Providing uncertainty estimates of the Sentinel-2 top-of-atmosphere measurements for radiometric validation activities

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ABSTRACT
As part of the Sentinel-2 mission, a Radiometric Uncertainty Tool (RUT) has been recently released to the community. This tool estimates the Sentinel-2 radiometric uncertainty associated with each pixel in the top-of-atmosphere (TOA) reflectance factor images provided by the European Space Agency (ESA). The use of such information enables users to assess the “fitness for purpose” of the data to their specific application. The work described here summarises the efforts and results of integrating the RUT for radiometric validation activities for the Sentinel-2 mission. Starting from the results provided by the RUT, the focus will be on providing a methodology to calculate the uncertainty associated with the mean TOA reflectance factor in a Region of Interest (ROI). Two different methods – one simple method directly using the RUT and a more rigorous one based on Monte Carlo method (MCM) propagation – are proposed and compared. These two methods focus on the effect of the spectral, spatial and temporal correlation of the errors in different ROI pixels and the impact of correlation on the uncertainty associated with the mean TOA reflectance factor. The study has also considered the impact of uncertainty contributions not included in the first version of the RUT.

Introduction

The first version of the Sentinel-2 Radiometric Uncertainty Tool (S2-RUTv1) provides calculations of the uncertainty per pixel of the S2 Level-1C (L1C) top-of-atmosphere (TOA) reflectance factor images derived from the multi-spectral imager (MSI) on-board S2. Such pixel-level uncertainty information can be directly applied as a quality indicator of the S2 L1C products.

However, when propagating pixel-level TOA radiance or reflectance factor products to higher levels in a processing chain, this pixel-level radiometric uncertainty must be treated carefully. Many applications of higher-level products aggregate data from different pixels in space and/or time using a simple, or a weighted, mean. To determine the uncertainty associated with the mean, it is not sufficient to know the uncertainty associated with a single pixel value; it is also necessary to consider whether there are systematic effects leading to common errors between different pixels. Similarly, higher level products also often involve combining data from different spectral bands. Again it is essential to understand whether there are systematic effects leading to common errors between different spectral bands.

In this paper we consider ways of estimating the error correlation structure in spatial, temporal and spectral dimensions. This case study is based on different regions of interest (ROIs) used in the radiometric validation of S2. This case study was chosen because it is a direct application of L1C products and their uncertainties and is of current interest.

Radiometric validation is a process that involves comparing the instrument under test with another reference measurement or model of the TOA radiance/reflectance factor. When both the instrument under test and the reference have an associated uncertainty estimate, it is possible to validate the test instrument’s uncertainty analysis using the performance criterion that the two should agree within their combined uncertainties (usually at the 95% confidence interval).

In order to reduce the effects of noise and/or to allow comparisons of sensors to references with a different spatial pixel size, such comparisons are usually performed by averaging over a specific ROI to obtain a “ROI best estimate”. This ROI is selected on the basis of certain criteria, such as a minimum site uniformity and viewing angle dispersion.

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1The version used here is S2-RUTv1.1 released on 23 June 2017 and accessible by J. Gorroño, Fomferra, and Peters (2016).
This manuscript defines a method for using the S2-RUTv1 that can provide an uncertainty estimate of the mean of the ROI for radiometric validation purposes. In “Concept of study, the limitations and the methodology”, we describe the concepts behind estimating the uncertainty associated with the ROI mean. We consider correlation in spatial, temporal and spectral dimensions and show both a robust Monte Carlo Method (MCM; BIPM et al., 2008b) and how an estimate of correlation can be obtained using the existing S2-RUTv1 by selecting and deselecting different uncertainty components. The Section “Qualitative assessment of the pixel-to-pixel correlation: Spectral, spatial and temporal dimensions” discusses the different sources of uncertainty in turn and considers error correlation structures in spatial, temporal and spectral dimensions. There are uncertainty effects that were not included in the S2-RUTv1 (Gorroño, Fomferra, et al., 2017); the Section “Impact of non-included contributors in a calibration site” discusses how significant these effects may be in determining the uncertainty associated with the mean value of a ROI. Finally, “An approximation to the ROI pixel mean uncertainty using the S2-RUTv1” provides an example for three locations used in radiometric validation of S2: the radiometric calibration network (RadCalNet) site at Gobabeb, the Boussole ocean buoy site and deep convective clouds (DCCs).

Concept of study, the limitations and the methodology

Error, uncertainty and correlation

The S2-RUTv1 provides users with the S2 L1C radiometric uncertainty per pixel. This radiometric uncertainty expresses the degree of doubt around the TOA reflectance factor measured at each pixel or, an interval around the TOA reflectance factor that encompasses a certain fraction of the distribution of values that could be attributed to the measured quantity (BIPM et al., 2008a). The actual error for a single pixel, that is the measured value minus the true quantity value (BIPM et al., 2012), is unknown, but is drawn from the probability distribution described by the uncertainty. In practice, the uncertainty (and resultant error) is caused by the combination of individual uncertainties associated with different effects, which are combined to provide an overall uncertainty.

Although we cannot know the error associated with any given effect for a given pixel, we can evaluate whether that error is likely to be the same for different pixels, times or spectral bands. It is this common error that creates error correlation.

Uncertainty over a ROI pixel mean

The direct results of the S2-RUTv1 cannot be directly used to determine the uncertainty associated with a ROI pixels’ mean. Neither the mean of the pixel uncertainties nor the standard deviation of the mean uncertainty represents a general scenario. Indeed, these two cases would correspond to the boundary scenarios where all pixels and contributions to the L1C radiometric uncertainty are positively correlated and fully uncorrelated respectively.

Consider the mean of 2 pixels that are scanned at two consecutive lines; effectively a $2 \times 2$ ROI. The equation to obtain the mean of the ROI pixels $\rho_{\text{ROI}}$ is

$$\rho_{\text{ROI}} = \frac{1}{4} (\rho_A + \rho_B + \rho_C + \rho_D)$$

where each term $\rho_i$ represents a pixel indexed in the spatial (across track) and temporal (along track) dimensions.

