Spectral Features, effects and cures

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ABSTRACT

The presence of structures, as observed in real data from earth observing satellites, that are due to the on-board diffusers are discussed. These structures are shown to be caused by the speckles created by the diffusers in the entrance slit of the spectrometer. A dedicated set-up for the study of these spectral features will be presented together with results on different types of diffusers, i.e. surface diffusers and volume diffusers. Finally, methods to reduce the amplitude of the spectral features will be presented. These methods become more important since the use of infra red channels at high spectral resolutions is aimed for in future missions.

1. INTRODUCTION

Earth observing satellites for spectroscopic analysis of the earth atmosphere take the sun as illumination unit. The spectra recorded after passage through the atmosphere are calibrated using direct sun observations. To mimic the scattering of the earth, an on-board diffuser is included in the satellites. An additional function of this diffuser is to get a homogeneous illumination of the entrance slit of the spectrometer and to monitor the aging of the instrument.

In the past years a number of reports^{1,2} have been made about wiggles that are observed in the calibrated spectra of earth observation satellites that can not be due to absorption in the atmosphere. In the 2004 SPIE annual meeting a complete session was dedicated to the discussion of these wiggles. During that meeting we presented our research³ in this field. We have created a setup that is designed for testing diffusers and to get insight in the means to minimize the wiggle amplitudes. This was presented in the 2005 SPIE annual meeting. This paper will shortly repeat the presentation of the setup and will then focus on the model to describe the wiggles. Novel results of the model and the experimental results obtained using our setup will be presented, showing a very good agreement. All new insights into spectral features reduction will be presented.

The present tendency in spectrometer design is to operate at longer wavelengths (above $2 \mu m$) at ever decreasing bandwidths per pixel (increasing spectral resolution). This means that Spectral Features will become a larger problem in the near future and that methods to reduce their amplitude are a necessity.

Definition of the Spectral Features Amplitude (SFA)

In order to have a simple quantity to relate to a given diffuser, that tells directly the amplitudes of the wiggles that are to be expected, we propose the use of the Spectral Features Amplitude (SFA). Spectral Features are those features in the spectra that are due to the diffuser (and are not due to absorption effects in the earths atmosphere or due to emission lines in the spectrum of the light source). The standard deviation of the normalized data is taken as the SFA. The SFA can be calculated over a spectral width containing a few periods of spectral features. Alternatively, the SFA can be calculated from a large number of independent spectra where the standard deviation is calculated per wavelength. Differently stated the Spectral Features Amplitude can be defined as: the deviation of the unwanted wiggles in the signal as measured in a spectrometer after eliminating all wanted features from the spectrum, e.g. by dividing two independent measurements.

2. CAUSE OF SPECTRAL FEATURES

When laser light (coherent or at least partially coherent⁴) is scattered by a rough surface speckles are observed. This is due to interference effects that occur in all locations of an observation screen. Each location on that screen receives light

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from many points on the scattering object. All contributions can interfere as long as the coherence length of the light source is long enough such that path length differences are smaller than this coherence length.

In case of an earth observation satellite the light source in use is the sun. The coherence length of the light emitted by the sun is very short such that speckle effects are not easily observed. However, since the spectrometer limits the wavelength band per pixel, the light reaching each pixel will show interference effects and thus also speckles. The effective coherence length L_c for a spectral width of $\Delta\lambda$ and a central wavelength of λ_0 is obtained via

$$L_c = \frac{\lambda_0^2}{\Delta \lambda}.$$
 (1)

The number of speckles present on each pixel changes with distances in the setup, illumination angle of the diffuser, etc. This means that the observed intensity per pixel will change over time. As a function of wavelength the intensity will even change for a perfectly stable setup. These intensity fluctuations with wavelength, that are due to changing speckle numbers and/or intensities, are what we refer to as Spectral Features. These Spectral Features can not be cancelled via a calibration scheme since they change with about everything. In a laboratory setup calibrating out the Spectral Features is feasible but in an operational satellite this is not an option. The fact that the speckle distribution changes with about everything is one of the best methods to reduce the spectral features: averaging!

