Short Term Scientific Mission Report
COST Action OPTIMISE: ES1309

STSM Applicant: Dr. Laura MIHAI,
laura.mihai@inflpr.ro
National Institute for Laser, Plasma and Radiation Physics / CETAL-PhIL,
Atomistilor 409, Magurele, Ilfov,
Romania

STSM topic: Development of procedures and protocols for the calibration of spectrometer systems for measuring reflectance and fluorescence for near ground support of ESA FLEX observations: Part 1 preliminary determination of spectrometer spectral response (full width half max) at selected wavelengths

STSM reference number: COST-STSM-ES1309-35225
STSM type: Regular (from Romania to United Kingdom)

Period: from 2016-10-30 to 2016-11-05

Host: Alasdair Mac Arthur,
alasdair.macarthur@ed.ac.uk
NERC Field Spectroscopy Facility,
University of Edinburgh, Edinburgh (UK),

Purpose of the STSM;

The main objective of this mission was to develop laboratory-based calibration and characterization procedures for spectrometers across the spectral range of the FLEX fluorescence imager, at sampling interval and band widths which will enable the detection of the solar flux in the telluric oxygen A and B bands reaching the Earth's surface measurements. These procedures should enable calibrations to be replicated at various facilities.
For this purpose, a Piccolo dual-field-of-view fiber optic-based spectrometers system with irradiance and radiance measuring capabilities with optical benches capable of measuring across the 400 nm to 950 nm (VNIR) range at 2048 sampling intervals and from 640 nm to 800 nm in 1044 sampling intervals was characterize and calibrated using different calibration systems.
As a primary calibration system we considered a selection of spectral line lamps.
Gooch and Housego OL 750 double monochromator system with different configurations (slits and light sources) was chose as a secondary reference system. The use of a high intensity light source was necessary to obtain FWHM values lower than 0.2 nm with very thin slits (0.05 nm). This enabled the use of spectrometers across telluric oxygen A and B bands.
The radiance source for calibration was an FEL lamp irradiance source and Hoffman integrating sphere. Both of these sources have current calibrations traceable to UK national standards.

Description of the work carried out during the STSM;

Fluorescence, the radiant flux emitted by chlorophyll molecules after excitation by photons, is the most directly measurable reporter of photosynthetic efficiency and hence a key indicator of the health and carbon fixation of photosynthesizing organisms. Measurements of fluorescence, at both the leaf and canopy level, can therefore greatly advance the understanding of the dynamics of photosynthesis, gross primary productivity, and ecosystem change over time (ESA 2015). The ESA Board and member states have just confirmed that the Fluorescence Explorer (FLEX) has been selected as the sensor system for the Earth Explorer 8 programme. The intention is for FLEX to fly in tandem with Sentinel-3 and the combined sensors to provide the necessary measurements to register vegetation reflectance and sun induced fluorescence (SIF). A ground validation network will now to be established along with instruments and locations selected by ESA to perform this function. This work could begin early in 2017 with a network established and operational for the launch of FLEX planned for 2022.

However, although a number of near-ground spectrometer system have been proposed (see Porcar-Castell, Mac Arthur et al 2015), so far no calibration protocols have been developed to calibrate spectrometers across the spectral range of the FLEX fluorescence imager and at sampling interval and band widths which will enable the solar flux in the telluric oxygen A and B bands reaching the Earth's surface to be measured. This is necessary for two reasons:

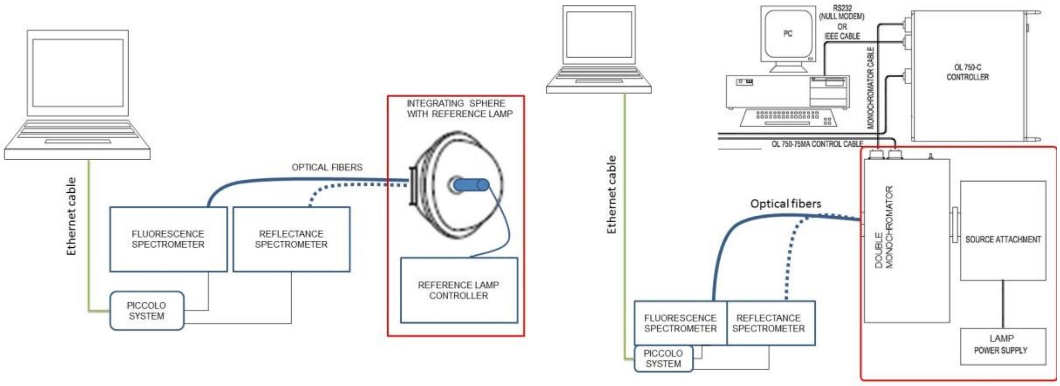
- first, to validate the space-based observations of SIF it will be necessary to develop models transform ground-based observations to the sampling intervals and spectral response of the space-based observations as both have different measurement characteristics. ESA will publish the sampling intervals and spectral response of the space-based imaging system but ground-based observation systems will have a range of different characteristics primarily dependent on the optical benches (spectrometer modules) selected.
- secondly, near-ground systems will be either mobile or fixed point and multiple instruments will be deployed possible across the Globe and, if not, certainly across the northern hemisphere. For reliable and replicable measurements and to enable measurements from one near-ground system to be compared directly with measurements from the other system, common calibration standards and laboratory calibration and field measurement protocols will be required.

The aim of this mission was to develop the laboratory-based calibration and characterization procedures for this work and to develop a protocol to enable calibrations to be replicated at different facilities.

A Piccolo dual-field-of-view fibre optic-based spectrometers system with irradiance and radiance measuring capability and with optical benches capable of measuring across the 400 nm to 950 nm (VNIR) range at 2048 sampling intervals and from 640 nm to 800 nm in 1044 sampling intervals was calibrated and characterized using two different methods: using selected spectral line lamps (Figure 1a) and using a double monochromator OL750D (Figure 1a).

The Gooch and Housego OL 750Dconfigured with high intensity light source and customized entrance slit were chose to enable the spectrometers spectral response to be characterize at 0.05 nm sampling intervals and FWHM of <0.2 nm and a tungsten light source for larger spectral resolution. This enabled the characterization of spectrometers across telluric oxygen A and B bands. A previous characterization of OL750D in different configurations was necessary before starting the Piccolo system calibration. The setup chose for OL750D characterization is presented in Figure 2 and the some configurations selected are specified in table 1.

Data obtained by Piccolo spectrometer system were processed and analyzed using MATLAB program. The experimental calibration setup diagram is presented in Figure 1.



a *b*

Figure 1. Wavelength characterization of Piccolo dual-field-of-view fibre optic-based spectrometers system characterization setups using: a) selected spectral line lamps and b) double monochromator.

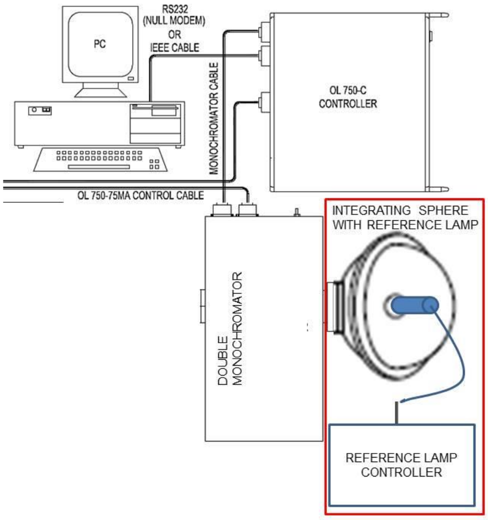


Figure 2. Setup used for OL750 D characterization.

Table 1. Configurations selected for OL750D characterization.

Slits	Aperture	Light Source	Range	Step
0.05, 0.5, 0.05	5.0mm	Neon	686-696 nm	0.05nm
0.05, 0.5, 0.05	5.0mm	Argon	758-768 nm	0.05nm
0.05, 0.5, 0.05	5.0mm	Argon	768-778 nm	0.05nm
1.25, 5.0, 1.25	5.0mm	Neon	686-696 nm	0.05nm
1.25, 5.0, 1.25	5.0mm	Argon	758-768 nm	0.05nm
1.25, 5.0, 1.25	5.0mm	Argon	768-778 nm	0.05nm
2.5, 5.0, 2.5	5.0mm	Neon	686-696 nm	0.05nm
2.5, 5.0, 2.5	5.0mm	Argon	758-768 nm	0.05nm
2.5, 5.0, 2.5	5.0mm	Argon	768-778 nm	0.05nm
5.0, 5.0, 5.0	5.0mm	Neon	686-696 nm	0.05nm
5.0, 5.0, 5.0	5.0mm	Argon	758-768 nm	0.05nm
5.0, 5.0, 5.0	5.0mm	Argon	768-778 nm	0.05nm

