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Interactive comment on "TanSat ACGS on-orbit spectral calibration by use of individual solar lines and entire atmospheric spectra" *by* Yanmeng Bi et al.

Yanmeng Bi et al.

qwang@cma.cn

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Discussion paper

Reply to interactive comments

September 2, 2020

Many thanks to the anonymous referee. These comments are very valuable and have greatly improved the quality of the manuscript. We have revised the manuscript following the comments.

General Comments

1. Abstract and introduction fall short in explaining the role of the two methods and to which kind of observation they are applied. Later in the manuscript it seems that Method 1 (using individual Fraunhofer lines) is applied to solar irradiance measurements only and allows the determinations of ground-to-orbit shifts and to monitor day to day variability as well as longer-term trends, and that Method 2 (using entire atmospheric spectra) is applied to Earth radiance measurements only and allows also the determination of intra-orbital variations. Please clarify this upfront, already in the abstract and the introduction.

Reply: We accept this very valuable comment and have revised the abstract and the introduction, where the role of the two methods and to which kind of observation they are applied are clarified.

2. It is stated that Method 2 is used for verifying Method 1 (Section 3.2) and that close

consistency has been found (abstract). Please clarify how this verification has been made and what exactly has been compared for this purpose. Have orbital averages from Method 2 been take for this? A figure with results from both methods depicted over the orbital phase would help to illustrate the level of consistency. Have longer time series of the two methods been compared? Please add such figures.

Reply: This comment and comment 1 make us further consider the role and relationship of the two approaches. As reference standards,the Fraunhofer lines possess much higher stability in nature than the synthetic spectra calculated by radiative transfer model (RTM). Therefore, the second method cannot be used to verify the first method. But, the second method can obtain the intra-orbit variation to complement the first one. We revised the 'verifying' to the 'complement' in abstract and section 3.2. In fact, for the assessment of the performance of ACGS, the first method is used as the main spectral calibration method because of its high accuracy and stability.

A simple comparison over Beijing in 2017 is performed for the two methods. We select these orbits according to some conditions. Only the cloud-free and clean scenes are selected because of the little aerosol effects. Dark ocean scenes are also excluded. Only 7 orbits are selected. We calculate the shifts in these orbits using the second method. Then the shifts in one orbit are averaged to obtain a shift. These averaged shifts are compared with those derived from the first method. For all field of view, the mean differences in O2A, WCO2 and SCO2 bands are -0.0017 nm, 0.0016 nm and 0.0020 nm, respectively. We add the figure of comparison. The intra-orbit shifts from the second method on 5 April 2017, is also provided as another case that is similar to that case on 23 April 2017 in Figure 10.

3. It is not clear whether the two spectral calibration methods are employed only for off-line analysis by hand or to which degree they are implemented in the systematic processing op to Level-1 (as suggested at Line 110 for Method 1). Please clarify this upfront.

Reply: The first method (using individual Fraunhofer lines) is used to process all the solar measurements to monitor the spectral variations on orbit. After the solar measurements are available, this method will automatically process the solar data. But the second method (using entire atmospheric spectra) is employed only by hand to some orbits. It is more complicated than the first method because it depends on the atmospheric condition (cloud and aerosol), the accuracy of RTM and the reanalysis data. Sometimes, the results are not outputted because the iterations fail in convergence.

4. Please introduce the spectral requirement(s). Are there separate requirements on a) shifts with respect to the ground characterisation, b) on in-flight spectral stability (at Level-0 prior to spectral calibration), and c) in-flight spectral knowledge at Level-1b(after spectral calibration). Please introduce the requirements explicitly. It would be nice if the spectral calibration requirements were introduced with a short discussion on the tracing to the CO2 product uncertainty requirement.

Reply: The spectral requirements include band coverage, spectral resolution, spectral sampling in FWHM, and the spectral calibration accuracy. Dr. Zhongdong Yang shows them in detail in the paper 'Laboratory spectral calibration of the TanSat atmospheric carbon dioxide grating spectrometer' published in 2018. Please refer to that paper about the detailed spectral requirements.