The speckle size σ_s scales linearly with wavelength,

$$\sigma_s = 0.61 \frac{\lambda}{\text{NA}},\tag{2}$$

which means that the number of speckles falling onto a one dimensional pixel scales inversely proportional to the wavelength. The effect of the increase or decrease of the number of speckles in the detection area by one is stronger for a few speckles than when many speckles are present. This means that the Spectral Features will be more pronounced for longer wavelengths. The NA in Eq.(2) stands for numerical aperture of the optical system. In the case that a lens is used in the system the NA is defined by the aperture of the lens and the distance between lens and observation plane (in this paper this is taken to be the entrance slit of the spectrometer). If no lens is used, free space propagation, the NA is defined by the width of the scattering surface and the distance between diffuser and observation plane.

3. DEDICATED SET-UP

The components in the layout drawing (see Figure 1) of the dedicated Spectral Features measurement setup are numbered alphabetically:

- A. Light source (QTH or Xenon type lamps)
- B. Re-imaging aspheric mirror optics, to image the lamp onto C
- C. Pinhole/diaphragm (changeable size)
- D. Collimation mirror (aspheric)
- E. Diffuser or sample holder
- F. Rotation table
- G. Spectrometer entrance optics (UV enhanced doublet to illuminate the entrance slit J)
- H. Optional polarization module
- I. Order filter wheel
- J. Entrance slit of spectrometer
- K. Collimation mirror
- L. Turret containing the diffractive optics (prism and grating)
- M. Detector unit ('Hamamatsu' CCD array)
- N. Darkened area
- O. Imaging mirror

This section only gives an overview of the components present in the setup. The stages will be discussed here, but many further details will be given in the following section where the input is required to explain the observed phenomena. The illumination unit is build on a rotation stage allowing us to change the angle of incidence on the diffuser. The diffuser itself is also placed on a, separate, rotation stage allowing the change of angle under which the diffuser is seen by the

spectrometer. Between the diffuser and the entrance slit of the spectrometer a lens is placed such that our system is in the so called mixed mode. A mixed mode is a mode where the 'imaging' from the diffuser onto the entrance slit consists of two or more of the following pure modes. The first pure mode is Free Space Mode. In this case no optical elements are used for the imaging. The second pure mode is the Imaging Mode. In the imaging mode the diffuser is imaged onto the entrance slit via a lens. The third and final pure mode is the Fourier Mode. Here the diffuser is placed in the front focal plane of the lens and the entrance slit in the back focal plane. In our setup we have a mix between Free Space Mode and Fourier Mode. The diffuser stands at about half a meter away from the front focal plane of the lens. The entrance slit is in the back focal plane.

The actual spectrometer consists of two types of dispersive elements. The first is a prism, and that one is used for the lowest wavelength band (Band I: 240 - 400nm). The other wavelength bands are measured with a grating as dispersive element (Band II: 390 - 550nm, Band III: 540 - 700nm, Band IV: 690 - 850nm, and finally Band V: 840 - 999nm). All these bands are measured using a 1024 pixels Si CCD detector. After replacing this detector with a 512 pixels InGaAs CCD detector also some near infrared bands can be measured, using a differently blazed grating to optimize the throughput in the NIR. The NIR bands (Bands VI through XV) are half the spectral width of the bands in the visible in order to arrive at similar spectral widths per pixel. The wavelengths measured in the NIR range from 920 through 1630nm.



Figure 1 Layout of the dedicated Spectral Features setup

The optics inside the spectrometer were designed such that the numerical aperture of the beam illuminating the entrance slit is smaller than the acceptance angles of the mirrors labeled K and O in Fig.1. In this way the number of speckles in the entrance slit is the relevant number is the spectral features calculations. All optical elements inside the spectrometer (except for the prism of course) are used in reflection to minimize chromatic effects.

4. RESULTS

This section gives an overview of the results obtained using the presented setup and compares these results with calculated spectra obtained from the spectral features model. In this setup we have tested several different diffusers of

which we will here show the result obtained for a real surface diffuser (Aluminum), a real volume diffuser (Spectralon), and a quasi volume diffuser (QVD). The presented results are the SFA values obtained from a spectrum divided by an independent spectrum to remove all spectral phenomena that are not related to the speckle effects. Each spectrum is on its own the result of many recordings during which the system is kept stable. In this way the noise levels in the spectra are reduced well below the expected spectral features levels.