According to the matrix-form of the Law of Propagation of Uncertainty (BIPM et al., 2008a), the variance associated to the term $\rho_{\text{ROI}}$ is given by

$$u^2_{\text{ROI}} = C^T U C$$

where the vector of sensitivity coefficients, $C$, is given by

$$C = \begin{pmatrix} \frac{\partial \rho_{\text{ROI}}}{\partial \rho_A} & \frac{\partial \rho_{\text{ROI}}}{\partial \rho_B} & \frac{\partial \rho_{\text{ROI}}}{\partial \rho_C} & \frac{\partial \rho_{\text{ROI}}}{\partial \rho_D} \end{pmatrix}^T$$

and the covariance matrix $U$ is given by combining a vector of individual uncertainties $V$ with a matrix of correlation coefficients $R$, through

$$U = V R V^T$$

The matrix operation in Equation (2) can be rewritten as

$$u^2_{\text{ROI}} = \frac{1}{16} \left[ u_A^2 + u_B^2 + u_C^2 + u_D^2 \right]$$

$$+ \frac{1}{16} \left[ u_A u_B r_{AB} + u_A u_C r_{AC} + u_A u_D r_{AD} + u_B u_C r_{BC} + u_B u_D r_{BD} + u_C u_D r_{CD} \right]$$

The terms in $V$, providing the uncertainty associated to each pixel, can be directly obtained by running the S2-RUTv1. However, the correlation terms, in $R$, cannot be directly obtained. Indeed, the level of correlation between pixels will depend on the scene type and/or the acquisition time.

For example, pixels measuring an ocean scene are expected to be largely uncorrelated due to the dominance of instrument noise over such low radiance.
scenes. On the other hand, pixels in a bright cloud scene will be highly correlated due to the dominant effect of systematic errors from a common calibration.

Thus, the pixel correlation in \( R \) is a consequence of the balance between the different uncertainty contributors of the S2 L1C uncertainty. To understand common effects, and hence the correlation coefficient for a particular scene, we have to consider the instrument characteristics and ground processing.

**Spatial, temporal and spectral dimension of the S2 MSI**

The focal plane of the S2 MSI instrument consists of 12 detectors in staggered formation. Figure 1 presents a schematic of the S2A VNIR focal plane.

Each detector contains several lines of pixels, each of which have a filter on top, which defines the spectral band of each detector line. For the SWIR bands, several such detector lines are combined with Time Delayed Integration (TDI). Each detector line has a total of 1296 pixels for the 10 m bands and 2592 for the 20 m and 60 m bands. The 60 m bands are obtained by spatial binning of the original 20 m pixels.

Thus, the spatial dimension is defined by the across-track (ACT) dimension of the focal plane and the temporal dimension is the result of the successive acquisitions of the pixels in combination with the satellite motion. The spectral dimension is defined by the spectral lines on the detector.

The effects of TDI and spatial binning will not be considered further since these processes are performed during the ground processing and the performance parameters, such as the instrument noise parameters or quantisation level, already include these effects. The discontinuity between detectors has an impact on the viewing angle continuity or the correlation between pixels. The ROIs studied here comprise a small fraction of the detector and are considered to be included in just one detector.

It is important to note that the discussion here does not fully account for the orthorectification process applied to the S2 Level-1B (L1B) products. The L1C products provide radiometrically corrected imagery with digital numbers (DN) proportional to TOA radiance values and in sensor geometry (ESA, 2017). This process consists on a B-spline interpolation of the L1B DN prior to their conversion to reflectance factor. This process fits the measurements onto an Earth grid that accounts for an elevation model with equally spaced sampling in Universe Transverse Mercator (UTM) coordinates.

As a result, the S2 L1C products do not keep the original spatial and temporal focal plane dimensions. However, in the absence of more detailed information, the North-up orientation of the L1C products is used to approximate the temporal dimension (North–South) as well as of the spatial dimension (East–West). This simplification is reasonable as the S2A orbit is a near-polar orbit with a 98.62° inclination.

**An approximation method: “select/deselect”**

The “select/deselect” method uses the capability of the S2-RUTv1 to generate uncertainty images for selected uncertainty contributors to estimate the total uncertainty of the average reflectance of a ROI.

In this approach we assign each effect to being either correlated (not reduced by averaging over the ROI), or uncorrelated (reduced by averaging over the ROI) and select only the correlated effects, assuming that the uncorrelated effects become negligible at the scale of the ROI. Each effect is discussed in the Section “Qualitative assessment of the pixel-to-pixel correlation: Spectral, spatial and temporal dimensions”, which describes how decisions were made. Note that effects may be correlated in one dimension (e.g. spatial) and uncorrelated in another (e.g. temporal or spectral). The associated correlation should be evaluated experimentally if feasible by studying the combined variations of the quantities or using any available additional data pertaining to their interrelationship. Additionally, in the absence of available data, information based on experience and general knowledge can be utilised (BIPM et al., 2008a). For the study

![Figure 1. VNIR focal plane schematic description. The image is reproduced with permission from Gascon et al., 2017.](image-url)
in this paper, the correlation will be based mostly on the latter method with the intention that, with access to further information and/or experimental data, a refinement of the values can be undertaken.

The method named “select/deselect” is intended to be as simple and quick as possible for the S2 L1C data users. In this method, the user interface incorporates a tick option to select individual effects, as shown in Figure 2.

The user just need to select the appropriate uncertainty contributions based on the correlation results that can be found below in Table 1. The mean value of uncertainty over a ROI in the output image can now be taken as an estimation of the uncertainty associated to the mean of TOA reflectance pixels in a ROI. The approach is very simple but has several limitations. For example, for ROIs of just a few pixels, the assumption that the random effects become insignificant may not be sufficient. Thus, this method must be tested to understand the validity of the ROI size at which this assumption is valid. The method also does not provide flexibility to cope with situations where the effect cannot be considered either perfectly correlated or perfectly uncorrelated. In such cases, the method has been adapted to produce two uncertainty images with the partially correlated contributions selected and deselected. The result is taken as the mean of the two ROI pixels for the two images.