For TanSat, there are no separate spectral requirements at stage of ground, Level-0 and Level-1b. The requirement on in-flight spectral accuracy is 5-10% of the spectral resolution, which has been added to Table 1 and also clarified at the end of the third paragraph in Section 1. The aim of this manuscript is to analyze if this spectral calibration requirement is satisfied. These requirements on the tracing to the CO2 product uncertainty requirement exceed the field of this manuscript, because CO2 product uncertainty depends on too many factors, such as your retrieval method(physical or regression), radiometric calibration at Level-1, instrumental model(SNR, ILS ...) , and so on.

5. The L1b users are certainly interested in the performance of the two methods, which is unfortunately not reported. If possible, please give estimates for the uncertainty of the spectral axis obtained by the two methods.

Reply: The first method has the high accuracy and stability in nature based on the Fraunhofer lines. We show its performance in Figure 4-6 and Figure 7-9. Figure 4-6 show that the first method has the ability to reveal the variation trend. Sorry for that we did not explain the error bar in figure 7-9. The horizontal axis is the spectral axis, the standard deviation is shown by the error bar for each FOV and each Fraunhofer line in the year 2017. After averaged for all FOVs and all Fraunhofer lines, the standard deviations in O2A, WCO2 and SCO2 bands are about 0.0039 nm, 0.013 nm and 0.021 nm, respectively. These estimations have been added at the last paragraph in Section 2.2.

The second method has the ability to reveal the spectral variation too. This method is not developed by ourselves. We simply apply the second method to our work without a full performance assessments made by ourselves. We strongly recommend the L1b users to refer to the paper published by Jos H.G.M. van Geffen and Roeland F. van Oss (Applied Optics, 2003), which is also given in the references. They develop this method to estimate spectral variations of GOME by using the earthshine spectra. Also, they shows the performance of this method.

Specific Comments

Abstract line 9: it is stated that the observed spectral variations are partly caused by vibrations. This is not understood. It is expected that mechanical vibrations within the spectrometer, in particular causing displacement of the slit with respect to the detector can cause a widening of the instrument spectral response, but not a shift of its barycentre.

Reply: We accept this comment and revise the statement. 'Vibrations' is deleted from the sentence at line 9.

Please introduce a blank space between numbers and units throughout the manuscript.

Reply: We have added a blank space throughout the manuscript.

Line 39: When discussing the aim of the study ("only study the wavelength offset or shift with respect to pre-launch spectral calibration.") please distinguish between ground-to-orbit change and in-orbit variability. Also please include a discussion of the spectral knowledge needs.

Reply: We accept this valuable comments and have revised the statement. '... study the wavelength offset or shift with respect to pre-launch spectral calibration' is changed to '... study the wavelength ground-to-orbit change with respect to pre-launch spectral calibration and the wavelength in-orbit variability.'

And, we have added the statement that shows the spectral knowledge needs at the end of the this paragraph.

Line 40: It is argued that the ILS can be assumed to be constant on orbit "because a common diffuser is used for solar observation". This is not understood. In what sense and across which elements is the diffuser "common"? Across the spectral bands? It is not clear how diffuser features or the use of different diffusers would possibly introduce spectral variation.

Reply: The transmissive diffuser is a special diffuser that allows light to transmit to reduce solar irradiance. This diffuser can subtly change the ILS due to its uneven illumination of the telescope aperture (see Sun et al., 2017). TanSat's diffuser is a 'general' or 'common' diffuser that only allows light to be reflected. We think this diffuser will not change the ILS.

Line 41: It is referred to "decon events". Please expand / clarify what is meant: de-contamination"? Line 41: Please complete the discussion of "decon events" by stating whether such events could affect spectral variability, e.g. by changes in thermo-

mechanical loads within the spectrometer.