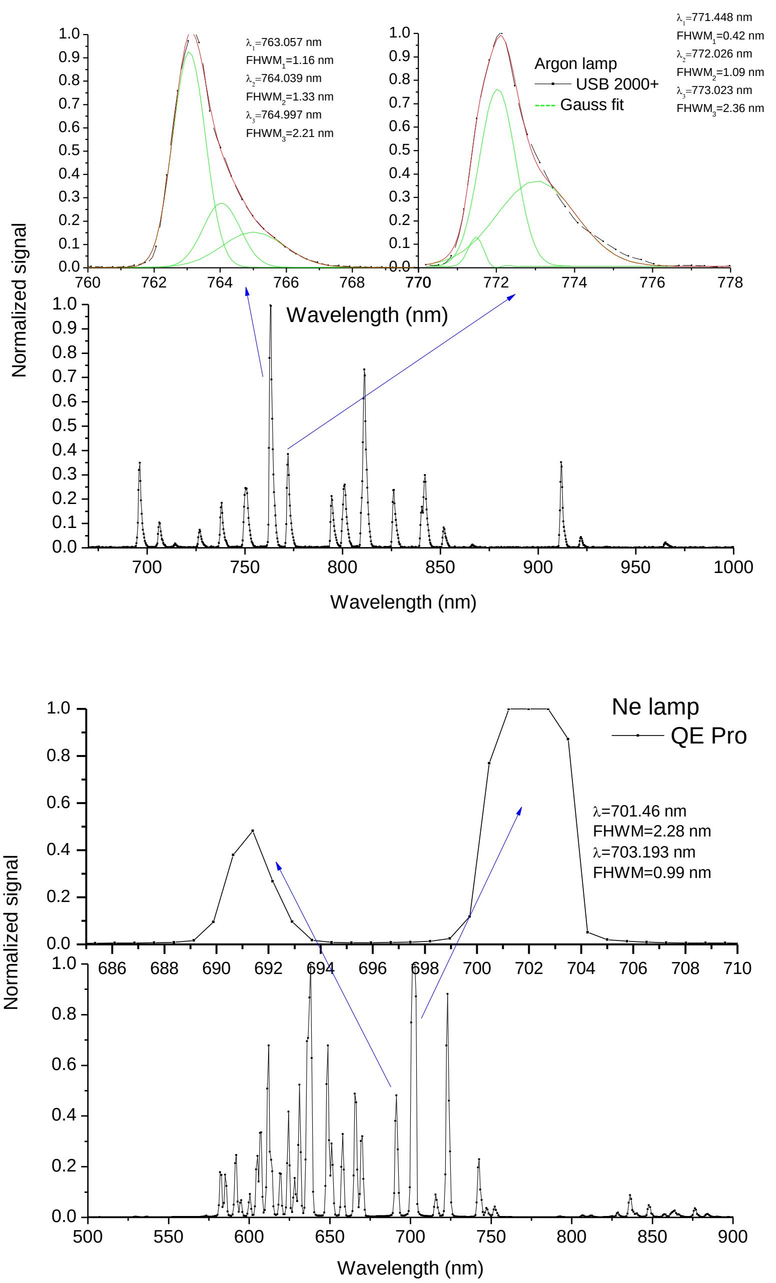
For irradiance a seasoned FEL lamp and for radiance a Hoffman integrating sphere was used. Both of these sources have current calibrations traceable to UK national standards.

Description of the main results obtained;

Only initial findings are presented in this preliminary report due to the extensive amount of data collected.