**MCM propagation**

In order to understand the potential limitations of the approximate approach, a comparison was made with a more rigorous method based on MCM propagation. The MCM determines the mean TOA reflectance factor for a ROI from the pixels over many iterations. At each iteration, the error associated with the reflectance factor is drawn from the distribution of each uncertainty contribution. If the uncertainty contribution is correlated between the pixels, the same sample is used for all the pixels in the ROI, whereas, if the uncertainty contribution is uncorrelated, a different error is drawn from the distribution for each pixel. Where there is partial correlation, two separate errors are drawn, one that is common to all pixels and one which is different from pixel to pixel. The distributions are set as normal or uniform distributions with a spread of values directly linked to the uncertainty as calculated directly from the S2-RUTv1. This uncertainty is obtained by generating an image of the specific uncertainty contribution. The method is illustrated in Figure 3.

The errors $\delta_{\text{corr}, i}$ and $\delta_{\text{uncorr}, i}$ in Figure 3 represent the two extreme cases for correlated and uncorrelated pixel errors. An error generated at the MCM propagation for a pixel $i$, uncertainty contribution $j$ and iteration $t$ can be mathematically written in a generic form as

![Figure 2. Image of the S2-RUTv1 dialog box with the tab “processing parameters” selected. This tab permits the selection and deselection of each uncertainty contribution.](image-url)
\[
\delta_{t,ij} = \alpha \cdot u_{RUT}^{ij} \cdot x_{ucorr}^{ij} + (1 - \alpha) \cdot u_{ucorr}^{ij} \cdot x_{ucorr}^{ij}
\]

where \(x_{ucorr}^{ij}\) are samples out of the normal \(N(0,1)\) or uniform distributions \(U(-1,1)\), \(\alpha\) denotes the weight of the uncorrelated components, and \(u_{RUT}^{ij}\) denotes the uncertainty in the reflectance factor for the pixel \(i\) and uncertainty contribution \(j\) obtained using the S2-RUTv1 (that is the standard deviation of the distribution from which the error is drawn).

The factors \(u_{ij} \cdot x_{ucorr}^{ij}\) and \(u_{ij} \cdot x_{ucorr}^{ij}\) represent the error at each Monte-Carlo iteration due to an individual effect and for an individual pixel. This effect may be fully correlated, giving the same error in each pixel, in which case \(\alpha = 0\). Alternatively, it may be fully uncorrelated, giving an independent error for each pixel, in which case \(\alpha = 1\). Intermediate cases are also possible.

**Qualitative assessment of the pixel-to-pixel correlation: spectral, spatial and temporal dimensions**

This section describes each one of the uncertainty contributions integrated in the S2-RUTv1. A full description of how these are determined is given by Javier Gorroño et al. (2017). Here, the description is focused on the correlation structure.

\[ u_{\text{noise}}: \text{instrument noise} \]

The instrument noise model is characterised in-flight by the calculation of the variance of dark signal (DS) and diffuser measurements. The noise model takes the DS standard deviation as the instrument noise in the absence of light. This model is scaled by the diffuser variance – see Javier Gorroño et al. (2017) – under the assumption that the increase of the noise with the light intensity is linear to the variance as if dominated by the photon shot noise.

In the temporal domain, the instrument noise can be considered completely uncorrelated between the acquisition lines. This point has been demonstrated (Javier Gorroño, Gascon, and Fox (2015)) for the S2 DS measurement using the Allan deviation (Allan, 1966, 1987), which disentangles higher and lower frequency components of the noise and provides an estimate of the upper bound of independent samples. The results showed that for the VNIR bands the number of independent dark samples was well above 1000. For the SWIR bands the number of independent samples could be more variable with some pixels showing values as low as 500 independent samples. For the validation activities using RadCalNet sites, ocean or deep convective clouds, the amount of temporal lines required is well below any critical limit. For example, even for the largest

\[ \text{Table 1. Summary of pixel correlation for radiometric validation sites.} \]

| S2-RUTv1 uncertainty contributors | Spatial | Temporal | Spectral |
|----------------------------------|---------|----------|----------|
| Instrument noise, \(u_{\text{noise}}\) | 0       | 0        | 0        |
| Out-of-field stray-light – systematic part, \(u_{\text{stray_sys}}\) | 0       | 1        | 1        |
| Out-of-field stray-light – random part, \(u_{\text{stray_rand}}\) | 0       | 0        | 0        |
| Crosstalk, \(u_{\text{crosstalk}}\) | N/A     | N/A      | N/A      |
| ADC quantisation, \(u_{\text{ADC}}\) | 0       | 0        | 0        |
| Dark signal stability, \(u_{\text{DS}}\) | 1       | 1        | 0.5      |
| Non-linearity and non-uniformity knowledge, \(u_{\text{gamma}}\) | 0       | 1        | 1        |
| Diffuser reflectance absolute knowledge, \(u_{\text{diff_abs}}\) | 1       | 1        | 1        |
| Diffuser reflectance temporal knowledge, \(u_{\text{diff_temp}}\) | 1       | 1        | 1        |
| Angular diffuser knowledge – cosine effect, \(u_{\text{diff_cos}}\) | 1       | 1        | 0.5      |
| Straylight in calibration mode – residual, \(u_{\text{diff_k}}\) | 1       | 1        | 0.5      |
| L1C image quantisation, \(u_{\text{L1C quant}}\) | 0       | 0        | 0        |

\[ \text{Figure 3. Schematic of the MCM propagation for the ROI mean uncertainty estimate.} \]
RadCalNet sites (1 × 1 km), the number of pixels in one dimension will be at most 100.

The VNIR detectors are monolithic complementary metal oxide semiconductor (CMOS) detectors, while the SWIR detectors are on HgCdTe detectors hybridised on a CMOS readout circuit (Drusch et al., 2012). This means that up to the pre-amp and voltage conversion, the noise is independent from one pixel to another. The voltage is further amplified at the front-end electronics (FEE) and video-chain unit (VCU). Thus, in the spatial and spectral dimension, the instrument noise can be considered independent between samples under the assumption that noise introduced by the post-amplification is not dominant. Note that at the FEE and VCU units, the coupling between signals may exist. This is independently accounted for at the sub-section $u_{xtalk}$: crosstalk.

$u_{stray sys}$: out-of-field stray-light – systematic part

The uncertainty contribution due to out-of-field straylight is added linearly in the proposed S2 L1C uncertainty budget in Javier Gorroño et al. (2017).