Reply: We have learned 'decon events' from the paper of Sun et al. (AMT, 2017). For OCO-2, it is necessary to decontaminate the ice(decon events) that accumulates on the antireflective (AR) coating of the FPAs in O2 A band. 'This effect will enhanced the reflectance of the FPA, and the reflected light might be scattered back to the FPA by the other optical components. This effect can be quantified as widening of the ILS wings'.

For TanSat, there are not this decon events. Therefore, the on-orbit spectral calibration of TanSat is easier than that of OCO-2.

Line 46: Please change "methods to evaluate the ACGS's wavelength calibration connecting each focal plane array (FPA) pixel to a specific wavelength." to "methods to assign a specific wavelength to each focal plane array (FPA) pixel of the ACGS."

Reply: We have changed this sentence.

Line 55: expand "shift and squeeze" to "shift and squeeze of the spectral axis".

Reply: We have expanded this sentence.

Typo: change "telescope aperture" to "spectrometer aperture". Section 2.1 It is not explained how the coefficients of the spectral axis (Eq 1) are derived from the in-flight spectral shifts determined at individual Fraunhofer lines. Please clarify.

Reply: The 'telescope aperture' has been changed to 'spectrometer aperture'. These coefficients of the spectral axis (Eq 1) have been derived from the spectral calibration test on ground. After launch, the coefficients C2-C5 remain unchanged to describe the non-linear effects of the wavelength on pixel index. In the first method, the C1 also remains unchanged. The C0 coefficients for each FOV and each band are corrected by subtracting the shifts. At each position of the selected Fraunhofer lines for each FOV and each band, a individual shift will be calculated at the reference position by: 'shift = measurement - reference'. Then, the shifts for a FOV in a band will be averaged to get

a shift.

We have added above statements at the end of Section 2.1.

Line 71: please add: the number of SPECTRAL pixels in the ... bands.

Reply: Spectral is added.

Line 72: please use the label "O2A band" as introduced earlier for the ACGS spectral band throughout the manuscript (as opposed to the "O2 A-band" as labelled by Fraunhofer in 1814).

Reply: The label 'O2A band' is used throughout the manuscript.

Line 72: typo: change "s" to "a". Line 72: please change "two pixels per full width at half maximum (FWHM)" to "two pixels per spectral resolution increment (defined as the full width at half maximum (FWHM) of the ILS"

Reply: 's' has been changed to 'a' at line 72. "two pixels per full width at half maximum (FWHM)" is changed to "two pixels per spectral resolution increment (defined as the full width at half maximum (FWHM) of the ILS".

Line 76: change "in three band" to "in the three bands"

Reply: 'in three band' is changed to 'in the three bands' throughout the manuscript.

Line 77: what is meant with "some middle pixels"? in the centre of the field? In the spectral centre of the bands?

Reply: 'some middle pixels' is very confused. We have revised this to 'three adjacent pixels located in the central section of the FPA for the three bands.'

Line 84: Please justify the adequacy of this parameterization e.g. by discussing the expected or observed smoothness of the wavelength as a function of pixel number. The polynomial used is a function of the index p rather than the index difference with respect to the centre pixel index. This asymmetry would cause instabilities to occur

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near the band edge with higher index numbers, if they occur. Please discuss if this is relevant here.

Reply: Thanks for this valuable comment. This parameterization that uses the index of pixels had been identified in the lab testing on ground in 2014. We did not notice this asymmetry effect. Another instrument called Greenhouse gas Absorption Spectrometer (GAS), the design of which is similar to the ACGS, is being developed for FenYun-3 satellite series. We will compare the two types of parameterizations.

Line 87: Please clarify what is meant with "the sampling resolution" of the Kurucz's spectra. Is it spectral sampling or spectral resolution?

Reply: Sorry for the confused expression. We have checked the Kurucz's spectra. "the sampling resolution of 0.001nm" should be 0.001 nm spacing. We have revised this at line 87.

