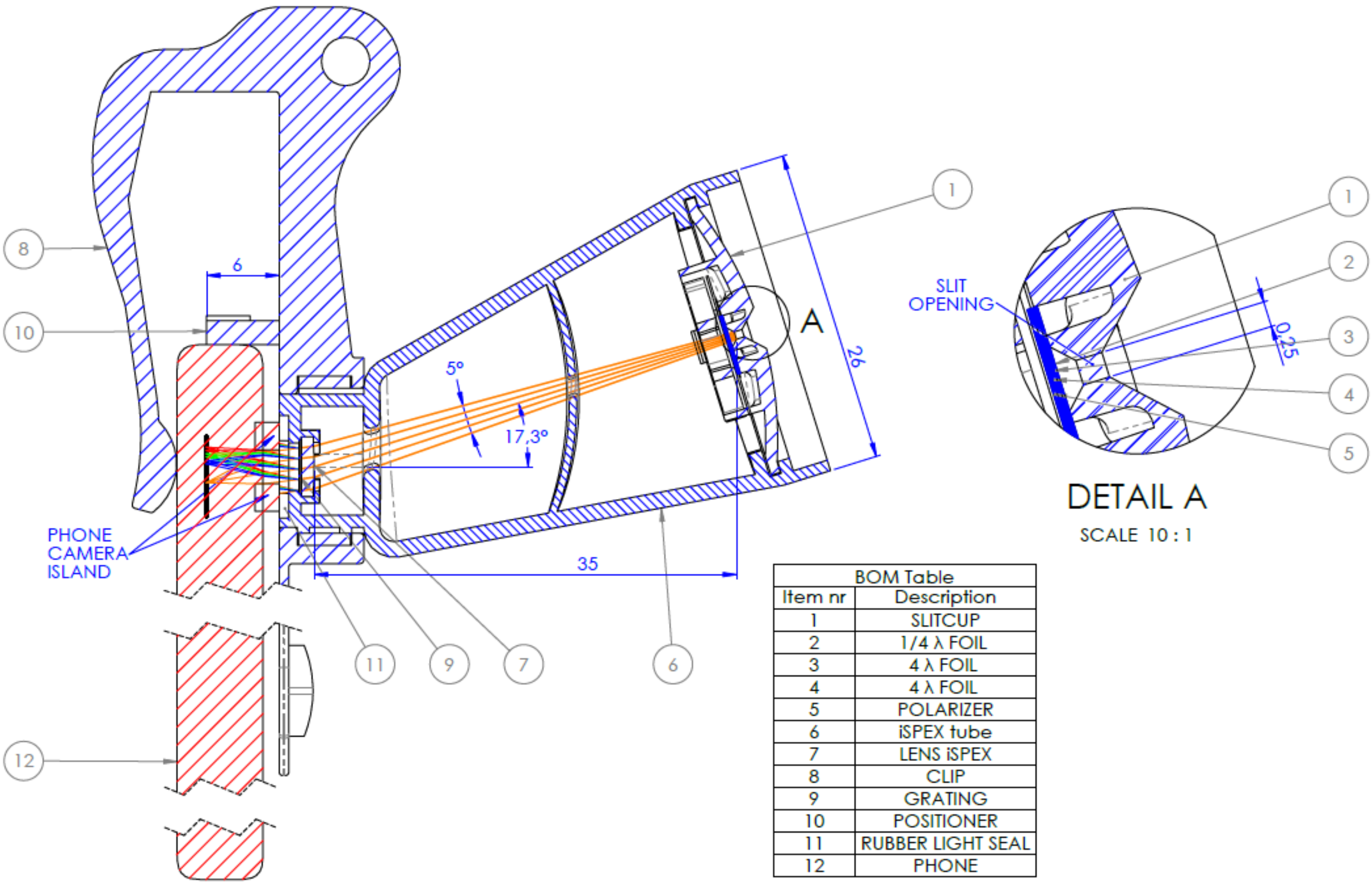
The iSPEX 2 optics consist of a double slit (side by side), the SPEX PMO (Section 6.2.2), a collimator lens, and a transmission grating, as shown in Figure 6.3. There are two slits, each 0.25 mm wide and 9 mm long, located side by side to measure in quasi-dual-beam mode. The PMO are placed directly behind the slits to minimise instrumental polarisation through stray light. A small plastic cradle holds the PMO foils in place. Dual-beam mode is achieved by having a horizontal ALP in the PMO behind the left slit and a vertical one behind the right slit. Dual-beam mode requires a uniform target between the two slits; this assumption holds in the center for smooth surfaces like sky polarisation [125], but not toward the edges. From the PMO, the modulated light propagates to a custom-made collimator lens ($f = 35$ mm) and a 1000 line/mm holographic transmission grating foil (Edmund Optics #52-116), dispersing the light onto the smartphone camera; the camera optics then register the spectra, as shown in Figures 6.2 and 6.7. A rubber seal blocks stray light, as shown in Figure 6.2.

The optics are located in a plastic tube, as shown in Figure 6.3. The tube itself is 35 mm long along its optical axis, which is angled +17.3° upwards to project the entire zeroth and

(a) iSPEX 2, whole.

(b) iSPEX 2, exploded view.

Figure 6.1: Render of the iSPEX 2 add-on, as a whole attached to a smartphone (left) and exploded into its three components (right). These are, from left to right, the smartphone clip, optical tube, and smartphone backplate. The smartphone is seen from the back.