The straylight generated by the Earth out-of-field contribution might vary due to the variation of the scene during the orbit. However, for any level of stray-light experienced, the result will be largely homogeneous over the VNIR and SWIR focal planes. The mirrors and splitter reflections tend to spread the stray-light entering the MSI instrument. The effect also does not arise from one source point but from a more extended source at each side apart from the focal plane, which further spreads the stray-light across the focal planes. The filters generate other non-uniform stray-light events such as ghosts that are accounted for in a case-by-case basis and are avoided or minimised for validation activities (e.g. by discarding products with a large extent of clouds in the ROI pixel vicinity).

A global figure of 0.3% of the reference Earth radiance will be used as a ROI mean error. The uncertainty combination in the work by Javier Gorroño et al. (2017) proposed a linear combination as a result of non-corrected systematic effect. This uncertainty is considered appropriate for land validation areas where the vicinity of the swath is expected to be dominated by land. However, the error estimate might be conservative for ocean measurements if the vicinity of the swath is dominated by a land scene.

$u_{stray rand}$: out-of-field stray-light – random part

The random component of straylight (i.e. that which varies across the focal plane) is produced by the lack of light tightness of the focal plane.

In the spatial dimension the effect is considered as fully uncorrelated. Experimental results in laboratory found out that the level was varying randomly from pixel-to-pixel in the ACT dimension.

In the spectral dimension, the effect is largely uncorrelated since the light tightness effect will vary between band detector lines, it can be considered independent.

However, in the temporal dimension the effect is largely correlated as the radiometric validation images are taken over uniform scenes. Very similar illumination conditions apply and, thus, very similar levels of light tightness for the same pixel are expected over the temporal scan lines.

$u_{xtalk}$: crosstalk

The contribution for crosstalk arises from the electrical signal coupling between spectral bands. The effect has an impact in the TOA radiometric performance for the SWIR bands. Due to the absence of a correction at the time of releasing the S2-RUTv1, the approach was to include the worst figures of contamination between bands (Javier Gorroño et al., 2017). However, a correction is now applied to S2 L1C images for this effect with the deterministic nature of the correction justifying a low correction residual hence this effect is not considered further here. Furthermore, the radiometric validation exercise presented here is carried out over uniform scenes which have been chosen to avoid nearby clouds (except for DCC methods).

$u_{adc}$: analogue-to-digital conversion quantisation

The analogue-to-digital (ADC) conversion at the VCU units has been modelled as an error distribution with an amplitude of 1/2 Least Significant Bit (LSB) and rectangular distribution.

This uncertainty is expected to be uncorrelated in the spectral, spatial and temporal dimensions; however, there are two possible problems with this assumption. First, the ADC conversion is shared at the VCU unit for several channels; however, this does not affect the uncorrelated nature of the uncertainty if the ADC does not introduce a large systematic effect. Second, the radiometric validation sites are selected on the basis of a radiometric uniformity and this could result in a correlated rounding between pixels in the temporal and spatial dimensions. Fortunately, the digitisation is performed with 12 bits meaning that even small scene variations represent a large variation in terms of LSB units.

$u_{ds}$: dark signal stability

The VNIR focal plane is not temperature controlled and an approximation for the variations with
temperatures can be described as follows (Hopkinson, Goodman, & Prince, 2004):

\[ DS(T_0 + \Delta T) = DS(T_0) \cdot e^{\frac{\Delta T}{C_0}} \]  

(7)

The HgCdTe detectors are passively cooled due to the larger sensitivity of the DS with temperature variations (Dariel et al., 2009). In addition, the offset level for the SWIR region could be marginally affected by the residual thermal emission.

The validation activities using RadCalNet sites, ocean or DCCs require the reading of a small fraction of pixels in the detector. In this situation, it is plausible to assume that the temperature gradient in the selected pixels will be very low and, if any thermal emission effect exists, it will be similar in the local vicinity. Thus, the DS stability is expected to be correlated in the spatial and temporal dimensions.

In the spectral dimension, the temperature variations cannot be assumed as perfectly correlated as the spectral lines are physically separated in the detector – or integrated in different VNIR and SWIR focal planes – and gradients of temperature along the detector could occur. In that case, a correlation of 0.5 can be considered.

\( u_{\text{gamma}} \): non-linearity and non-uniformity knowledge

The knowledge over the non-linearity and non-uniformity correction \( \gamma(p,b,d,Y(p,l,b,d)) \) is given as 0.4% for the S2-RUTv1 (Javier Gorroño et al., 2017).

Since all the pixels in the ROI measure a similar radiance level at calibration sites, the non-linearity estimate can be considered highly correlated over the spatial and temporal dimension. In the spectral dimension; assuming that the pre-flight characterisation is dominated by drifts and correlated sources in the spectral dimension (Gardner, 2004), a spectral correlation is assumed here too.

The knowledge of the non-uniformity correction is largely limited by the focal plane noise (FPN). The residual after this correction has a random nature across the field-of-view. Thus, in the spatial dimension its effect is uncorrelated between pixels. The same parameters and similar radiance levels are measured between pixels in the temporal dimension and, thus, can be assumed as correlated error. The non-uniformity correction residual for different pixels in different spectral lines must be considered as partly correlated since the residual is not expected to be proportional on a one-to-one pixel basis but lower frequency components are expected to be largely correlated.

Depending on the validation scene (e.g. level of radiance), either the non-linearity residual or non-uniformity residual will dominate the uncertainty contribution. The final correlation figures showed in Table 1 are set as an intermediate case with the expectation that in future refinements a separate uncertainty for the non-linearity and non-uniformity can be assessed.

\( u_{\text{diff.abs}} \): diffuser reflectance absolute knowledge

The diffuser reflectance factor is obtained through a complex process which involves the interpolation and/or fitting of on-ground measurements and its convolution to account for a different pupil projection of the on-ground measurements and the MSI measurements and is reported by Mazy et al. (2013).

The bidirectional reflectance factor (BRF) uncertainty accounts for several separate effects: BRF absolute characterisation knowledge, BRF spatial knowledge, polarisation effect, diffuser illumination and viewing angle knowledge, and other effects – e.g. thermal cycling impact (Javier Gorroño et al., 2017).