Line 87: The solar reference spectrum by Chance and Kurucz (JQSRT, 2010) has a spectral resolution of 0.04 nm and a spectral sampling of 0.01 nm. Please correct or clarify. Please clarify which spectrum is used for which spectral domain, as the solar reference spectrum by Chance and Kurucz does not cover wavelengths larger than 1000 nm. Please specify spectral sampling and resolution of the reference spectrum by Fontela et al.

Reply: Kurucz's spectrum atlas are widely used for radiative transform model and data retrieval in the scientific community. We have found the two paper published by Fontela, Chance and Kurucz when we look for the solar spectrum. Because it introduces the reference spectrum in many details from 200-1000nm, we list them as the references in our manuscript. Indeed, the paper shows the solar spectra with 0.04nm resolution and 0.01 nm sampling. And, this spectrum was developed for GOME, SCIAMACHY et al.

But the resolution of the spectrum used in our research are not the

same as that described by Chance and Kurucz's paper. The spectrum in O2A band with spacing of 0.001 nm are also released via his web(http://kurucz.harvard.edu/sun/IRRADIANCE2005/). Also, the high resolution of near 0.001 nm in WCO2 and SCO2 band can be found in another directory of IRRADIANCE2005.

I guess these spectra used in my research might be produced or updated after Chance and Kurucz's paper was published, because in the header of spectra, Kurucz writes that "this work was financially supported in part by the NIES GOSAT Project, Center for Global Environmental Research National Institute for Environmental Studies, Japan". So, the bands expand from O2A to CO2 bands. At current, the resolution of Kurucz's solar spectra is the highest among our all solar reference spectra. Some solar spectra provided by the RTM model can not meet our needs.

Line 90: The statement that the spectral resolution of the solar reference spectra is one order of magnitude higher than the spectral resolution of the ACGS seems not valid (see comment on Line 87). Please correct or clarify.

Reply: We have deleted this statement at line 90.

Line 109: change "are" to "is"

Reply: 'are' is changed to 'is' at line 109.

Line 114: Reformulate "The wavelength offsets of each band have annually variation in a year." Proposed "The wavelength offsets of each band exhibit an annual variation."

Reply: This sentence at line 114 has been reformulated.

Line 116: Reformulate "There are little thermal gradient" to something like "thermal gradients are small", please quantify.

Reply: This sentence is changed to 'The small thermal gradients can lead to the slight change of the geometry of major optical components such as slit, collimator, grating

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and FPAs.'

Line 117: The slit is missing in the listing of relevant optical component in this context. Please add.

Reply: slit is added.

Line 118: changeS

Reply: 'change' is revised to 'changes'.

Line 118: It is stated that "offset which are similar for each FOV". Please clarify if that is expected because of the spectrometer design or whether this is simply a finding of this analysis.

Reply: That is expected. We have revised this statement to 'offset which is expected to be similar for each FOV'.

Line 124: Please add "insensitivity" to "insensitivity of the spectral response".

Reply: 'insensitivity of the spectral response' has been added at line 124.

Line 126: it is not clear in which sense the detector material is relevant for the sensitivity to thermal variations. Please explain. Is it about thermal expansion of the detector?

Reply: The original statement explaining the effect of temperature on larger shifts is inaccurate. The sentence 'The O_2 A-band uses the silicon .... to minor variations in temperature' has been deleted. From the perspective of the whole ACGS design, O2A band locates in the middle of the instrument, while the two CO_2 bands locates on the both sides. The thermal gradients in CO_2 bands are larger than that in O2A band.

Line 129: Change "in UV-visible bands" to "in the O2A band". ACGS does not cover the UV.

Reply: Yes, we have changed this sentence.

Equation 3: The contributions to the cost function are weighted by the inverse of the

measurement noise, so the weight is lower in the Fraunhofer and their wings lines as compared to the continuum. It is not clear whether this weighting strategy is useful, in view of the fact that the spectral information is exactly in these spectral regions. Please discuss / consider

Reply: We did not consider this question when we use this method. We simply apply this equation developed by Geffen et al. (2003) in our work. In principal, this weighting strategy is reasonable because the measurement contains noise which can affect the convergence of the cost function. Re-examining this weighting strategy demands clear physical insight about the two kinds of spectra, i.e, measurement and simulation. We think this need to be further studied.