BOM Table	
Item nr	Description
1	SLITCUP
2	1/4 λ FOIL
3	4 λ FOIL
4	4 λ FOIL
5	POLARIZER
6	iSPEX tube
7	LENS iSPEX
8	CLIP
9	GRATING
10	POSITIONER
11	RUBBER LIGHT SEAL
12	PHONE

Figure 6.2: Cross section of iSPEX 2 (blue) attached to a smartphone (red) with a zoom on the slit (detail A). Five rays are traced from the slit to the grating in orange, then dispersed onto the camera chip. Sizes are in mm.

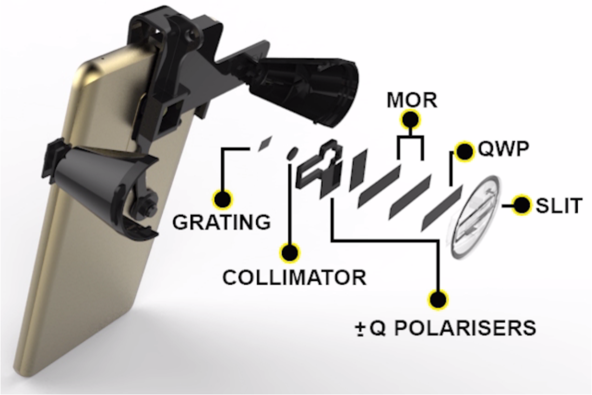
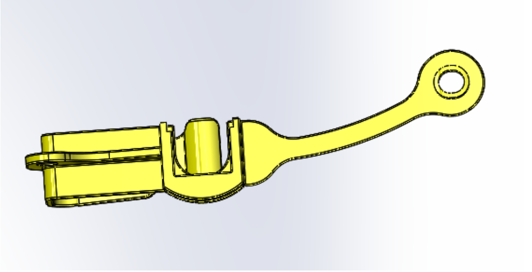


Figure 6.3: Exploded view of the iSPEX 2 optical tube with the slit, quarter-wave plate (QWP), multi-order retarder (MOR), 0° and 90° polarisers, collimator lens, and grating foil indicated.

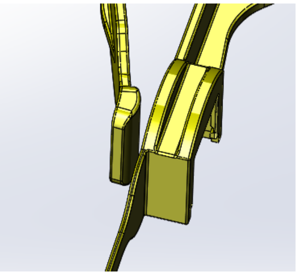
first orders of the spectrum on the smartphone camera. The tube consists of two halves (left and right) which are produced separately and click together along its length (Section 6.4.4). A baffle is located halfway along the tube, consisting of overlapping protrusions from either tube half. This ensures overlapping coverage and thus reduces light leakage. The slit end of the tube has two 'ears' to which additional add-ons can be attached, such as a cuvette holder for transmission spectroscopy. The camera end has two ridges to which the clip (Section 6.3.2) attaches; these can also be used for custom attachments for different cameras.

6.3.2 Smartphone clip

iSPEX 2 attaches to smartphones using a clip, as seen in Figure 6.1. The clip design is shown in detail in Figure 6.4. It attaches to the smartphone with a clamp on the front (screen) side, directly behind the camera. This clamp is 14 mm wide and made from soft plastic to prevent scratching. It is attached to the clip over the top of the smartphone. Additionally, the clip has a 'clapper' extending 49 mm below the camera along the back side, with a suction cup at the end. This attaches to the flat back surface of the smartphone. This double attachment



(a) Smartphone clip.



(b) Zoom on clamp.

Figure 6.4: CAD model of the iSPEX 2 smartphone clip. The optical tube and backplate slot into the central opening, opposite the clamp. The long, curved extension is the 'clapper' with a suction cup at the end. Ridges along the clip provide stiffness and strength. The clip is fabricated in black.

prevents rotation of the add-on and ensures the slit is always projected horizontally onto the camera. The clapper is curved 11 mm to the right of the camera (seen from the back, as shown in Figure 6.5) so the suction cup does not fall off the edge on devices with cameras near the edge, such as iPhones.

Several iterations of the clip design were necessary. Originally, the clip had no clapper and attached to the right side of the smartphone (seen from the front), but this acted as a lever and caused the add-on to rotate under its own weight. This was solved by having the clip attach over the top, so its weight rests on the smartphone, and adding a clapper. The clapper originally had a small magnet at its end instead of a suction cup, but smartphone backsides were found to be only weakly magnetic in only a few places.

6.3.3 Smartphone backplate

iSPEX 2 is placed in front of the smartphone camera using a backplate unique to each smartphone model, as shown in Figure 6.5. Smartphones with multiple backside cameras typically feature one wide-view camera with generic optical properties and a focal length of 3.8–4.5 mm (corresponding to a field-of-view of 60°–75° × 45°–55° [281]), which is used for iSPEX 2. The backplate consists of a universal plate with two positioners with different positions for each smartphone model. One rests on top of the smartphone, the other on the right (seen from the back). Since most smartphone cameras are in the center or on the left, this design ensures that most of the weight of iSPEX 2 rests on the smartphone, rather than create a lever.

The positioner locations depend on the dimensions of the smartphone, the curvature of its top corners, and the locations of buttons along the side. We are compiling a database of popular smartphone models including these parameters. The top positioner has a small notch to accommodate the iPhone SE, one of the few popular models with buttons along the top. The positioners are 21.5 mm (side) and 30 mm (top) long and 6 mm wide, providing sufficient coverage even on smartphones with curved edges.

Figure 6.5: Render of iSPEX 2 attached to several smartphones with different dimensions and camera locations, seen from the back. Each has a backplate with unique positioner locations to place the optics directly in front of the camera.