The data points below the 900nm were recorded using the Si CCD camera while the extra points (in the near infra red, above 900nm in the shown results) were recorded using an InGaAs CCD camera. Both cameras have the same mounting and are from Hamamatsu (C7222-1006 in visible, and C8061-01 in the near infrared). The pixel sizes were according to the data sheet 25μ m×1.4mm and 25μ m×0.5mm, respectively. Due to the length difference between the two detectors the SFA is expected to be different. For the Al diffuser we have measured all visible wavelength bands and three NIR bands. The longest VIS band overlaps with the shortest NIR band. A scaling by a factor of 0.7 (30% reduction) for the NIR SFA values made the results match in this overlap region. This scaling factor is applied to all measurements, and as can be seen from the presented results the data points seems to fall on a understandable, non discontinues, curve. The physics behind the shape of the curves will be explained in the discussion section. Here the building blocks behind the theory will only be introduced.

SFA on Aluminium - comparison measurement & model



Figure 2 Results of the spectral features measurements on an Aluminum diffuser. The shown line gives the simulation results

For the Aluminum diffuser the only effects that are important are the surface roughness of the diffuser (determines the visibility of the speckles and thus the amplitude of the SFA), the number of speckles in each detector pixel, and the spectral width of each detection pixel. Owing to averaging effects within a pixel the SFA will reduce. As will be shown in the discussion, the period of the spectral features scales quadratic with the wavelength. The reduction in SFA with wavelength will therefore reduce. This effect can be seen in Fig.2.

In Figs.3 and 4 the results are shown for a quasi volume and a real volume diffuser. The same effects have to be taken into account as for Aluminum plus some extra effects. These effects have to do with the coherence length pertaining to the spectral bandwidth of a pixel, and to the enhancement in the averaging effect owing to the opening angle of the beam of light that illuminates the diffuser. These effect make the apparent curve to bend upwards. For Al the curve bends downwards. For QVD the curve has a tendency to bend upwards, and for Spectralon the line is nearly linear with wavelength.

QVD is a flat quartz window that has been ground on both surfaces, and from which at the back surface aluminum has been deposited to enhance its reflectivity.



SFA on QVD comparison measurement & model

Figure 3 Results of the spectral features measurements on an Quasi Volume Diffuser (QVD)



SFA on Spectralon - comparison measurement & model

Figure 4 Results of the spectral features measurements on a volume diffuser (Spectralon)

5. DISCUSSION

Before entering the actual discussion it has to be stated that the results as shown here are valid for our optical arrangement. By changing the optical layout the SFA curves will change. A diffuser that performs best in one optical arrangement can be far worse in a different arrangement.

The spectral features are due to speckles caused by the diffuser in the system (and any other rough surface that the light happens to get scattered by). The speckles are a random phenomenon which makes the analysis statistical in nature. The amplitude of the spectral features for a given wavelength can change with e.g. angle of incidence on the diffuser. The statements given hereafter are therefore always average values. Single measurements can yield results that are different from these average values. For this reason we have adopted the standard deviation as measure for the spectral features amplitude, which makes the discussion less sensitive to large peaks in the spectral features spectrum.

In the following we give a full discussion on all effects as observed during the measurements on the different types of diffusers. From numerical analysis we found that the spectral features amplitude scales linear with wavelength. This is not observed for any of the measured diffusers. The reasons for this non compliancy with theory will be discussed.

5.1 Surface diffuser

As surface diffuser we have used an aluminum diffuser with a surface roughness far larger than the wavelengths used during the measurements. This means that the speckle patterns that will be created using this diffuser will have a visibility of unity⁴. The surface diffuser is the easiest to model. No coherence effects have to be taken into account. As observed in Fig.2, the SFA has two distinguishable regions. The first corresponds to the prism dispersed part of the spectrum, the other to the grating dispersed parts. In the prism dispersed part the SFA is about constant (Band I: 240 - 400nm). This is explained by the fact that the spectral width per pixel increases with wavelength. Due to the spectral width per pixel the SFA is not an exact measurement but only an average over that particular bandwidth.

For all other measured bands the SFA is found to increase with wavelength but the slope of the SFA decreases with wavelength. This is again explained by inter pixel averaging and the fact that the period of the oscillations increases with wavelength (see Sec.6). The SFA as measured is different from SFA values that are calculated. In a measurement the angular extend of the light source is always taken into account. This angular extend results in an averaging since many independent speckle patterns are created simultaneously. The number of independent speckle patterns depends on the solid opening angle of the illumination beam and on the wavelength. Since the speckles scale linear with wavelength the amount of averaging decreases according to a quadratic function with the wavelength.

