Sentinel-5: a novel measurement approach to quantify diffuser induced spectral features

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SENTINEL-5: A NOVEL MEASUREMENT APPROACH TO QUANTIFY DIFFUSER INDUCED SPECTRAL FEATURES

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I. INTRODUCTION

Many current and future earth observation satellites include spectrometer instruments, due to their suitability for identifying atmospheric gases through spectral signatures. Space based spectrometer instruments, such as the Sentinel-5-UVNS instrument (S5)\textsuperscript{1} for the polar-orbiting MetOp Second Generation satellite, require appropriate calibration to incident sunlight in order to provide radiometrically accurate data. To ensure homogenous illumination of the entrance slit of the spectrometer during sunlight calibration, a diffuser is used to scatter the incoming light \cite{1}. One contribution to inaccuracy in sunlight calibration is spectral features, an interference phenomenon resulting from scattering off the calibration unit diffuser \cite{2}.

The scattering of the incident light at the diffuser induces path differences, which yield a speckle pattern in the entrance slit. These speckles are still present at the focal plane of modern spectrometers through a combination of the high spectral and spatial resolution \cite{2} \cite{3}. Spectral features originate from the spectral integration of speckles in the slit to the spectrometer detector plane and further integration by the detector pixels \cite{1}. The spectral variation following pixel integration is known as spectral features. The magnitude of this error is evaluated in terms of the Spectral Features Amplitude (SFA), the ratio of the signal standard deviation with its mean value, within a specific wavelength range \cite{4}.

This work proposes a novel measurement technique. This method is based on the acquisition of monochromatic speckle patterns in the slit over a finely sampled wavelength range. The net spectral features at the spectrometer detector are evaluated through post processing, by integrating acquired speckle patterns along the spectral resolution, and detector pixels. A key advantage of the proposed technique is the fine sampling and observation of the interference structures that make up spectral features, below the level of a spectrometer pixel. The simplified optical system and simulation of an idealised spectrometer reduces the error contributions when compared to measurement using an entire spectrometer.

The goal of this investigation is the measurement of the S5 spectral features amplitude associated with the Heraeus Optical Diffuser (HOD), a volume diffuser, and the TNO quasi volume diffuser (QVD), in conjunction with qualitative insight into the mechanism behind speckle induced spectral features, supporting the design of future spectrometers.

This paper is structured as follows: Section II details the system designed to acquire monochromatic speckle patterns. The monochromatic speckle patterns are obtained using a tuneable laser capable of wavelength steps below the speckle decorrelation wavelength, as investigated in III. Section IV outlines how monochromatic speckles are integrated to spectral features, and reports the SFA values for the HOD and QVD. The spectral features results are discussed in light of this inference in Section V, with conclusions presented in Section VI.

II. EXPERIMENTAL SYSTEM

An optical system was devised with sufficient spectral and angular degrees of freedom to study the spectral features phenomenon. Tuneable NIR and SWIR lasers are used as the light source, with nominal tuning ranges of 750-790nm and 1540-1620nm respectively. The laser wavelength is independently monitored by a wavemeter, which is used in a PID controller to stabilise the laser wavelength. The laser beam is expanded directly from a fiber through a linear polariser. A plain glass window placed at 45\degree reflects \textasciitilde 4\% of the beam through a lens onto a photodiode, for independent power monitoring.

The expanding laser beam is then incident on the diffuser sample and passes through a rectangular aperture defined by the nominal S5 aperture. Subsequently, it enters a telescope and is directed onto a NIR-SWIR camera placed at the focal point.

The source optics and telescope were mounted on rotation tables such that the system could be configured to the S5 geometry. The diffuser sample is mounted on rotation and translation stages to allow for fine control during alignment.
A. Diffusers
In this work, two diverse diffusers are investigated, a quasi volume diffuser (QVD) and a real volume diffuser. All tests are performed for both the QVD and HOD diffusers, to allow comparison.