Line 142: It is not satisfactory to state that "the search routine" is used to find the minimum of equation (3). Please specify the minimization routine, at least by specifying its class / type, maybe the library from which this routine is taken.

Reply: We have checked our routine to identify that fmincon routine in MATLAB package is used to find the minimum of a nonlinear function.

Line 148: The statement "Hence, the result of this method is independent of solar lines and can be compared with the calibration results shown in section 2." Is confusing. Please discuss in which sense the two methods bring different information and what has been learnt. Please discuss the parts of the orbit in which solar irradiance and Earth radiance spectra are acquired and in which the two methods are applied. Please discuss the thermal behavior of the spectrometer as a function of the orbital phase.

Reply: We want to express that the two methods use different references and different processing techniques to obtain the spectral variations. Then, the results of two methods can be compared. The statement 'Hence, the result of this method is independent of solar lines and can be compared with the calibration results shown in section 2' is revised to 'The result of this method can be compared with that shown in section 2'.

In the reply to comment 2, we discuss the parts of the orbit in which the results from solar irradiance and Earth radiance spectra are compared. These discussions have been added to the third paragraph in Section 3.2.

The author and co-authors have few knowledge about the thermal behavior of the ACGS as a function of the orbital phase. We had a talk with the expert who knows the thermal variation, and learned that the thermal behavior of ACGS is very complex because it can be affected by different observation modes which are nadir, glint, target and solar modes. The temperature is cooled to -30 degree Celsius for FPAs in CO2 bands and to -5 degree Celsius for other components. In addition, The ACGS and CAPI are integrated designed. The platform controls the thermal balance for the two instruments. The temperature maybe has fluctuations of ± 2 degree in one orbit.

Line 155: the statement "Totally, ACGS has 1242x9, 500x9 and 500x9 different ILS tables in O2 A-band, WCO2 and SCO2 band, respectively." Is not understood. Are so many ILSs stored in the tables?

Reply: Yes, the all ILSs are stored in the Level-1b files in HDF5 format.

Line 170: Please clarify which Earth radiance scenarios are eligible for the spectral calibration. It is assumed that the O2A band all scenes are eligible, while in the SCO2 and WCO2 bands dark ocean scenes might have to be excluded due to low signal and hence low signal to noise ratio levels. It is expected that cloudy scenes are eligible for spectral calibration in view of the high signal to noise ratio and the presence of Earth atmospheric signatures.

Reply: We clarify the conditions for calibration in the reply to comment 2. Yes, Dark ocean scenes are excluded. Cloudy scenes are also excluded because we can not simulate the measurement due to the limitation of RTM when clouds exist.

Line 176: Please discuss the implication of the observation that "shifts derived from this method agree closely with that calculated from solar spectra". Please discuss what can

be learnt on the orbital variations.

Reply: We think that the agreements imply that the spectral performance of ACGS spectrometer is stable on orbit. The abnormal variations determined from solar spectra can provide warning signature for the instrument status. The second method provides the intra-orbit variation and the first method provides longer-term variation trends. Therefore, they complement each other.

Figures 4-6 caption: Please specify for which year(s) the data are plotted. Clarify whether the wavelength changes shown are averages of spectral shifts determined at a set of Fraunhofer lines, or band-averaged shifts.

Reply: The year is 2017. The wavelength changes are averages at the selected Fraunhofer lines. We have added the explanation in the text where the figure is cited.

Figure 6 caption: Typo. Change "spectral resolution in WCO2 band" to "spectral resolution in SCO2 band".

Reply: Yes, this figure is for SCO2 band.

Figures 7-9 caption: Please specify over which domain and range the statistics are evaluated (is it the temporal variation in the domain as shown in Figures 4-6?