6.4 Production

6.4.1 Multi-order retarder foils

As described in Section 6.2.2, iSPEX 2 uses polymer retarder foils to produce the SPEX polarisation modulation. The first units use two Meadowlark B4 foils [462] with 4λ retardance (at 560 nm) each, as did the original iSPEX [94], for a nominal total retardance of 8λ at 560 nm. This induces a modulation with 7 full periods across the typical spectral range of smartphone cameras (as seen in Figure 6.10b), which is 390–700 nm [281].

These foils are produced by stretching transparent sheets of polymer, such as polyvinyl alcohol (PVA), polycarbonate (PC) or poly(methyl methacrylate) (PMMA) [462]. While the pre-fabricated foils provide the desired retardance with great consistency, they are prohibitively expensive for low-cost CS purposes.

To enable high-volume throughput, integrated in our production line, we are exploring internal production of MOR foils, based on a setup previously used to stretch sheet metal [463]. Initial experiments are focused on finding the optimal material from PVA, PC, PMMA, polyethylene terephthalate (PET), and Zeonor cyclo olefin polymer, at various thicknesses from 50–200 μm. Further experiments will determine the efficacy of softening the foils through heat (up to 80 °C) and the maximum achievable retardance. Visual inspection and spectrally resolved measurements through a crossed polariser setup will be used to measure the retardance of sections of the foil during the stretching process, as spatial variations in retardance and fast axis orientation are expected [462]. The end goal is to mass produce low-cost MOR foils with sufficient quality for iSPEX 2, not necessarily for high-end commercial purposes.

6.4.2 Injection moulding

Like the original [94], iSPEX 2 is produced through injection moulding. This is inexpensive yet precise. Components that can be injection moulded include the collimator lens, optical tube, smartphone clip, and backplate. The suction cup (Section 6.3.2) and optical foils (Sections 6.2.2 and 6.3.1) are purchased or self-produced by other means (Section 6.4.1).

Various plastics are used for iSPEX 2. Thin parts, including the tube and backplates, are manufactured from polycarbonate-acrylonitrile butadiene styrene (PC-ABS) coloured black with masterbatch (MB). PC-ABS and polypropylene (PP) are being evaluated as materials for the clip. The collimators are produced separately from Zeonor 330 plastic.

The optical tube and clip are manufactured from a single mould (Figure 6.6), while a separate mould is used for the backplate. The backplate mould is complex, requiring two sliders to account for the device-dependent positioners. By parameterising the slider positions based on the smartphone dimensions, the mould can instantly be adjusted to a different device.

6.4.3 3D printing

Except for the optical components, iSPEX 2 units can also be 3D printed, for which we will provide model files. This was used extensively in the development phase for quick testing and will be useful for future compatibility. For example, this allows users to self-produce backplates tailored to new smartphone models not included in our database. Local production through 3D printing also reduces the unit cost, especially valuable in resource-poor areas, one of the prime target audiences for smartphone spectroscopy [143].

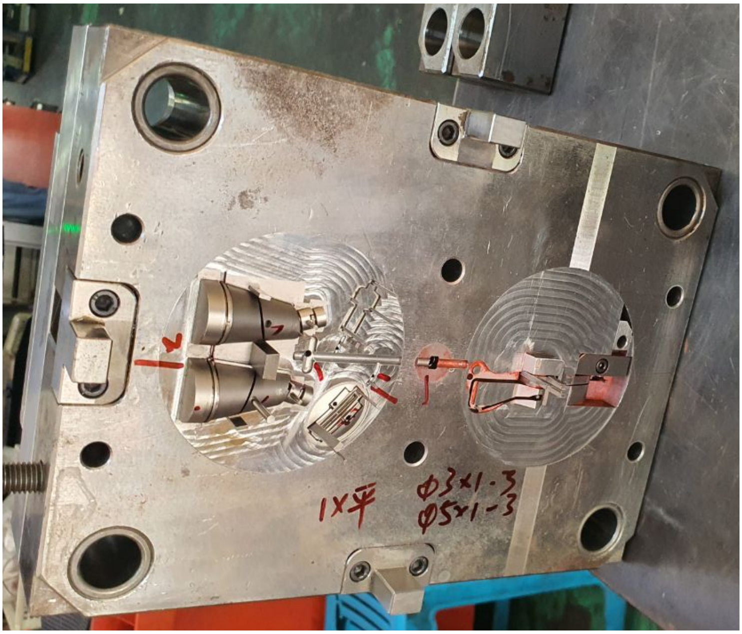


Figure 6.6: Injection mould used to produce the iSPEX 2 optical tube and smartphone clip.

However, 3D printing introduces several difficulties. First of all, the PMO and grating foils cannot be 3D printed and thus must still be purchased and cut to size. Second, low-cost 3D printing techniques inherently have wider production tolerances than injection moulding. With 3D printed prototypes we often found it necessary to manually file or cut components to make them fit tightly. Finally, some 3D printing materials such as PA nylon are translucent; we found this easiest to counteract by covering the entire unit twice over with a felt-tip pen. Because of these complications, we use 3D printing only for prototyping, not production.

6.4.4 Assembly

Assembly of iSPEX 2 units is straight-forward. First, the PMO foils are placed in their cradle in the correct orientations. Next, the cradle, collimator lens, and grating foil are placed into the corresponding slots in the tube halves, which are then clicked together. When used with a smartphone, the optical tube is then slotted into the smartphone clip, followed by the backplate corresponding to the smartphone model. The backplate is easily removed for use with a different device. For other uses, a custom attachment between tube and camera can easily be manufactured by the user. The tube can even be used with the naked eye for a qualitative measurement or a demonstration.

For the injection moulded units, the PMO and grating foils are punched into an asymmetric shape to prevent confusion of their optical axes; the cradle has corresponding protuberances. Like with the original iSPEX, a calibration setup in the factory is used to verify that all optics are oriented correctly [94]. For 3D printed units, this must be done carefully by hand.