A quasi-volume diffuser (QVD) has a number of roughened surfaces arranged in transmission or reflection configuration. The QVD in this work is a $24 \times 24 \times 50$mm, $45^\circ/45^\circ/90^\circ$ prism with three diffusive surfaces. The hypotenuse is reflective and the legs are transmissive. It is made of fused silica and manufactured by TNO. In a true volume diffuser, the predominant scattering mechanism is Mie scattering by structures within the volume. The HOD volume diffuser in this work is a $3$mm thick, $80$mm diameter synthetic fused silica volume diffuser, with a fire polished surface finish, manufactured by Heraeus.

B. Detectors
The detector is placed in the setup at a place representative for the S5-slit. An InGaAs detector is used to capture oversampled ($640 \times 520$ pixels) S5 samples for the SWIR wavelength range. A Si detector is used to perform measurements for the NIR wavelength range, also oversampled at $2750 \times 2200$ pixels. The detectors are sized such that they both significantly oversample a single S5 slit sample with a field of view (FOV) of $0.2^\circ \times 0.5^\circ$.

III. EXPERIMENTAL PROCEDURE

The system is aligned such that the incidence and observation angles are representative of a sample centered on the S5 baffle field of view.

To measure the SFA, monochromatic speckle images are acquired at the spectrometer entrance slit over a large wavelength window, approximately 15nm wide, sampled every 4pm. To verify that this step size would be sufficient, the correlation of individual speckle patterns with varying wavelength was examined.

To investigate speckle correlation change with wavelength, the laser is tuned in steps of 1pm for the first 30pm and then coarser steps of 60pm. The HOD is measured over a range of 0.1nm, and the QVD is measured over a range of 0.9nm. Three speckle images are taken per wavelength, to confirm the system repeatability. This measurement is performed for both NIR and SWIR wavelength ranges.
The correlation coefficient, $\rho(X, Y)$, commonly assessed in the image processing community, measures the linear dependence between two vectors, $X$ and $Y$:

$$
\rho(X, Y) = \frac{\sum_{i=1}^{k}(x_i - \bar{X})(y_i - \bar{Y})}{\sqrt{\sum_{i=1}^{k}(x_i - \bar{X})^2 \sum_{i=1}^{k}(y_i - \bar{Y})^2}},
$$

where $k$ is the number of pixels in the images $X$ and $Y$, and $\bar{X}, \bar{Y}$ are the respective image mean values. The quantities $x_i$ and $y_i$ are the values of the $i^{th}$ pixels in images $X$ and $Y$, respectively.

Speckle correlation curves are generated by computing the correlation between an average image, $X$, generated from measurements taken at the initial parameter set, and each subsequent $j^{th}$ image in the dataset, $Y_j$, with the variation of the requisite parameter. This change in speckle pattern will manifest itself as a decrease in correlation, $\rho_j(X, Y_j)$, relative to the average of the initial images, $X$.

Correlation curves provide a measure of the rate of change of speckle pattern with respect to parameter variation, useful for diffuser and configuration comparison. The multiple measurements indicate the repeatability of the setup.

![Speckle correlation curves](image)

**Fig. 3.** a) NIR speckle decorrelation with wavelength for the HOD and QVD diffusers. b) SWIR speckle decorrelation with wavelength for the HOD and QVD diffusers. The data is fitted to a power series model.

With wavelength as the requisite parameter Fig. 3. a) displays a comparison between HOD and QVD correlation curves in the NIR spectral range, clearly showing the considerably more rapid decorrelation of the HOD. This more rapid decorrelation is expected to result in a lower spectral feature amplitude for the HOD, due to increased speckle averaging in the spectral dimension. Panel b) displays the curves for the SWIR spectral region. These curves confirm that the chosen spectral sampling of 4pm is sufficiently fine for the spectral features measurements.

A variety of decorrelation metrics are quoted in literature regarding the study of speckle patterns generated from rough surfaces. Defined in this paper are the wavelength displacement required to achieve a correlation coefficient of 0.5 and 0.05 or less, respectively denoted $\lambda_{0.5}$ and $\lambda_{0.05}$.

A summary of the obtained decorrelation wavelengths is presented in Table 1. A step size of 4pm is justified for the SFA measurements as it is approximately eight times lower than the HOD $\lambda_{0.05}$ and 100 times lower than the QVD $\lambda_{0.05}$.