Piccolo dual-field-of-view fibre optic-based spectrometers system characterization in wavelength using selected spectral line lamps.

a) For each lamp (neon and argon) were obtained two spectra corresponding to each of the optical benches used in the Piccolo spectrometer system (Ocean Optics USB2000+ and QE Pro). Example of spectra obtained for Piccolo system characterization using the reference lamps are presented in Figure 3. From these spectra we selected some spectral ranges (see Table1) around the lamps main emission peaks and we repeated these measurements with the OL750 D using different lamps system as reference sources.



a

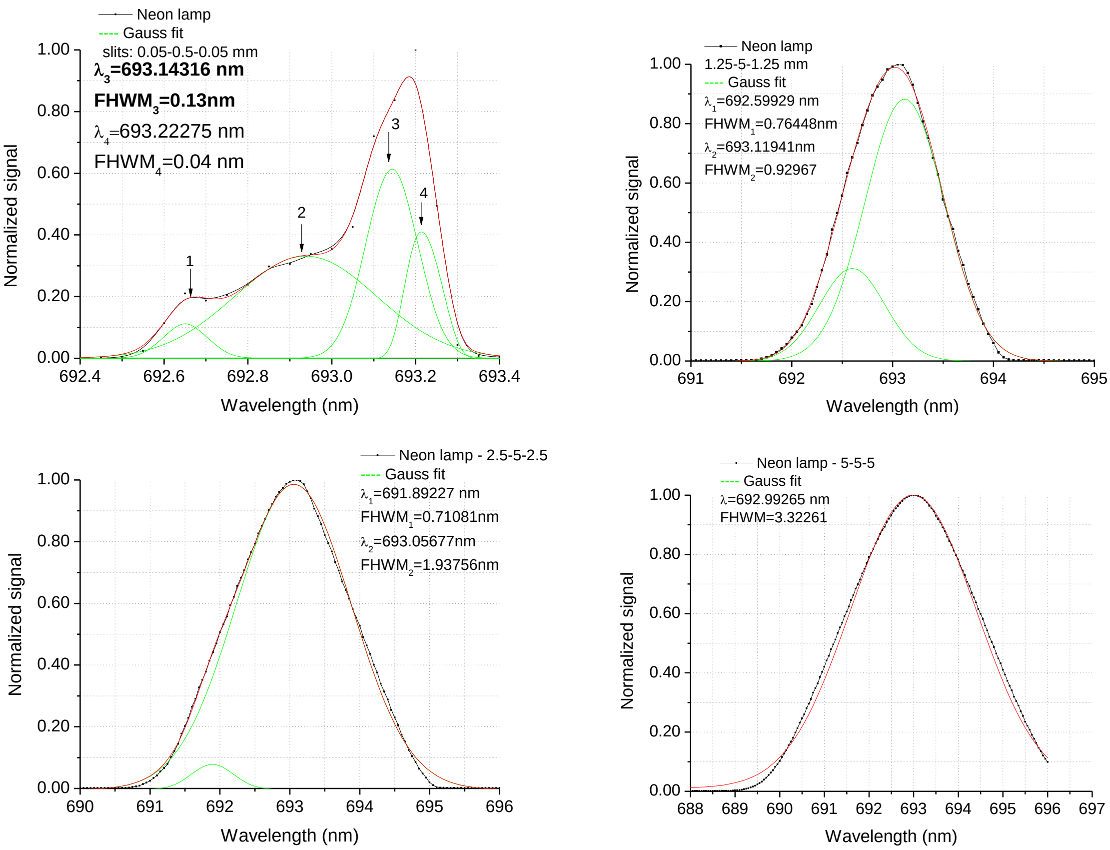
b

Figure 3. The absorption spectra corresponding to: a) argon lamp measured with the USB+2000 spectrometer and b) neon lamp measured with QEPro spectrometer.

b) **OL 750 double monochromator characterization using spectral line lamps and integrating sphere**

In order to evaluate the system characteristics at different performance levels, previous to this step, the OL750D double monochromator system was characterized considering different configurations (four different slits/apertures sets, two different gratings, two different reference lamps, associated to different absorption lines). Some of the results obtained for OL750D performances are presented in Figure 4.

As it can be noticed from the Figure 4, values of FHWM were between 0.13 and 3.32 for the purposed configurations using slits between 0.05 and 5 mm at the OL750D input with either a high intensity laser driven light source or a standard tungsten lamp source. The FHWM values were calculated applying a Gaussian fit for multiple selected peaks.