5.2 Volume diffuser

The same mechanisms that are responsible for the SFA versus wavelength for a surface diffuser are also at work for volume diffusers. The difference is that an additional mechanism has to be taken into account. Since the scattering particles are now positioned throughout the diffuser material, the speckle pattern will now be formed by contributions from all those particles. There where the surface roughness of a surface diffuser is small as compared to the coherence length per pixel, for the volume diffuser the particles can be deeper into the material than one times the coherence length. In most cases the thickness of a volume diffuser will be several times the coherence length. In our setup the bandwidth per pixel is about 0.2nm which lead via Eq.(1) to a coherence length of 1.25mm for 500nm light. For $1\mu m$ the coherence length will be 5mm which is about equal to the thickness of our used Spectralon sample.

The number of sub-layers that have to be added incoherently is found by multiplying the thickness of the diffuser by its refractive index and divide it by the coherence length. Twice this value is the number of sub-layers for a volume diffuser used in reflection. For the case where the penetration depth is less than the thickness of the sample, this penetration depth has to be used instead of the sample thickness.

5.3 Quasi Volume diffuser

The situation for the QVD is similar to that of the volume diffuser. The important difference is that the scattering is not distributed over a large number of sub-layers as for a volume diffuser, but is now concentrated on three interfaces, with effectively two interfaces that create speckle in the entrance slit.

These three interfaces are: the top interface where the light partially diffusely reflects and transmits, the back surface where all light diffusely reflects, and finally the top interface again where again the light partially diffusely transmits and reflects. As long as the separation between the surfaces is large enough, their contributions have to be added incoherently.

As stated before, the first surface (the top interface) scatters the light partially towards the entrance slit (Speckle pattern I), while the remaining light is transmitted towards the back surface where a speckle pattern is created as illumination source. All light is here scattered and the light that transmits through the top surface forms the second speckle pattern in the entrance slit. Owing to this passage through scattering surfaces, and relatively large separation between interfaces,

the resulting overall speckle pattern in the entrance slit will be highly sensitive to angular changes of the illumination beam. This means that the averaging effects due to opening angle of the light source are for a QVD very large.

6. MODELING AND DISCUSSION

To reduce measuring time and to get more detailed insight in spectral features a MatLab program has been written to model the different types of diffusers in all possible configurations that can be envisaged. To validate our model we have implemented the optical layout of our in-house spectral features setup. The results of the modeling show identical features as observed in experiments and the obtained SFA graphs are shown in one figure together with the measured data in a previous section. This tells us that our model can be used to predict the trends of the SFA with wavelength, and to compare different optical arrangements. In order to get an exact quantitative agreement the model should include all optical elements with there actual dimensions. This is found to be to slow in terms of computation time. We have therefore adopted the approach where we only simulate layouts and diffusers, where the sizes have been scaled down, to get a qualitative comparison between different types of diffusers and different optical layouts. The final scaling to get a match with experimental data is obtained via a few measurements. The model gives then the interpolation and extrapolation of the spectra. Interpolation is used for parts of the spectra that have not been measured between measured wavelength bands. Extrapolation in used for spectral regions outside of all measured bands, but also to get information what would happen if the optical arrangement would be changed.

As mentioned before our setup consists of the mixed mode, i.e. a part of free propagation followed by a Fourier mode. These two modes can be altered, removed, and the imaging mode can be added to it. In the previous SPIE annual meeting paper³ the model has been described. In the following our present understanding of spectral features will be described.

The period of the spectral features has in some form to do with the speckle size. Since we observe the spectral features in the spectral domain we are interested in the speckle size as a function of the wavelength and the rate of change of the speckle pattern with changes in wavelength. Figure 5 shows the wavelength shift required to obtain an uncorrelated speckle pattern, as a function of beginning wavelength. The stars are the calculated speckle widths for correlations equal to 0.5 and the line is a quadratic line fitted through these data points. This indicates that the spectral speckle width scales via a quadratic function with the wavelength. For the graph shown in Figure 5 a free space propagation of 540mm was followed by a Fourier transform via a lens. The small spectral widths of the speckles are mainly due to the free space propagation. It was calculated that for 400nm light the spectral width equals 20nm for the case where the free space propagation is not included.