6.5 Data acquisition and processing

This section describes the acquisition, calibration, and processing of iSPEX 2 data. These are acquired as RAW images on a smartphone using an app based on SPECTACLE [281], described in Section 6.5.1. Currently, these RAW data are manually uploaded to a PC for calibration and processing. Our goal is to move as much of this as possible to the smartphone, possibly with additional cloud computing in a back-end server for devices with insufficient computational power.

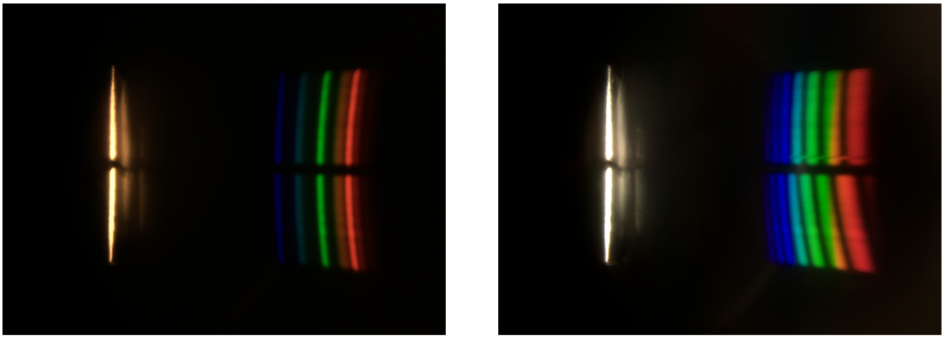
6.5.1 Smartphone app

Data acquisition on smartphones is done using a custom-designed app, based on SPECTACLE [281], currently in development for iOS and Android. Significant changes to iOS mean few elements from the 2013 iSPEX app [94] can be reused for iSPEX 2. However, user feedback on the original app is taken into account. For example, some users misunderstood the scientific aims and methods of iSPEX because these were not explained clearly [256]. Difficulties in installing the add-on and interpreting feedback from the app were also noted [297].

Data are obtained in RAW image format because of its high linearity and dynamic range [281]. This is in contrast to the JPEG images taken with the original, where non-linearity and white balance introduced significant problems [94, 281]. Two examples, taken with a 3D printed prototype, are shown in Figure 6.7. Aside from problems due to faults in the prototype, such as stray light, which will be reduced in the final product, these images are representative examples of iSPEX 2 data. Processing of these images (Section 6.5.2) is currently done on PC, but will be done in-app in the future.

The following data acquisition protocols will be included in the initial release of the app:

- Wavelength calibration: Single observation of a fluorescent light, as described in Section 6.5.3.



(a) Fluorescent light. (b) Reflected sunlight through a 100% polariser.

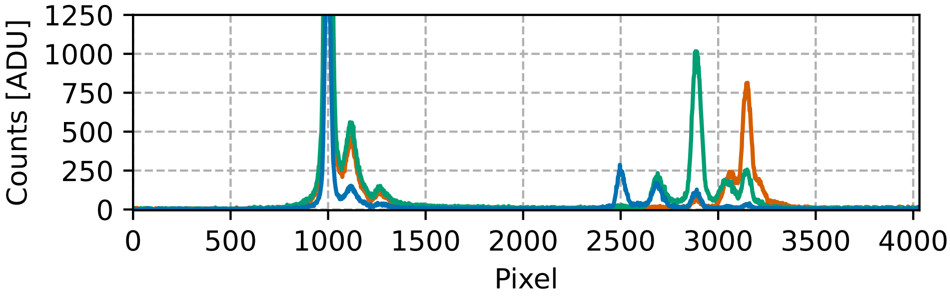
Figure 6.7: Spectra taken with an iSPEX 2 prototype on an iPhone SE. The fluorescent light spectrum (left) is used in the wavelength calibration, and clearly shows the smile and keystone effects. The 100% polarised image (right) shows the SPEX modulation in the two $\pm Q$ spectra, with an additional curvature due to variations in retardance. The small glitch in the top spectrum and the stray light are due to manufacturing faults in this prototype. These images were taken in RAW format and converted to JPEG for visualisation; all data processing is done on RAW images only.

- Aerosols (AOT): Series of observations from horizon to zenith along the principal (observer-Sun-zenith) plane, as with other SPEX variants [94, 125, 177]. The optimal number of observations is to be determined based on data quality and computational considerations, specifically the speed at which RAW images can be saved on smartphones.

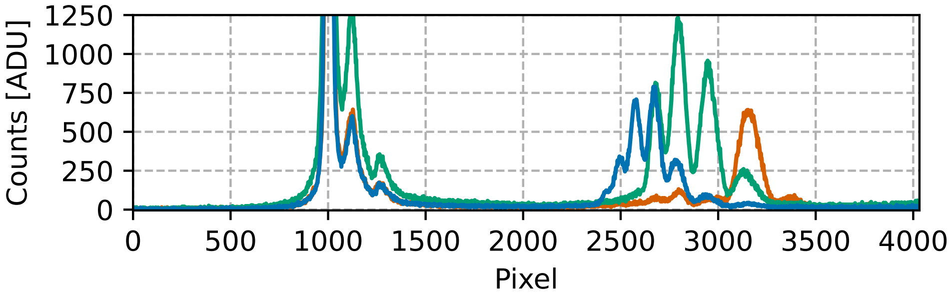
- Water (R_{rs}): Series of observations according to the Mobley protocol [209], measuring sky radiance at 40° from zenith, upwelling radiance at 40° from nadir, and downwelling irradiance with a grey card at 40° from nadir. The same protocol is used in the HydroColor app, which does multispectral (RGB) measurements [121].