<table>
<thead>
<tr>
<th>Wavelength Range [nm]</th>
<th>Diffuser</th>
<th>$\lambda_{0.5}$ [nm]</th>
<th>$\lambda_{0.05}$ [nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>770-770.1</td>
<td>HOD</td>
<td>0.003</td>
<td>0.03</td>
</tr>
<tr>
<td>1570-1570.3</td>
<td>HOD</td>
<td>0.015</td>
<td>0.05</td>
</tr>
<tr>
<td>770-770.8</td>
<td>QVD</td>
<td>0.055</td>
<td>0.40</td>
</tr>
<tr>
<td>1570-1571.2</td>
<td>QVD</td>
<td>0.055</td>
<td>0.50</td>
</tr>
</tbody>
</table>
IV. SPECTROMETER SPECTRAL FEATURES

To understand the origin of spectral features, consider a simplified model of the spectrometer operation, downstream from the diffuser as follows. Fig. 4. a) shows light from the slit plane entering the collimation system. Note that the spectral and spatial dimensions of the slit, as imaged by the spectrometer, are denoted as along track (ALT) and across track (ACT), according to the orientation of the satellite orbit, for a push broom spectrometer.

The collimated light is then incident on a dispersive element, a grating in case of Sentinel-5. The dispersive element redirects the light to different angles dependent on wavelength. The camera optics subsequently map this light to different spatial positions on the spectrometer detector.

Fig. 4. a) Schematic of one of the spectrometer optical trains for Sentinel 5. b) Functional representation of spectrometer operation, displaying how the ALT dimension of the slit is imaged onto oversampled pixels in the spectral dimension of the detector for varying wavelengths. \( \lambda_1 \) and \( \lambda_2 \) are so called edge wavelengths, for which the slit is imaged onto independent oversampled pixels, defining the spectral resolution of the instrument. The depicted wavelength, \( \lambda_3 \), illustrates the contribution of wavelengths intermediate to \( \lambda_1 \) and \( \lambda_2 \) to the spectral features observed at point P on the detector.

To enable modelling of spectrometer spectral features based on individual speckle patterns, it is important to understand that any such features are the net result of all dispersed wavelength contributions within the spectral resolution of the instrument.

The proposed approach to spectral features modelling requires a datacube of speckle patterns acquired at different wavelengths. In this work, a speckle datacube refers to the dataset containing the experimentally obtained images of speckles sampled over a range of wavelengths in increments of 4pm. The wavelength range of this datacube is defined by the spectral resolution of the instrument in question and the range of spectral features to be modelled.

Consider the simplified linear spectrometer equations:

\[
\begin{align*}
    a &= M_x x , \\
    b &= M_y y + k\lambda ,
\end{align*}
\]

where the S5 detector coordinates are \( a \) (spatial direction) and \( b \) (spectral direction), the slit coordinates are \( x \) (ACT) and \( y \) (ALT), the respective magnification factors are \( M_x \) and \( M_y \), the wavelength of light is \( \lambda \) and the dispersion constant \( k = \frac{db}{d\lambda} \).

This analysis makes the further simplifying assumption that magnification factors are constant with wavelength. Consider the polychromatic light emanating from the slit, subsequently collimated and dispersed ALT. The ALT dimension is mapped to some number of pixels in the spectral direction, corresponding to the spectral resolution of the instrument. For example, the S5 NIR instrument has a spectral resolution of \( \sim0.4\text{nm} \), corresponding to three pixels in the spectral dimension, \( b \).
A point, $P = (a, b)$, on the detector sees contributions from the “bottom” of the slit in the “red wavelength”, $\lambda_1$, and contributions from the “top” of the slit in the “blue wavelength”, $\lambda_2$, (and all intermediate wavelengths in between). This is critical to interpreting the mapping of a datacube of individual speckle patterns to spectrometer spectral features.