The BRF absolute characterisation is dominated by systematic effects that are translated in a correlated nature between pixels. The propagation of the radiometric standards through the traceability chain includes contributions associated to long-term drifts. As a consequence, the BRF absolute characterisation is expected to be dominated by systematic effects that are largely correlated in the spectral domain (Gardner, 2004).

For two pixels separated by a small distance in the focal plane, the pupil projections on the diffuser overlap significantly (the pupil projection is shown in Mazy et al. 2013). Consequently, effects such as uniformity and polarisation error will be correlated between the ROI pixels. Similarly, the BRF angular knowledge is correlated due to the similarity in the viewing angle between pixels separated by a small fraction of the focal plane.

Based on the previous reasoning, this contribution is considered correlated for the ROI pixels (spatial and time dimensions) and between the bands (spectral dimension).

\( u_{\text{diff.tmp}} \): diffuser reflectance temporal knowledge

This contribution is also considered as a linear addition by Javier Gorroño et al. (2017) as for the section \( u_{\text{stray.syn}} \): out-of-field Stray-light – systematic part.

In this specific case, the error estimate was based on a dedicated on-ground qualification programme (J. Nieke, personal communication, 3 August 2017). Further, in-flight experience with similar diffuser material indicates a comparable degradation estimates as described for the MERIS instrument by Delwart and Bourg (2011) allowing an interpolation to the S2 acquisition timestamp. The degradation rate for the pixels in the ROI is expected to be very similar since, again, the pupil projection of the ROI pixels is
very similar and any rate gradient will be negligible. Thus, the estimated error for this contribution can be also considered as the mean error over the ROI.

\( u_{\text{diff, cos}}: \text{angular diffuser knowledge – cosine effect} \)

The angular knowledge over the cosine correction is limited by the diffuser planarity or lack of knowledge of the diffuser angular coordinates. The error from the measured value between two pixels in the selected ROI will be of similar level and sign since the pupil projection of two pixels in a ROI and across different bands is shared at a large extent for a small ROI (similar discussion in section \( u_{\text{diff, abs}}: \text{diffuser reflectance absolute knowledge} \)). Therefore, the uncertainty is largely correlated between pixels in any of the three dimensions.

\( u_{\text{diff, k}}: \text{straylight in calibration mode – residual} \)

This contribution arises from the imperfect knowledge of a bias correction due to the multiple reflections of the Sun and Earth illumination introduced during the Sun diffuser calibration. The bias has been estimated at 0.7% of the calibration radiance level for all bands – see (Gascon et al., 2017) – and a conservative residual of 0.3% has been associated to the correction knowledge (Javier Gorroño et al., 2017).

The stray-light during calibration has been characterised both in absolute terms and also in terms of its uniformity level across the focal plane. Similarly to the contribution in \( u_{\text{stray, sys: out-of-field Straylight – systematic part}} \), the combination of rays tends to homogenise the effect across the focal plane. The major source of stray-light in this situation is the Sun that can be largely considered as a point source. Nonetheless, since the contribution arises after the multiple reflections from the Calibration and Shutter Mechanism, the effect must be considered as the combination of several scattered rays entering the optical system. Nevertheless, this type of residual is not directly accounted for by the absolute calibration coefficient \( A(b) \) but as part of the FPN noise at the non-uniformity correction in \( y(p,b,d,Y(p,l,b,d)) \) (see section \( u_{\text{gamma: non-linearity and non-uniformity knowledge}} \)). With a conservative residual of ±0.3%, the differences in the focal plane cannot be considered the dominant limitation of the correction knowledge but the absolute characterisation of the stray-light levels. Furthermore, if the ROI used for validation is at 1 x 1 km or smaller, these variations will be even lower. Thus, it is justified to assume that the uncertainty residual will be largely correlated in the spatial dimension as a consequence of a “common” absolute error.

In the spectral dimension, the residual is expected to be partly correlated. The use of a common bias for any of the 13 bands implies that the residual errors will fluctuate around a normal distribution with a scale of 0.3%. Between two spectrally adjacent bands, the fluctuation over the residual will be very similar. However, the more spectrally distant the bands are – e.g. B1 and B12 – the more uncorrelated the residual is expected to be.

In the temporal dimension, the stray-light residual is fully correlated since the effect applies to the calibration coefficient \( A_{\text{NTDI}} \) which is constant in this dimension.

\( u_{\text{ref, quant}}: \text{L1C image quantisation} \)

The L1C images of reflectance factors are codified in JPEG2000 format with a maximum number of 16 bits. The rounding effect has been discussed to be very low in relative units (<0.1%) except for very low reflectance values (e.g. ocean scenes). The nature of this uncertainty contribution is to be uncorrelated on a pixel-to-pixel basis.

Summary pixel correlation for validation sites

Impact of non-included contributors in a calibration site

This section considers the impact of uncertainty contributions that were not included in the S2-RUTv1 (Gorroño et al., 2017).

Deconvolution residual and other sources of straylight

The Point Spread Function (PSF) describes the response of the imaging system to a point source. The correction of the image for the PSF is planned as part of the S2 L1C processing but has not yet been implemented in the operational product.

The radiometrically uniform nature of validation sites largely minimises this effect because the signal that is lost by one pixel towards its neighbours is compensated by a gain from the neighbouring pixels’ optical path towards it. The same reasoning is applied for a diffuser calibration where the uniformity of the diffuser source minimises the internal straylight and only the out-of-field component must be accounted for (see \( u_{\text{diff, k: straylight in calibration mode – residual}} \)).

Ghosting effects due to the effect of crosstalk have been previously discussed in \( u_{\text{crosstalk}}: \text{crosstalk} \). However, a further source of ghosting can be identified due to the filter inter-reflections. This effect can be minimised when the ROI selected during validation is carefully selected to avoid images with high radiance clouds nearby.
Polarisation error

This is an error introduced by the sensitivity of the instrument to a difference in the light polarisation. If both the response of the instrument and the TOA signal are characterised for the polarised components of the light, this error can be corrected for. In the absence of such an information, it must be treated as an uncertainty contribution.

The polarisation sensitivity of the MSI instrument is <3% and the expected degree of polarisation (DoP) for scenes such as the RadCalNet Gobabeb site or the DCC is below 10%. However, for bands dominated by larger atmospheric components such as B1, the DoP could be significantly higher (Sun, Baize, Lukashin, & Hu, 2015).