Users are guided through these protocols with text explaining what to do and, for example, arrows to guide them in the right direction, using the smartphone compass and accelerometers. Citizen scientists have been involved in the development of these protocols from the start, to ensure user-friendliness. Optimal exposure settings for each protocol are currently hard-coded but in the future will be determined automatically.

6.5.2 Data pre-processing



(a) Fluorescent light.



(b) Reflected sunlight through a 100% polariser.

Figure 6.8: Two adjacent rows of pixels (one GR, one BG_2) in the spectra shown in Figure 6.7, split into the RGB channels. The G_2 channel is not shown here. The slit and several ghosts are visible from 800–1500 pixels, the first order spectrum from 2300–3500 pixels. The data have been corrected for bias and flat-field.

Data are processed according to the SPECTACLE method [281], which was originally developed for iSPEX 2. A Python library for data processing specific to iSPEX 2 is currently in development[20]. iSPEX 2 data are corrected for bias and flat-field using SPECTACLE; in spectra taken with prototypes, dark current is negligible compared to stray light, but this may change with injection moulded iSPEX 2 units or on certain devices.

The corrected image is split into the $\pm Q$ component spectra, currently based on hard-coded windows for specific cameras but in the future automatically, and demosaicked. The $RGBG_2$ channels of the Bayer-filter camera are treated separately rather than combined through interpolation, since interpolated data add no extra information [281]. After demosaicking, there are eight separate spectra, namely the combinations of $\pm Q$ and $RGBG_2$. Figure 6.8 shows two examples of demosaicked RGB spectra. Finally, each row is convolved with a Gaussian kernel ($\sigma = 6$ pixels) corresponding to an FWHM of ~3.8 nm (see Section 6.5.3). This reduces the noise on the spectrum without reducing the spectral resolution, being narrower than the image of the slit.

6.5.3 Wavelength calibration

The pre-processed data are then wavelength-calibrated. As seen in Figure 6.7, iSPEX 2 data exhibit significant smile (variations in dispersion along the slit) and keystone (deformation of the spectrum into a trapezoid). Both effects are common in long-slit spectrometers [177,464]. Smile is corrected by doing the wavelength calibration per pixel row; a keystone correction is still in development.

The wavelength calibration is done using a reference spectrum of a fluorescent light, like that shown in Figure 6.7a. These have three sharp spectral lines corresponding to the $RGBG_2$ channels, at 611.6 (R), 544.5 (G/G_2), and 436.6 (B) nm. Because of mosaicking, the raw data have R and B values only in every alternate row and column, while combining G and G_2 gives full row coverage but in alternating columns. The column gaps are filled in by the Gaussian kernel convolution (Section 6.5.2), which also reduces noise. The maximum value per channel in each pixel row is determined to find the line centers. A quadratic fit is made to these, and the resulting fitted line centers are used. This fills in the gaps in R and B and reduces the effect of noisy rows. Figure 6.9 shows the line centers thus derived from the spectrum in Figure 6.7a.

A wavelength solution map, with the central wavelength for each pixel, is generated by fitting a quadratic relation between the spectral line wavelengths and the line centers from Figure 6.9. The resulting dispersion is typically ~0.27 nm/px, depending on the camera optics, exposure settings, and pixel position (as seen in Figure 6.9). For the images shown in Figure 6.7, where the slit is ~35 pixels wide (FWHM), this gives a spectral resolution (FWHM) of 9 nm. The FWHM varies slightly based on camera optics and exposure settings, mainly focus. 9 nm resolution is comparable to common ocean colour sensors such as the TriOS RAMSES and HyperOCR [283] and satellite instruments like Sentinel-3/OLCI [283] and HARP-2 [86], and only 2–3 times wider than PACE/OCI (5 nm) [86] and SPEXone (2–3 nm) [86, 184].

The overall wavelength map is converted into individual wavelength maps for the $RGBG_2$ channels by demosaicking it, as if it were an image itself. Finally, all rows are interpolated to the same 390–700 nm range in 1 nm steps, giving wavelength-calibrated spectra as shown in Figure 6.10.

[20] https://github.com/burggraaff/ispex2

6

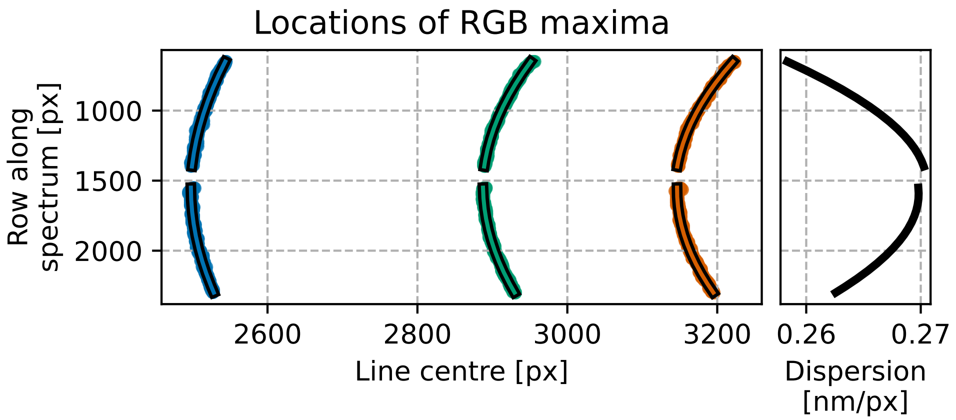


Figure 6.9: Pixel positions of the spectral lines in Figure 6.7a (left) and the derived dispersion (right). The coloured dots indicate the maxima in the B, G/G_2, R (from left to right) channels, while the coloured lines with a black outline indicate the fitted positions. The fits are done separately for the $\pm Q$ spectra. The smile effect is clearly visible. The mean dispersion between the B (436.6 nm) and R (611.6 nm) lines is shown; a smaller value in nm/px corresponds to a wider dispersion.