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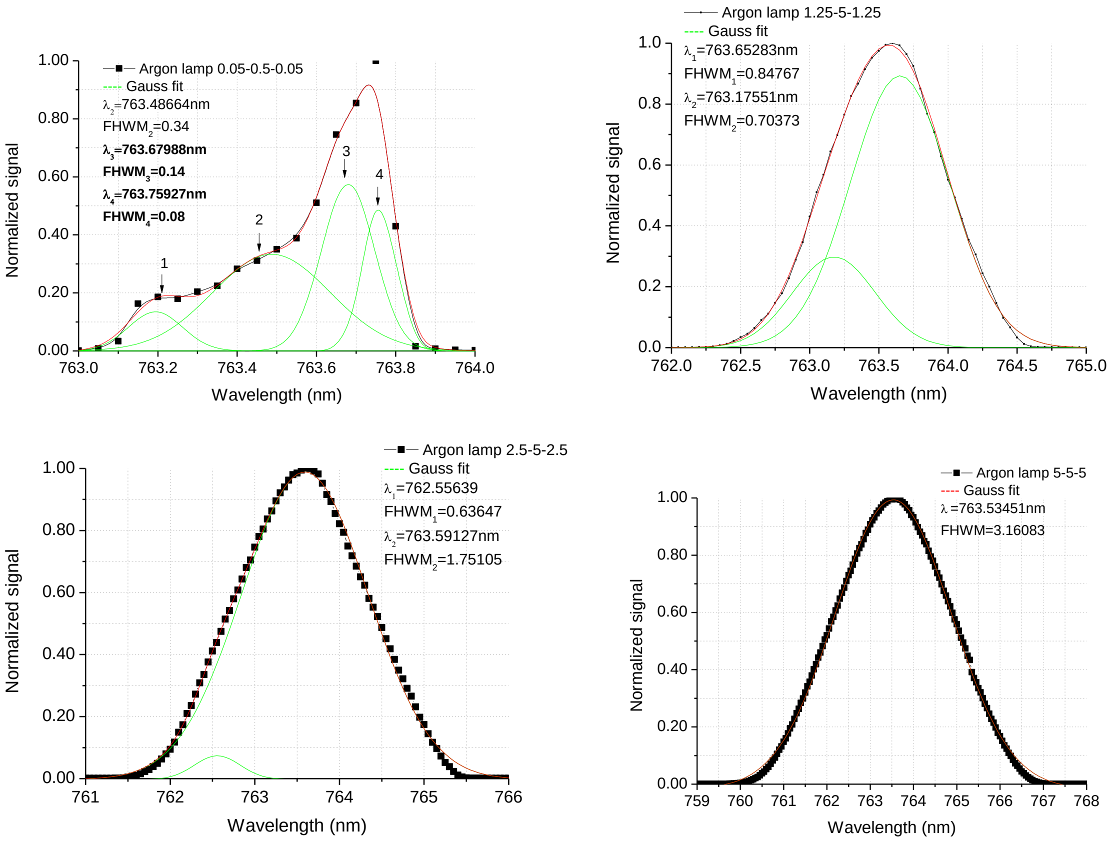