For ocean scenes, the variations of DoP will be different with wavelength, angular configuration, as well as the scene characteristics such as wind speed or aerosols (Sun & Lukashin, 2013). Thus, depending on the previously mentioned factors, the polarisation error can range from an almost negligible to an important effect when close to the polarisation sensitivity of the instrument.

Orthorectification uncertainty propagation

This processing step is introduced at the S2 L1C products and has been discussed in section “Spatial, temporal and spectral dimension of the S2 MSI”. The radiometric interpolation has two effects on the S2 L1C radiometric uncertainty.

First, orthorectification will reduce the uncorrelated components of the TOA radiometric uncertainty (Javier Gorroño, Banks, Gascon, Fox, & Underwood, 2016). The impact on the uncertainty of a mean ROI however is that the uncertainty values will, in real terms, converge faster to a minimum value than the predictions using the S2-RUTv1.

Second, there is an uncertainty associated with the interpolation inherent in orthorectification. This is expected to be negligible for radiometric validation sites since the radiometric variations of these sites are expected to be low.

Non-uniformity spectral residual

The non-uniformity correction is updated by deploying the diffuser in-flight. There is a disagreement between the Sun spectral signature and the TOA spectral signature that introduces a systematic effect. A reference to the potential impact of this contribution can be found in the work by Barsi, Lee, Kvaran, Markham, and Pedelty (2014) for the Landsat-8 (L8) Optical Land Imager (OLI).

The results presented for both soil and vegetation show a spectral residual below 0.2% for any case and a root mean square (RMS) value below the 0.1%. Thus, for a similar sensor as the S2 MSI, the impact of this contribution is to be expected low. Nonetheless, a specific study for this effect is necessary that defines specific figures for this contribution.

Spectral knowledge

This contribution is the consequence of the imperfect knowledge of the spectral response characterised pre-flight and its potential variation during launch and once on orbit. The work by Javier Gorroño et al. (2016) presented a preliminary assessment for this effect. The results show that assuming a spectral response uncertainty of 0.2 nm \((k = 1)^2\) for systematic and 0.1 nm \((k = 1)\) for random spectral calibration knowledge, the dispersion of the data was below 0.3% using a desert site as example. Nonetheless, the study did not consider the equalisation (as part of the gamma correction) of the S2 L1C data and the impact of the pre-flight knowledge is expected to be significantly lower.

In the study to describe the potential impact of spectral variations, a spectral shift was added to the spectral response function bands of Sentinel-2. As indicative values, the degradation rates measured in-flight by the Spectroradiometric Calibration Assembly on-board the Terra MODIS mission (Xiong, Che, & Barnes, 2006) were used. The approximate values used for the S2 VNIR bands are: −0.33 nm (B1), −0.26 nm (B2), 0.04 nm (B3), −0.03 nm (B4), −0.05 nm (B5), −0.07 nm (B6), 0.1 nm (B7), 0.2 nm (B8) and −0.18 nm (B8A). The error in reflectance factor for all the bands was below the 0.1% with the exception of B1 which increased to 0.3%. The SWIR bands are not included since they represent a specific case where icing introduces an additional interference and specific evaluation is required.

As described in the section “Non-uniformity spectral residual”, the impact of these contributions is not expected to be significant for the uncertainty budget of most radiometric validation sites but they require a specific scene evaluation to provide quantitative figures and integrate them in future versions of the S2-RUTv1.

Geometric knowledge

Geometric knowledge describes both the impact of geolocation accuracy and the angular dispersion of the observed pixels in a ROI.
The geolocation knowledge results by Gascon et al. (2017) describe values either for refined or non-refined S2 L1C products below the 12.5 m \( (k = 2) \) specification. Recent work by Javier Gorroño et al. (2017) describes the impact of this uncertainty as a function of the geolocation knowledge for the Libya-4 and La Crau radiometric calibration sites. With the reported geolocation knowledge of the S2A L1C products the expected impact for the calibration sites is expected to be generally below the 0.1%.

A fair approximation of the angle dispersion of the pixels in a ROI can be obtained if a linear relationship is applied to the full swath angular dispersion. For a full swath, there are 14,376 pixels across 20 m bands – from Figure 1 (1296 pixels/detector = 98 blind pixels) \( \times \) 12 detectors. If a linear relationship is assumed, the 20.6° field-of-view of the instrument, a ROI of 20 \( \times \) 20 pixels of 20 m bands (the example represents a 400 m ROI) covers an estimated 0.07° peak-to-peak. Thus, the effect of this angle dispersion can be expected as negligible unless the target scene and the angular configuration is specifically affected by the BRDF hot-spot.

**An approximation to the ROI pixel mean uncertainty using the S2-RUTv1**

**Case study locations**

The study is performed over three different sites that correspond to different methodologies of TOA radiometric validation: the RadCalNet site at Gobabeb, the Boussole buoy site and DCCs. These sites have a different balance of uncertainty contributions and were chosen to determine how this changes the level of pixel correlation for each case. Here there is no discussion of the uncertainty associated to the validation methods themselves, simply the S2 MSI uncertainty estimates.

RadCalNet (www.radcalnet.org), once it becomes fully operational, will provide users with an operational (routine) service for nadir-view TOA reflectance factor data from several instrumented ground sites in the spectral region 400 nm to 1000 nm or 2500 nm, depending on available instrumentation. The site-measured surface reflectance and atmospheric data are propagated to TOA through a common processing chain by NASA-Goddard using MODTRAN (MODerate resolution atmospheric TRANsmission).

As part of the RadCalNet prototype phase, a new site is being established jointly between ESA, CNES and NPL near to the Gobabeb research station in Namibia (Bialek et al., 2016). The site is in the gravel plains at the edge of the Namib Desert and was chosen through an extensive search for a site with high spatial uniformity and stable atmospheric conditions on a flat location (Bialek et al., 2016). The ground-monitoring instrument installed at Gobabeb (in July 2017) on a 10 m high mast is an adapted CIMEL CE 318 BRDF 12-filter Sun Photometer which measures in 12 spectral bands from 414 nm to 1640 nm. The instrument takes measurements in a pre-determined sequence, scanning across the ground and sky. The data are processed by fitting the reflectance data to a BRDF Roujean model (Roujean, Leroy, & Deschamps, 1992) and extracting the nadir data to provide the surface reflectance for input to the RadCalNet portal (Meygret, Santer, & Berthelot, 2011).