Since fluorescent lights are less ubiquitous than in the past, and will likely be fully replaced by LEDs in the foreseeable future, an alternative method may become necessary. For example, common features of SRFs such as the ~580 nm edge in R bands [281] may be used instead of spectral lines.

6.5.4 Spectral response calibration

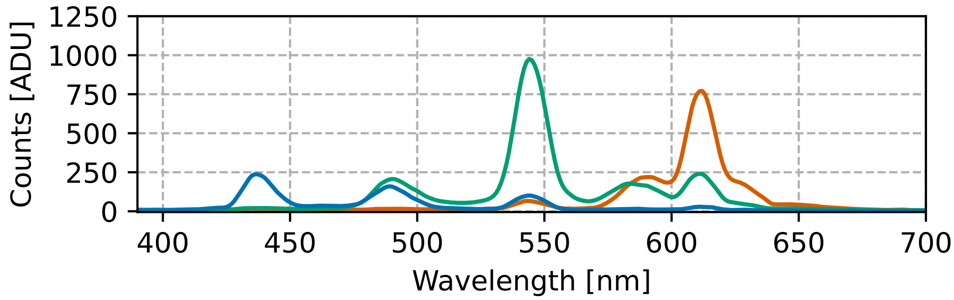
The wavelength-calibrated spectra are corrected for the $RGBG_2$ spectral response functions (SRFs), again using SPECTACLE [281]. The SRFs are interpolated to the same wavelengths as the data, after which the data are divided by the SRF. This gives radiances, a constant factor away from absolute radiometric units [281], as shown in Figure 6.11. To prevent amplifying noise and stray light, currently only wavelengths where the SRFs are >0.15 (in relative units) are used. This restriction will be relaxed with better stray light reduction and correction. Even so, both spectra in Figure 6.11 show excellent agreement between the RGB radiances. For fully unpolarised light measurements, this is the final calibration step.

For cameras without SPECTACLE SRFs, iSPEX 2 itself can be used to measure these using a known light source. This has been attempted with the original iSPEX using skylight reflected off white paper, with an RMS error of 5% compared to reference data, increasing towards longer wavelengths [281]. The skylight spectrum was model-based, introducing assumptions that cannot be tested in the same measurement. For this reason, it may be preferable to instead use consumer lamps, such as those characterised in the LICA database [381].

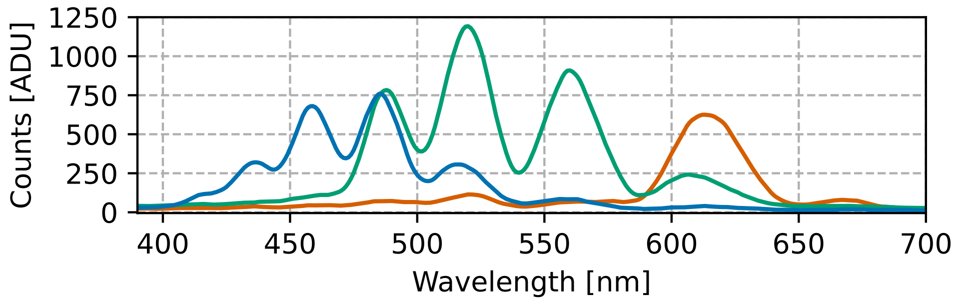
6.5.5 Polarimetric demodulation

Finally, the DoLP and AoLP are retrieved by inverting Equation (6.4) to demodulate the calibrated spectra. First, the retardance and polarimetric efficiency of the instrument must be

6



(a) Fluorescent light.



(b) Reflected sunlight through a 100% polariser.

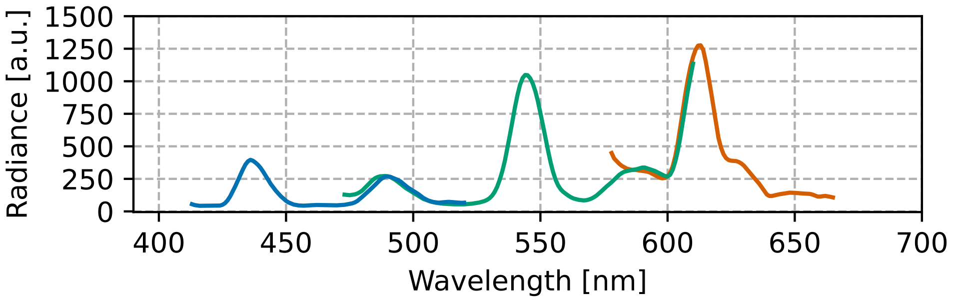
Figure 6.10: Spectra from Figure 6.8 after wavelength calibration.

calibrated using a known 100% polarised light source [177]. For iSPEX 2, we plan to do this upon assembly using a rotating wiregrid polariser.