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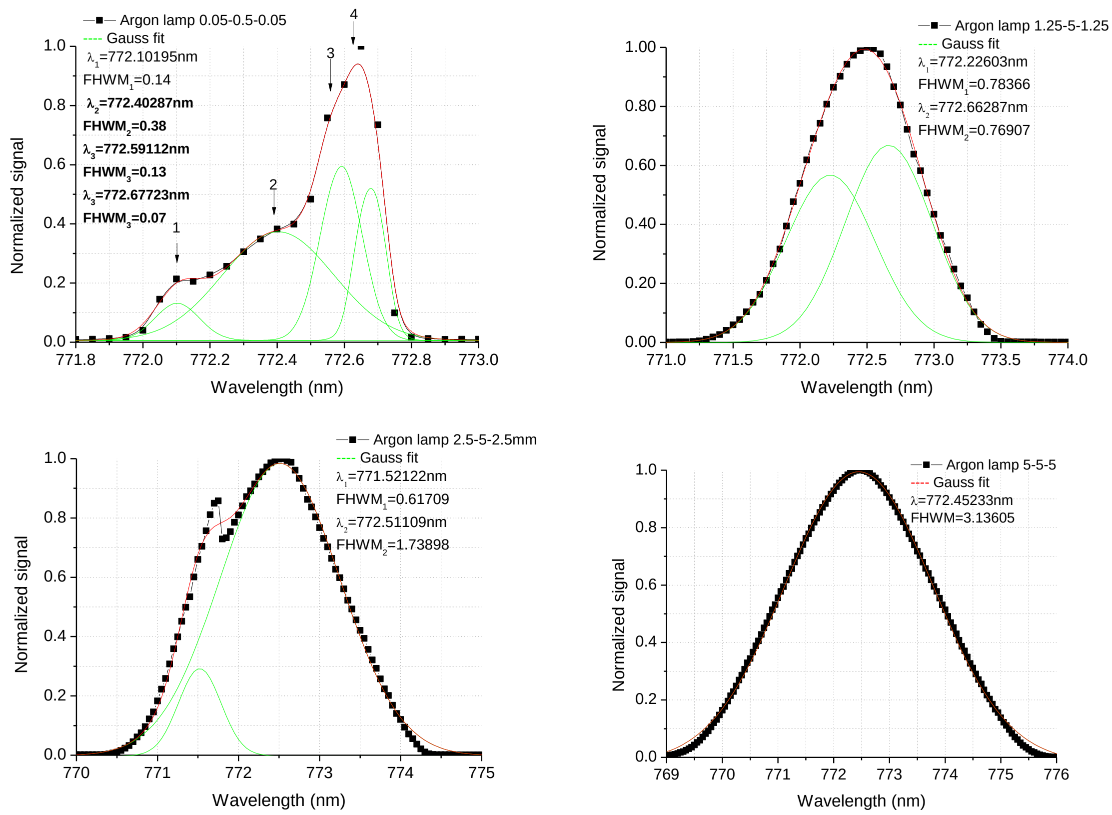

c

Figure 4. Monochromator performances using: a) a neon lamp; b) an argon lamp for the spectral range of 760 – 767 nm and c) an argon lamp for the spectral range of 770.5 – 774.5 nm.

c) **Piccolo dual-field-of-view fibre optic-based spectrometers system characterization using the OL750 monochromator**

Examples of spectra obtained for the Piccolo system characterization using the OL750 monochromator are represented in Figure 5. The optimized monochromator configuration was used. The difference between the QEPro spectrometer measured value and the wavelength set at the monochromator was equal to 0.365 nm with a standard deviation of around 0.027 nm, and -0.426 nm for the USB+ spectrometer, with a standard deviation of ± 0.014 nm.