Edge wavelengths, $\lambda_1$ and $\lambda_2$ are related to point $P$ and the ALT slit dimension, $Y$, by considering (3):

\begin{align*}
\lambda_1(y = 0, b) &= \frac{b}{k}, \\
\lambda_2(y = Y, b) &= \frac{b - M_y Y}{k}.
\end{align*}

The intensity in the detector plane, $I_{\text{det}}(a, b)$, at point $P$, from a datacube of speckle patterns, $I_{\text{slit}}(x, y, \lambda)$, collected at the S5 slit is some summation through the datacube, limited by the ALT size of the slit:

$$I_{\text{det}}(a, b) = \sum I_{\text{slit}}(x, y, \lambda).$$

Formulating $x$ as a function of $a$ and $y$ as a function of $\lambda$ and $b$, using (3):

$$I_{\text{det}}(a, b) = \sum_{\lambda = \lambda_1}^{\lambda_2} I_{\text{slit}} \left( \frac{a - b - k\lambda}{M_x, \frac{-M_y \lambda}{M_y}}, \lambda \right) \frac{\Delta \lambda}{\lambda_2 - \lambda_1},$$

where $\Delta \lambda$ is the step size between consecutive speckle images in the datacube. The factor $\frac{\Delta \lambda}{\lambda_2 - \lambda_1}$ correctly weights the summation. Equation (7) at one point, $P = (a, b)$, can be visualized as the summation along the red line in Fig. 5.

![Fig. 5](https://www.spiedigitallibrary.org/conference-proceedings-of-spie) Images in false colour correspond to monochromatic speckle measurements. The yellow rectangle defines the $0.2\times0.5^{\circ}$ FOV S5 slit sample. The red line represents the summation through a speckle datacube corresponding to a single point on the detector.

One can now visualise the wavelength dependent summation of all points between the top and bottom of the slit, required to obtain one point on the detector for an idealised spectrometer. This reasoning can be extended to the case of multiple points along the detector spectral dimension, $b$. This extension is visualised as the parallel diagonal red lines, each corresponding to an individual value of $b$, in Fig. 6.
Fig. 6. Multiple summations along the spectral dimension, with varying $b$.

Noting that the wavelength limits can be expressed as a function of $b$:

$$I_{\text{det}}(a, b) = \sum_{\lambda = \lambda_1(b)}^{\lambda_2(b)} I_{\text{slit}} \left( a \lambda \frac{b - k\lambda}{M_x}, M_y, \lambda \right) \frac{\Delta\lambda}{\lambda_2(b) - \lambda_1(b)}. \quad (8)$$

Equation (8) is visualized, for one entire S5 sample, as the summation along the planes in Fig. 7.

Fig. 7. Visualisation of ALT and ACT datacube contributions to spectral features.

In Fig. 8. a) we see a varying intensity pattern, reminiscent of fundamental speckle patterns. We will refer to such a pattern as “spectral speckles”. The black lines in Fig. 8. a) represent the S5 detector pixels. Spectral features are visualised as the integration over these pixels in Fig. 8 b).

It is apparent that the variations in intensity incurred by the spectral speckles generates spectral features. The spectral features are compared for across track samples of 0.5°. This is how the spectral features amplitude is estimated by measuring a datacube of individual speckle patterns over a specified wavelength range.
Fig. 8. a) Spectral speckles on the S5 detector. b) Spectral features on the S5 detector. Note the integration in ACT is over a third of the sample for visualisation.

The spectral features amplitude (SFA) is standard deviation of the 0.5’ ACT spectral features, normalized to the mean of the datacube. Table 2 presents a summary of the spectral features, as calculated by integration through the speckle datacube, to the S5 detector. The SFA is given as a percentage of the mean intensity value.

Table 2. Measured SFA values.

<table>
<thead>
<tr>
<th>Range [nm]</th>
<th>Sample</th>
<th>SFA [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>758 - 775</td>
<td>HOD</td>
<td>2.3</td>
</tr>
<tr>
<td>755 - 780</td>
<td>QVD</td>
<td>2.8</td>
</tr>
<tr>
<td>1545 - 1565</td>
<td>HOD</td>
<td>3.7</td>
</tr>
<tr>
<td>1545 - 1565</td>
<td>QVD</td>
<td>4.3</td>
</tr>
</tbody>
</table>

A comparison of the spectral features for the entire 0.5° ACT sample is provided in Fig. 9.