The Boussole buoy site is a superstructure deployed in the deep waters (~2400 m) of the northwestern Mediterranean Sea (7° 54’ E, 43° 22’ N). It is composed of radiometers at above surface, 4 m, and 9 m depth and additional set of instruments as fluorometers or backscattering meters. All this instrumentation provides the necessary inputs to estimate the water leaving radiance and its further normalised water leaving reflectance. These quantities have been directly used for the vicarious radiometric calibration of satellite ocean colour sensors but are also applicable to the validation of Level-2 biophysical products and the long-term monitoring of ocean colour missions and site radiometric properties (Antoine, Guevel, et al., 2008; Antoine et al., 2008).

DCCs are very vertically extended and opaque clouds with very bright and cold tops close to the tropical tropopause. Their reflectance spectrum, after correction of stratospheric gaseous absorption if seen from space, is near lambertian and very spectrally flat in the VIS with amplitude primarily driven by cloud optical thickness. Their daily occurrence within the intertropical convergence zone as well as their large horizontal extent allows high rates of observation from remote sensing. DCCs are consequently often used as spectral invariant targets to monitor the radiometric response degradation of reflective solar bands of earth observation sensors (Fougnie & Bach, 2009; Lamquin, Bruniquel, & Gascon, 2018; Wang & Cao, 2016). MSI products containing observations of DCCs covering few to hundreds of kilometres can be extracted from a series of radiometric tests such as thresholding reflectance in water vapour absorption bands (especially B10, 1375 nm) to detect high opaque cloudy features (see Lamquin et al. (2018) for details).

**RadCalNet Gobabeb site case study**

For the RadCalNet Gobabeb site we selected a product with minimum cloud image percentage. The product corresponds to an overpass on 9 June 2017 and UTM tile T33KWP.

The ROI pixels were selected with centre at lat/lon \(-23.6°, 15.119°\) with a size ranging from one pixel up to 500 m. This ROI was also checked for any potential pixels masked as cloud, cirrus, no data or defective.
The results in Figure 4 show the evolution of the ROI mean uncertainty as a function of the ROI size as calculated using the MCM. The first point on the left side of the figure corresponds to the per-pixel uncertainty directly obtained from the S2-RUTv1.

The decrease of the uncertainty is in the range of 0.2–0.8%, depending on spectral band and the different correlation levels of different bands. For B1, the uncertainty only decreases by 0.1%; this is because this band has already been binned, for 3 × 3 20 m pixels, and the correlation between pixels is lower because of the low noise component – this band has reported SNR well above 1000 (Gascon et al., 2017). For all bands the uncertainty levels stabilised at around ROI sizes of 200 m or less.

Figure 5 presents the comparison of the results in Figure 4 versus the approximation method “select/deselect”.

Figure 4. Evolution of the ROI uncertainty (k = 1) with the ROI size for the RadCalNet Gobabeb site using the MCM technique.

Figure 5. Evolution of the difference between the MCM and select/deselect technique as a function of the ROI size for the ROI uncertainty (k = 1) of the RadCalNet Gobabeb site.
The results confirm an agreement between the two methods at the level of 0.1% above 200 m. A sensitivity analysis of the MCM method varied some of the contributions by adding (or not) a compensation of 0.05% to account for the truncation of images of the S2-RUTv1. This sensitivity study gave similar results to those in Figure 5 thus suggesting that the small level of disagreement between the methods may be produced by the truncation.

**Boussole site case study**

For this case study, the same criteria has been followed as for the “RadCalNet Gobabeb site case study”. The product selected here corresponds to an overpass on 28 March 2017 and UTM tile T32TMP. Figure 6 presents the uncertainty calculated by the MCM propagation for different ROI sizes at the Boussole site for the studied S2 bands. Figure 7 presents

![Figure 6](image6.png)

**Figure 6.** Evolution of the ROI uncertainty \((k = 1)\) with the ROI size for the Boussole site using the MCM technique.

![Figure 7](image7.png)

**Figure 7.** Evolution of the difference between the MCM and select/deselect technique as a function of the ROI size for the ROI uncertainty \((k = 1)\) of the Boussole site.
the corresponding agreement between the MCM propagation and the “select/deselect” approach.

For this site, the uncertainty decreases up to a larger ROI size compared to the RadCalnet Gobabeb case study. Figure 7 indicates that the stability is reached at around 400 m for all the studied bands. This is an expected result since at such a low radiance, the pixel reflectance factors contain a much higher uncorrelated component. The rise visible for B12 for a 50 m ROI is the consequence of the S2-RUTv1 truncation. The uncertainty maximum value is 25.5% (maximum is 255 in coded in a single byte) (Javier Gorroño et al., 2017).

Even for a large ROI, the uncertainties are higher compared to the RadCalnet Gobabeb case study. This is due to a large component from systematic out-of-field stray-light, which has been assessed as 0.3% of the reference radiance and which assumes a constant albedo of the Earth outside of the field of view. In an ocean site the radiance of the field of view can vary strongly. It is expected that the stray-light contributions of those scenes closer to the field of view have a larger impact than the ones further away. Figure 8 presents the sensitivity of the 500 m ROI uncertainty with variations in the out-of-field straylight from 0% up to 0.3% of the reference radiance.

The values in Figure 8 are provided in absolute reflectance factor with mean reflectance factor of the ROI pixels as follows: 0.12 (B1), 0.085 (B2), 0.048 (B3), 0.027 (B4), 0.022 (B5), 0.019 (B6), 0.016 (B7), 0.013 (B8), 0.012 (B8A), 0.0027 (B11) and 0.0015 (B12). The uncertainty levels in Figure 8 are small if compared to most of the measured TOA reflectance factors over land scenes. However, these levels become important for such low reflectance factor levels measured in water scenes.

Figure 9 shows the S2A overpass at the Boussole site obtained by the COVE tool (Kessler et al., 2013).