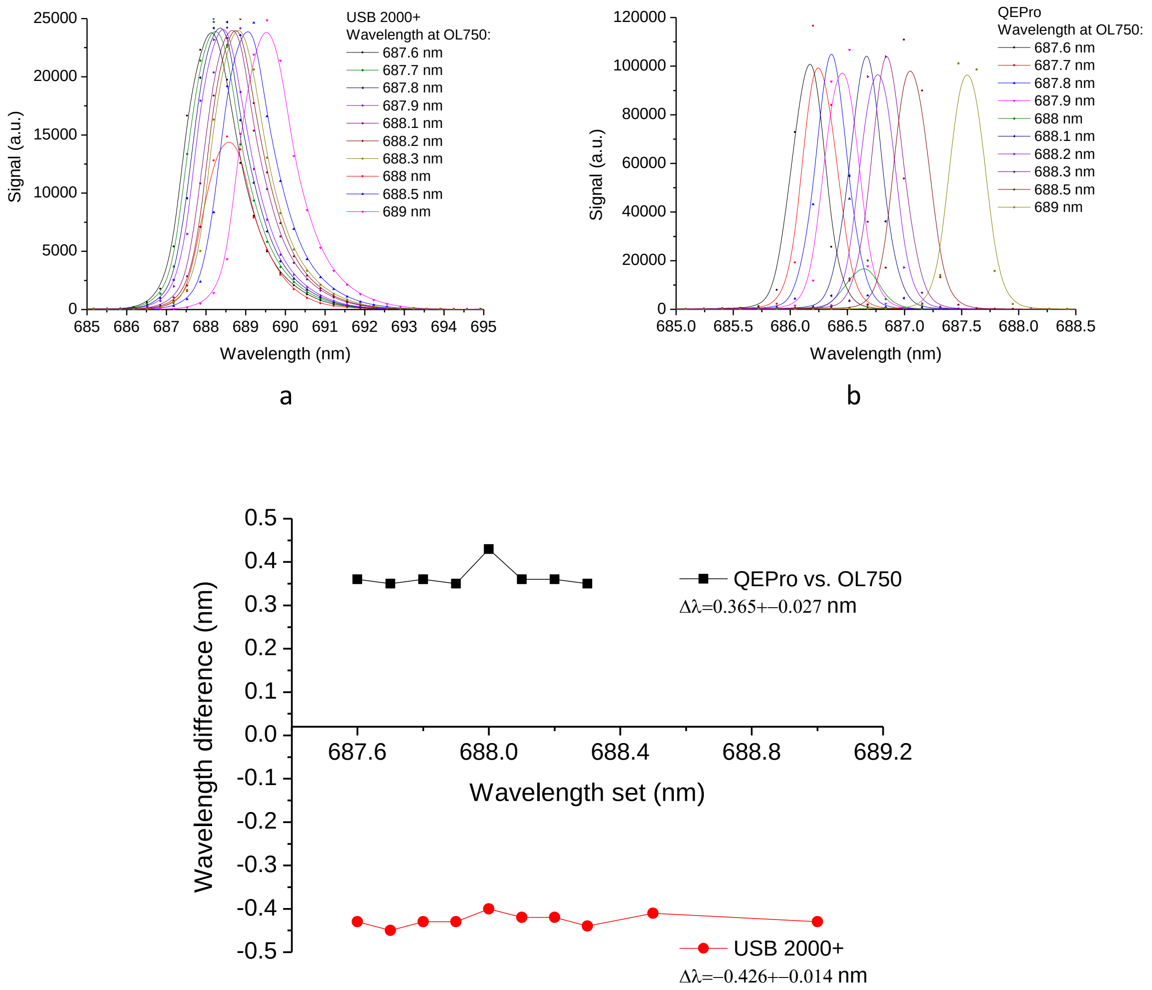

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Figure 5. The monochromator spectra measured with the Piccolo spectrometers system integrating the QEPro and USB2000+ spectromters.

A better spectral resolution was obtained at this stage for the QEPro spectrometer, equal to 0.26±0.009 nm, compared with the USB2000+ spectrometer that had a FHWM = 1.507±0.04 nm.

Preliminary conclusions:

During the STSM at NERC Facility / University of Edinburg the wavelength characterization and calibration of a Piccolo dual-field-of-view fibre optic-based spectrometers system has been done using two different methods. At this point, firstly was determined the FWHM and the shape of the OL750D source for different configurations, establishing the monochromator system performances.

Secondly, the FWHM values and the spectral response peaks shapes were determined for the spectrometers system. In this direction, more investigations has to be done in the future to establish the errors and uncertainties for each system. Also, a better characterization OL750D system spectral response has to be done with more spectral lines lamps.
The next steps will be also to assess the radiance, irradiance and FOV calibration methods and to delevope the procedures to support FLEX hnear-ground instrumentation.
The general protocol and calibration procedure for a dual field system was established during the STSM, the next step being to repeat the procedure for the applicants own laboratory, in order to verify the procedure repeatability.

Future collaboration with the host institution (if applicable);

The collaboration will continue repeating the establish procedure during the STSM, so the procedure repeatability will be checked. Also the investigation on all systems uncertainties will be extended for full validation of the procedure.

Foreseen publications/articles resulting from the STSM (if applicable);

An abstract reporting the results obtained during this STSM was submitted for presentation to EARSeL workshop, to be held in Switzerland, in April 2017.

Confirmation by the host institution of the successful execution of the STSM;

(it might be separate document written and signed by the Host - confirmation of acceptance from a senior Researcher affiliated to the Host institution formally accepting the scientific report.)