Since the spectral width scales quadratic with wavelength, the period of the spectral features should also scale quadratic. The exact period of the spectral features does not have to be identical to the 50% spectral width of the speckles. It can be expected that the period is a few times larger. Not every speckle movement results in a speckle walking in or out of the detection area.

Measurements using polarization filters in the beam revealed that the effect of polarization is either nothing, or a reduction of the SFA by a factor of square root of two. For an aluminum diffuser polarization has no effect. This is due to the fact that a polarized beam is not depolarized by an aluminum diffuser. The same holds for the QVD. This diffuser does also not alter the state of polarization. For a volume diffuser like Spectralon it was found that the reduction of a square root of two holds. Spectralon was found to scramble the state of polarization. The factor of a square root of two is valid since we have now two independent, non interfering speckle patterns that yields thus a reduction in SFA by the square root of two.



Figure 5 Spectral width of the speckles as a function of wavelength

The inner pixel averaging effect results in a reduction of the SFA that depends on the number of spectral features periods within the bandwidth of a single pixel. Since the period scales quadratic with wavelength the averaging reduces with wavelength. A calculation that was performed to get insight in the averaging effects within a pixel resulted in the graph shown in Figure 8. Figures 6 and 7 show calculated and measured normalized spectra, respectively. From these figures the change in period with wavelength can clearly be seen, as well as the increase in amplitude with wavelength.



Figure 6 Calculated spectral data after normalization.



Figure 7 Measured normalized data.



Figure 8 SFA as simulated to show the effects of inner pixel averaging.

The first band in Fig.8 pertains to the prism dispersed band. For this band the band width per pixel increases with wavelength. The two other bands pertain to grating dispersed bands. For these bands the band width per pixel is constant. The amplitude of the spectral features was taken to increase linear with wavelength while the period scaled according to a quadratic function. Comparison with Fig.7 shows that the measured SFA scales similar to this simulated

graph, indicating that inner pixel averaging is real. For the simulations used to obtain Fig.6, a cosine like function, with changing amplitude and period was modeled and the integral was taken over changing intervals. For fully resolved measurements the SFA should be a linear line that passes through the origin. All fits shown in the measurements results indicate that due to averaging the zero crossings takes already place between 100 and 200 nm, a clear indication for inner pixel averaging.

The coherence effects are only important for the QVD and real volume diffusers. This means that QVD and volume diffusers will also perform better in terms of reducing SFA values. These averaging effects have been modeled in the case of real volume diffusers by applying a scaling factor that is equal to the square root of the number of independent speckle patterns. This number is found by dividing the penetration depth of the light into the diffuser by the coherence length. For QVD the modeling is different. Here the coherence function is calculated to obtain the degree of interference between the contributions from the different surfaces. For a QVD a thickness that is small with respect to the coherence length the coherence function will yield unity while for thicknesses larger than the coherence length the coherence function reduces to zero.

A final modeling step that still has to be implemented are the averaging effects due to the angular extend of the light source. The idea is to calculate the angular change in the illumination beam that is required to get a non correlating speckle pattern with respect to a pattern calculated prior to the angular change. Once this angle is known the full opening angle of the illumination beam can be divided into a number of sub beams that each create an independent speckle pattern. The total averaging effect is than equal to the square root of the result of that division.



Figure 9 Simulated spectral features spectrum. (left hand side image)16 sampling points per nm along the x-axis. The pertaining SFA is 4.5%. (right hand side image) One sampling point per nm along the x-axis. The pertaining SFA is 11.8%.

Figure 9 shows results obtained from simulations. In these spectra all features can be seen that are also observed in measured spectra. The fast oscillations (not fully resolved by the chosen sampling in Fig.9, left hand side) is what is currently understood as the effect of a speckle moving into or out of the detection area. The detector measures above this fast oscillation also a slower oscillation. This slower oscillation is also seen in the simulations. These slow oscillations are also spectral features, i.e. they are also due to the speckle effects. It is our current understanding that the slow modulations are not due to single speckle events, but to more than one speckle events. If for instance 20 speckles are present in the entrance slit of the spectrometer (or on a detector pixel), one speckle extra or less would yield an intensity change of 5%. If one speckle were to move out for a longer time (i.e. for a wider spectral range), another speckle moving in or out of the detection area would yield an intensity change of about 5% on a 5% offset due to the already missing speckle. These offsets are expected to be the origin of the slow oscillation.