Figure 9 shows the large variation of out-of-field scene for an orbit of S2A over the Mediterranean sea. For the Boussole site, the immediate out-of-field scene is composed of water bodies; however, it is immediately afterwards dominated by land. The selection of the site just above or below can provide a completely different combination of out-of-field scene. In addition, the cloud coverage of the scene might further vary the levels. Thus, it is beneficial for the S2 radiometric performance over water scenes that more detailed predictions of the out-of-field straylight are set. This means a more detailed systematic error assessment – and, if possible, correction – dependent on the out-of-field scene distribution.

**Deep convective cloud case study**

The selected DCC product corresponds to an overpass on 21 December 2015 and UTM tile T51LVH. The DCC occupies almost the entire tile size and, for this example, the selected ROI corresponds to an approximate centre of the tile (precisely 11.383, 122.617 in lat/lon degrees).

The ROI uncertainty in this case converges quicker than in the previous cases and at a lower value. This
is the consequence of a lower relative uncertainty – i.e. as a percentage of the ROI mean value – due to the high radiance of the scene. Specifically, the remaining uncertainty is dominated by the diffuser calibration uncertainty.

DCCs are commonly used for inter-band monitoring and radiometric validation by exploitation of the spectral flatness (or whiteness) of their spectra. One reference band is supposed well calibrated so that the signal above the DCC (i.e. TOA corrected from stratospheric gas absorption) must be comparable from one band to this reference band. Per band deviation from this expectation, which is further refined using radiative transfer modelling of the clouds predicting the supposedly exact spectral shape, are then interpreted as inter-band calibration residuals. As an example here, the S2 bands are calculated as ratios of the B4 which is one of the band used as reference for MSI by Gascon et al. (2017) and Lamquin et al. (2018).

Figure 10 presents the uncertainty calculated by the MCM propagation for different ROI size at the selected DCC and for the studied bands. Figure 11 presents the corresponding agreement between the MCM propagation and the “select/deselect” approach.

Figure 12 presents the uncertainty associated to the ratio of each ROI-mean of the S2 bands with respect to the ROI-mean of B4. The results are
presented for all ranges of spectral correlation values of the diffuser calibration uncertainty $u_{\text{diff,abs}}$ as this is the dominant contribution.

The results show that the uncertainty associated with this ratio can be much smaller if the contribution due to the diffuser calibration is considered as largely correlated (as this is a ratio, the sensitivity coefficient is $-1$). For high spectral correlation of $u_{\text{diff,abs}}$, the ratio uncertainty is around the 0.5% for the VNIR bands whereas it increases up to 1% for the SWIR bands. Although the spectral correlation value of $u_{\text{diff,abs}}$ specified in Table 1 is set to 1, the actual correlation is expected to decrease the further apart the bands are spectrally. That is, spectrally closer bands (e.g. B3) might present a large spectral correlation while the correlation is lower for bands such as B11 or B12 which are in a different focal plane.

Figure 11. Evolution of the difference between the MCM and select/deselect technique as a function of the ROI size for the ROI uncertainty ($k = 1$) of the DCC site. The simulation used a spectral correlation of $u_{\text{diff,k}}$ of 0.5 and $u_{\text{diff,abs}}$ of 1.

Figure 12. Evolution of the ratio of ROIs uncertainty ($k = 1$) with the variation of $u_{\text{diff,abs}}$ spectral correlation for the DCC site using the MCM technique. The simulation used a spectral correlation of $u_{\text{diff,k}}$ of 0.5.
Discussion and conclusions

This study has defined a method to produce an uncertainty estimate associated to the mean TOA reflectance factor of the ROI pixels by using the S2-RUTv1. The method named "select/deselect" can be directly used by the S2 L1C data users and has been designed to be as simple and quick as possible.

The method has been compared with a more robust MCM propagation approach. The results showed, in general, that for ROI pixels above ~200 m (400 m for low radiance sites) the methods agree within 0.1%.

The correlation in the spatial, temporal and spectral dimensions has been extensively discussed in the section “Qualitative assessment of the pixel-to-pixel correlation: spectral, spatial and temporal dimensions”. For several uncertainty contributions just a qualitative assessment provides sufficient description of the correlation (e.g. instrument noise). However, for some uncertainty contributions, this qualitative assessment has not been sufficient and more involved studies are required. For example, Figure 8 has shown the importance of understanding the out-of-field straylight, particularly for ocean scenes. Nonetheless, it is also important to recognise that quantitatively describing the correlation of some contributions might be challenging where required data are nonexistent or for contributions that are complex.

In addition to the correlation assessment, it is important to analyse the effect of those uncertainty contributions that are not included in the S2-RUTv1. For the specific case of a ROI pixels under uniform sites, several of these contributions will have a small impact. For example, the ghosting effect produced by the filters is minimal or avoided by cloud screening the ROI pixels and the neighbouring area. Other effects such as the polarisation might have a larger impact for specific bands and angular configuration, particularly for ocean sites.

The results presented here have shown the importance of considering the pixel correlation for the ROI mean uncertainty.

The method here described can be applied to support the majority of S2 radiometric validation activities and can also be applied to other processing activities. For example, this same study is useful to determine the required binning in water applications and/or can be adapted to produce uncertainty estimates to S2 L1C spatially binned products.

The application to radiometric activities using Pseudo-Invariant Calibration Sites (PICS) would require further study. The assumption in this work is that the ROI pixels encompass one single detector. This assumption is not usually valid for PICS monitoring where the ROI pixels will be likely to be split in between detectors. In addition, the larger ROI size required means that some of the assumptions presented in the section “Qualitative assessment of the pixel-to-pixel correlation: spectral, spatial and temporal dimensions” might not hold validity. Therefore, for PICS more complex correlation structures are needed.

The development of the S2-RUT is an iterative process and as such, the intention of this work is to move forward towards new features and refinements from the S2-RUTv1 presented by Javier Gorroño et al. (2017). Here, the limitations, but also potential improvements, have been highlighted with the expectation that they will be revisited in future iterations. Furthermore, this work has the purpose of training the S2 users on how to use the S2-RUT uncertainty estimates in a final application. It is important that the community becomes familiar with these metrological concepts so that the tool can be successfully used and integrated in further processing applications.

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