Fig. 9. a) NIR spectral features amplitude for HOD and QVD. b) SWIR spectral features amplitude for HOD and QVD.

As expected, the spectral features are larger for SWIR wavelengths, as the speckle size is proportional to wavelength. As the HOD has a more rapid spectral decorrelation with wavelength compared to the QVD, it was expected that the HOD spectral features amplitude would be significantly lower. Contrary to this, the HOD spectral features are only marginally lower than the QVD spectral features. This is discussed in the next section.

V. DISCUSSION

Based on the considerably more rapid spectral decorrelation of HOD speckle patterns compared to the QVD, as presented in Table 1, a substantially lower SFA value could be expected. However, an important outcome of this activity is that this has not been observed, evidenced by the SFA values in Table 2.

The rapid spectral decorrelation for the HOD diffuser does not necessarily translate one to one to the spectral features domain. A spectrometer puts significantly more weight in the ALT speckle size rather than the decorrelation characteristic of the diffuser. Therefore, the ALT speckle size is the driving parameter determining the spectral feature amplitude. When integrating a speckle datacube, the reduction in spectral speckle contrast is achieved through the summation of independent patterns. For the case of a spectrometer, both spectral and spatial averaging occur in the integration step, as the integration plane sums across a diagonal region in the datacube.
One can imagine the summation of independent patterns as the number of independent speckles that the diagonal integration plane intersects. It is apparent that the number of independent speckles in both the ALT dimension of the slit, and the $\lambda$ range corresponding to the spectral resolution, determines the total number of independent patterns intersected.

The number of independent patterns in the slit is independent of the diffuser, and determined by the individual speckle size, constrained by the aperture airy disc, and the slit ALT dimension. The number of independent speckle patterns in the spectral domain is a property of the diffuser and determined by the corresponding speckle decorrelation wavelength.

Considering this understanding of speckle contrast reduction by integration to the S5 plane, it becomes apparent as to why the performance of the QVD and HOD are more similar than would be expected from their spectral decorrelation curves. A heuristic argument is that the gradient of the integration plane through the datacube weights the number of independent pattern intersections, between ALT and $\lambda$ contributions. This gradient is directly proportional to the dispersion constant, $k$, which, in the case of a spectrometer, should be a relatively large value, to provide sufficient spectral resolution. Thus, contributions related to independent speckle in the ALT direction are found to be more heavily weighted in the generation of diffuser spectral features.

A more rigorous argument is the focus of ongoing work towards predictive statistical models. It should be emphasised that the overall long term goals of this project should be the development of a consistent model of spectral features, that can be derived from first principles knowledge of speckle size, speckle contrast, decorrelation wavelength and decorrelation angle.

An ultimate validation of this novel method would involve direct comparison with a test bed spectrometer, with matching geometry and diffusers. Further investigations promise valuable technical insight regarding the spectral features induced radiometric errors expected in the development of future spectrometers.

VI. CONCLUSION

The novel method of evaluating spectral features from monochromatic speckle patterns in a representative slit plane and simulating the spectrometer operation has proven to be a valuable step into a more comprehensive understanding of the origin of spectral features. Valuable understanding has been gained into the spectrometer mixing of spectral and spatial speckle decorrelations resulting in integrated spectrometer speckles and spectral features.

Estimates for the SFA of S5 have been acquired confirming marginally lower values for the HOD compared to the QVD in both SWIR and NIR wavelength ranges. This is consistent with the measured decorrelation of individual speckle patterns with wavelength, which was observed to be considerably more rapid in the HOD compared with the QVD. Despite the rapid decorrelation of the HOD, this did not correspond one to one for measured SFA, due to the inherent mixing of spatial and spectral decorrelation during spectrometer integration. This has been judged to be the main contributor driving the spectral feature amplitudes for future spectrometers.

This novel approach was justified on the basis of sampling requirements, complexity reduction, budget and time constraints and signal to noise. Most importantly, however, this approach provided additional qualitative insight into the mechanism behind speckle induced spectral features. Future verification using a test bed spectrometer would be highly valuable in validating this approach.

VII. REFERENCES