The simulated spectra in Fig.9 show that the SFA scales linear with the wavelength and that the period of the oscillations increases with wavelength. A better linear increase with wavelength is obtained by averaging out many spectra. The exact relation between period of the features and the wavelength can not be given from these spectra. For the calculations at the larger wavelength we have reduced the sampling by a factor sixteen while the wavelength was increased by a factor of four. This quadratic scaling was chosen on the basis of Figure 5.

6.1 Spectral Features Reduction

In this paper several mechanisms have been mentioned that can be used, or are always present, to reduce the amplitude of the speckle induced wiggles in the spectra. This section will give a short resume of the before mentioned techniques.

6.1.1 Angular extend

The angular extend of the light source used yields a number of independent speckle patterns. The extend of the sun is for instance already 0.5 degrees. The speckle patterns are independent when their contributions do not interfere and when the speckle patterns have no correlation. This mechanism for SFA reduction is always present but can be optimized by choosing the proper diffuser and optical arrangement. Longer optical paths and a QVD or volume diffuser will lead to a stronger reduction based on angular averaging.

6.1.2 Number of speckles per detector pixel

The SFA scales inversely proportional with the number of speckles per pixel. This means that increasing the size of the pixels, or reducing the size of the speckles will help reducing the SFA.

6.1.3 Polarization

Since two orthogonally polarized beams can not interfere, these two beams will result in two independent speckle patterns. This will yield a reduction by the square root of two. Since the polarization state of the light source is in general a given fact the only extra reduction that can be achieved is by choosing a diffuser that will scramble the polarization state. In our research only Spectralon showed polarization scrambling.

6.1.4 Movements

The speckle pattern will change strongly by a translation and/or rotation of the diffuser. These movements are therefore a very useful tool to reduce the SFA. If during a recording of the spectra the diffuser is being moved, the speckle pattern will smear out and will thereby be reduced in contrast. This is a very strong method to reduce the SFA. The drawback is that an actuator has to be implemented in the setup. One standard movement is to use a longer integration time, since the sun will move with respect to the satellite.

6.1.5 Pixel bandwidth

The spectral features have apart from their amplitude also a period. It was found that depending on the mode in which the diffuser is used the period can be smaller than the spectral bandwidth of the detector pixels. This leads to an averaging within the pixels. This averaging method can be optimized by increasing the bandwidth of the pixels. This is directly a degradation of the achieved resolution and therefore not a good approach. The alternative is to optimize the optical arrangement to decrease the period of the spectral features. The present tendency is to design spectrometers with reduced spectral bandwidths per pixel.

6.1.6 Diffuser

The type of diffuser is the most straightforward means to influence the spectral features. An aluminum diffuser will in general produce far stronger features than a volume diffuser or a QVD. QVD is in particular very good in reducing spectral features for illumination sources with a 'large' opening angle. Both QVD and the real volume diffusers can be used advantageously for small coherence lengths. These coherence lengths pertain to the bandwidth for each pixel on the detector.

6.1.7 Optical arrangement

That the optical arrangement can be optimized to reduce the SFA is more or less obvious. This arrangement dictates the size of the speckles and hence the number of speckles per detector pixel. It also defines the period of the spectral features and therewith the averaging within a detector pixel. And finally, the averaging due to the opening angle of the illumination source is, amongst others, determined by this arrangement.

CONCLUSION

It has been shown that spectral features can be fully explained by speckle theory and that speckles have therefore to be seen as the source of spectral features. A single quantity has been introduced, the SFA (spectral features amplitude), that can be used to arrange different diffusers in terms of spectral features reduction capabilities. A special setup has been presented together with results obtained using this setup. The MatLab program that has been written for the modeling of spectral features has been mentioned and results using this program in the field of the spectral width of speckles, the inner pixel averaging, and actual spectra have been shown.

In the final section a summary has been given for all methods that can be used to reduce the spectral features. These suggestions should be kept in mind while designing a new satellite based spectrometer.

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