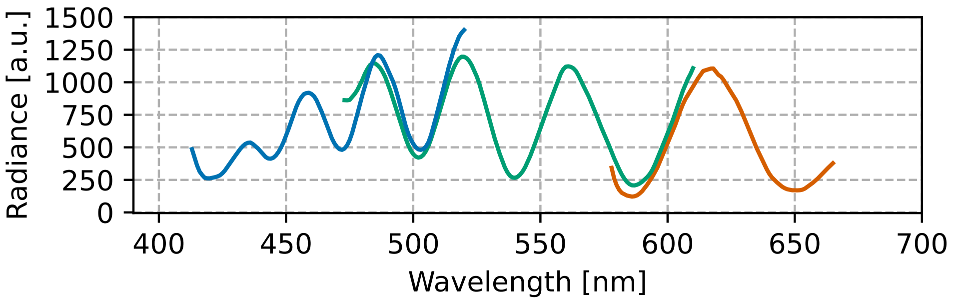
6

As can be seen in Figure 6.12, variations in retardance and efficiency exist along the $\pm Q$ slits of 3D-printed prototypes. These are partially due to fabrication issues, such as MOR foils flexing in their bracket due to wide production tolerances (Section 6.4.3), which will be resolved in the injection moulded product. However, they are also partially due to issues including nonnormal incidence, since the optical path length and refractive index vary with the direction of propagation [465]; this will persist in the final product, necessitating a spatially dependent calibration of retardance and efficiency. We are currently characterising these effects. A final complication is the fact that different sections of the slits see different targets, meaning inherent variations in DoLP and AoLP exist. The demodulation pipeline will have to account for this too.

The demodulation algorithm is in development. An iterative approach is likely necessary, fitting not only DoLP, AoLP, and the unpolarised spectrum $I_{in}(\lambda)$, but also instrumental effects including the QWP and MOR retardance, alignment and orientation of foils, the relative transmission between the two slits, and variations in the source spectrum along the slits [125, 177]. The derived DoLP, AoLP, and $I_{in}(\lambda)$ are used to determine AOT for aerosol and R_{rs} for ocean colour measurements. The typical spectral resolution in DoLP and AoLP is approximately the modulation period [175] of 25–60 nm, though this can be lowered to the native spectral resolution of ~9 nm (Section 6.5.3), albeit with a lower accuracy [176]. The



(a) Fluorescent light.



(b) Reflected sunlight through a 100% polariser.

Figure 6.11: Spectra from Figure 6.10 after spectral response calibration.

original iSPEX had a polarimetric accuracy (typical uncertainty) of ~0.03 in DoLP, mostly limited by defocus due to lacking camera controls [94]. Having solved these problems [281], we hope to increase the accuracy to sub-percent levels which enable retrieval of parameters such as effective radii and refractive indices (real and imaginary) [466].

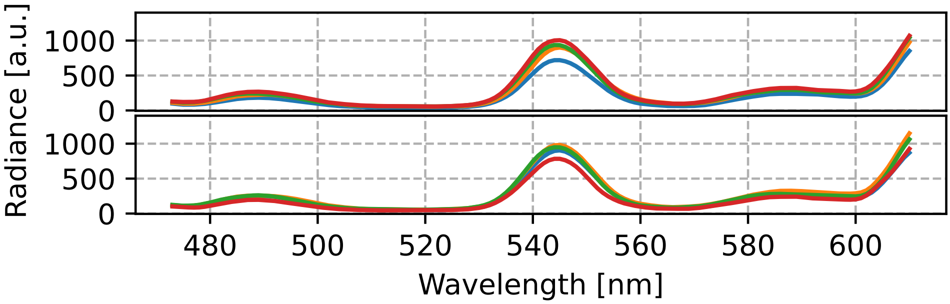
6.6 Future perspective

This section describes the ongoing calibration and validation efforts for iSPEX 2 as well as current and future scientific applications and opportunities.

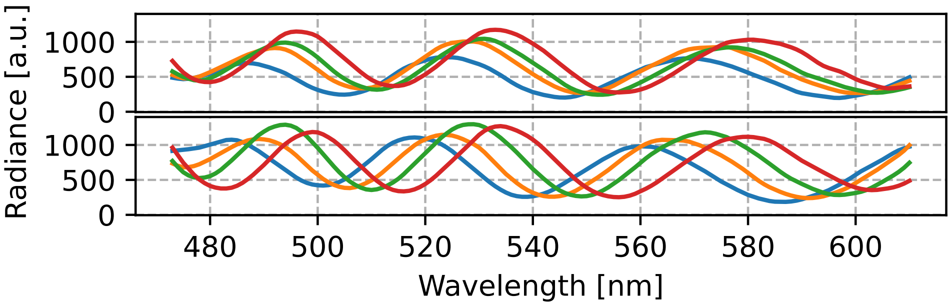
6.6.1 Calibration & validation

Each iSPEX 2 unit will be factory-calibrated for retardance and polarimetric efficiency with a 100% polariser (Section 6.5.5) and a small number will be validated in the lab at various DoLP and AoLP using a glass plate setup [457]. This will allow for a thorough comparison in performance between iSPEX 2 and other sensors, as well as between iSPEX 2 units and between smartphones. The calibration data for each iSPEX 2 unit will be linked to its serial number in a database, from which the app will retrieve them.

iSPEX 2 AOT and R_{rs} measurements are being validated through simultaneous observations with other instruments. For both, this will include groundSPEX, which is based



(a) Fluorescent light.



(b) Reflected sunlight through a 100% polariser.

Figure 6.12: Four rows in the G-band $+Q$ (top) and $-Q$ (bottom) spectra from Figure 6.7. Each coloured line corresponds to a row in the spectrum, though these are not the same between $+Q$ and $-Q$. Large variations are seen in the 100% polarised spectrum but not the unpolarised fluorescent light spectrum.

on the same principle but with a much higher spectral resolution and a polarimetric accuracy of ~1% [125]. AOT match-ups will also be done with MicroTOPS II, a handheld Sun photometer [122], and AERONET [134]. AERONET has previously been used to validate groundSPEX [125]. R_{rs} match-ups are being performed with WISP-3 handheld and TriOS RAMSES shipborne spectroradiometers, similar to the HydroColor app [121]. Validation has thus far taken place largely within field campaigns organised through the MONOCLE consortium[21]. Opportunities for further validation are under investigation.

An initial experiment comparing iSPEX 2 and WISP-3 R_{rs} measurements showed good agreement overall but also highlighted several areas of improvement (Figure 6.13). The spectra were similarly shaped, particularly the CDOM-phytoplankton absorption slope at 400–570 nm. The B- and G-band spectra showed residual modulation at $\lambda \leq 500$ nm, which will be reduced in the future through an improved demodulation algorithm. Future work on the SRF calibration (Section 6.5.4) will reduce edge effects such as that seen in the G-band at 470 nm.

[21] https://monocle-h2020.eu/

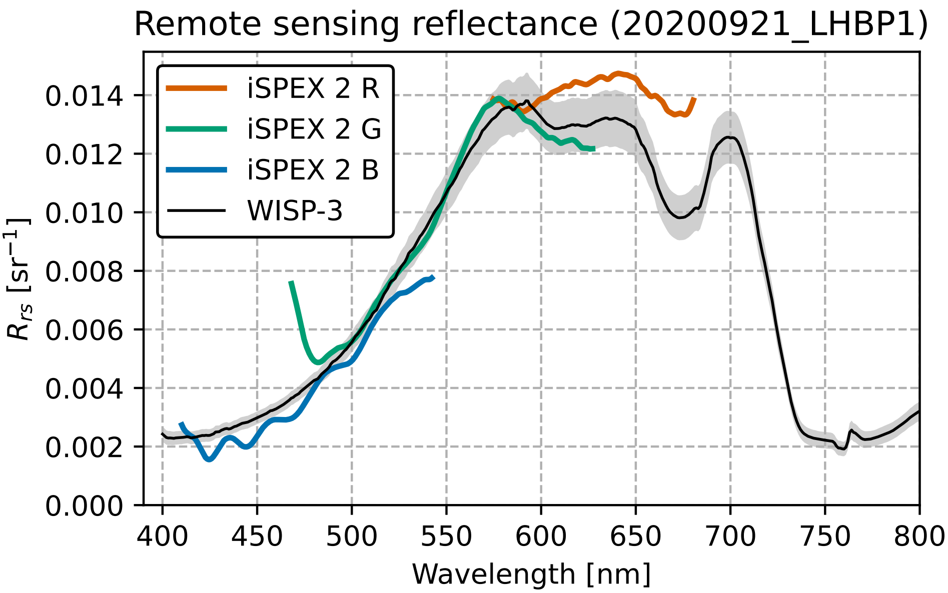


Figure 6.13: Comparison between near-simultaneous iSPEX 2 (red, green, blue) and WISP-3 (black) R_{rs} spectra. Data were gathered on 21 September 2020 at a pond in Leiden, the Netherlands (52°10'2.5"N 04°28'23.7"E). The iSPEX 2 spectra were normalised to the WISP-3 spectrum following [282]. The overall agreement between the two instruments is good, but there are some areas of improvement (Section 6.6.1).

6.6.2 Scientific applications

The main application of iSPEX 2 is as a low-cost instrument for citizen science remote sensing of air and water, specifically measuring AOT and R_{rs}. Both top-down and bottom-up approaches will be used for this. In the top-down approach, citizen scientists will be prompted by researchers to observe at a certain place or time, similar to the original iSPEX [94]. Conversely, in the bottom-up approach, citizen scientists can use iSPEX 2 independently, with researchers only providing support such as data processing and interpretation.

Planned top-down scientific applications of iSPEX 2 include high spatial resolution measurements of AOT and R_{rs}, extension of existing time series, and validation of satellite or airborne instruments. iSPEX 2 provides point measurements in arbitrary locations, facilitating extremely high spatial resolution. For example, a small group of citizen scientists standing along a lake shore can simultaneously map its reflectance (and thus its inherent properties) on meter scales. iSPEX 2 can also be used to fill in gaps in existing time series, for example if clouds prevented measurements during a satellite overpass. Finally, push notifications can be used to prompt citizen scientists to take validation measurements during a satellite overpass.

6.6.3 Future opportunities

In addition to the currently planned applications, more experimental work with iSPEX 2 is also possible. For example, while we are currently focused on unpolarised R_{rs}, polarised R_{rs} may provide additional information on water composition [174, 238]. However, an optimal protocol for measuring polarised R_{rs} will need to be found. Additionally, extending the principal plane measurements to the solar aureole, almucantar, and horizon may improve the AOT data and particle size distributions [134,460,461]. Outside remote sensing, iSPEX 2 will also be useful as a low-cost device for lab or field-going spectroscopy, for biological assaying and point-of-care diagnostics, among other purposes [98, 143].

Non-smartphone platforms also provide interesting opportunities. Unmanned aerial vehicles (UAVs) and webcams like the Raspberry Pi have cameras capable of professional-grade radiometry [281]. Raspberry Pi-based systems could be used as low-cost autonomous field-going spectroradiometers. Already, UAVs with pushbroom spectrometers are delivering data products like R_{rs} with high spatial and spectral resolution in a single fly-over [136]. Using iSPEX 2, any camera can become a hyperspectral and polarimetric sensor.

Funding

European Commission Horizon 2020 programme (grant nr. 776480, MONOCLE).

Acknowledgements

The authors wish to thank Akupara and Sanjana Panchagnula for providing pandemic-proof laboratory space. Data analysis and visualisation were done using the AstroPy, Matplotlib, NumPy, and SciPy libraries for Python.

6