Reply: The statistics are evaluated based on each individual Fraunhofer line in each band in 2017. The positions of each lines are also shown in Figure 3. The bars represent the standard deviations. We have revised the caption to 'The statics-stics of wavelength change derived from individual solar line for all spatial FOVs in O2A/WCO2/SCO2 band in 2017' Figure 4-6 show the averaged change in a band for the all selected Fraunhofer lines shown in Figure 3.

Figure 10 caption: Please mention that results from the second method applied to Earth radiance spectra are shown. Add labels to the three panels indicating the spectral bands.

Reply: The caption is revised to 'The wavelength change derived from the second method applied to Earth radiance spectra. These results are for each FOV and each band along latitude in one orbit on April 23, 2017 (DOY 113). The top panel is for the O2A band, the middle panel is for the WCO2 band and the bottom panel is for the SCO2 band.'

Figure 11 caption: Change "plus squeezed" to "and squeezed"

Reply: 'plus' has been changed to 'and'.

Table 2 Caption. It is not clear over what exactly the mean and the standard deviation are evaluated. Is it the statistics shown in Figures 7-9? Is it the spectral variation in all irradiance spectra or in all radiance spectra acquired on the specified day (or something else).

Reply: It is the statistics shown in Figure 10. It is the spectral variation in all radiance spectra in one orbit on April 23, 2017.
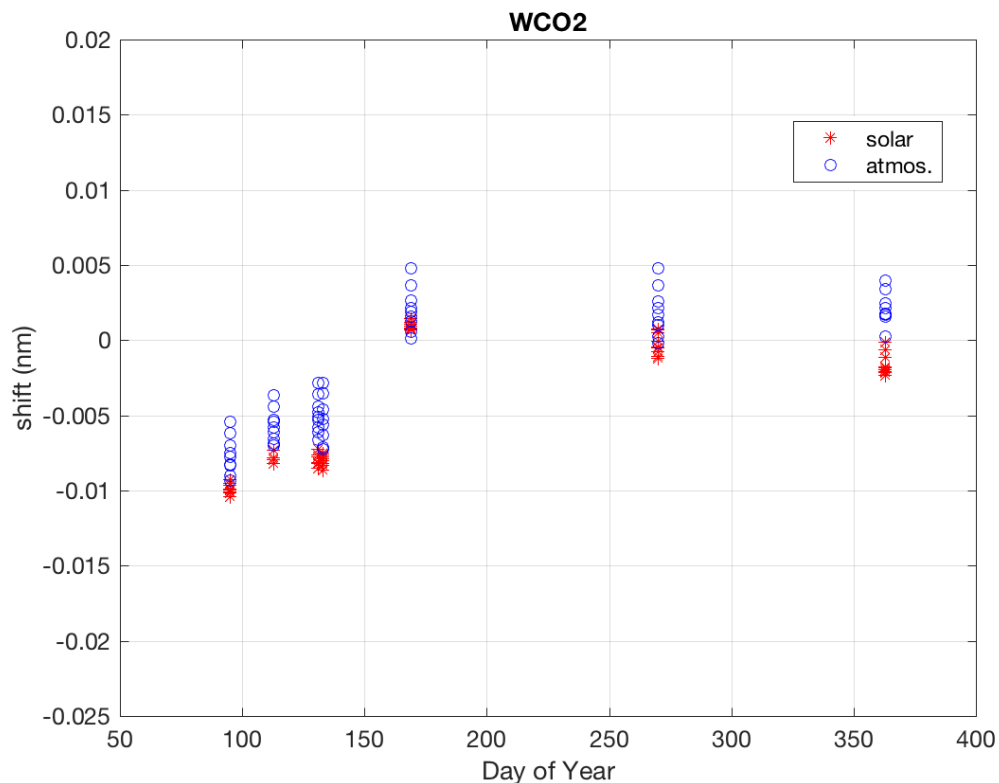
Fig. 1. Comparison of shifts from the two methods for nine FOVs in WCO2 for the orbits over Beijing, China, in 2017. The shifts derived from the second method are averaged in one orbit for each FOV.
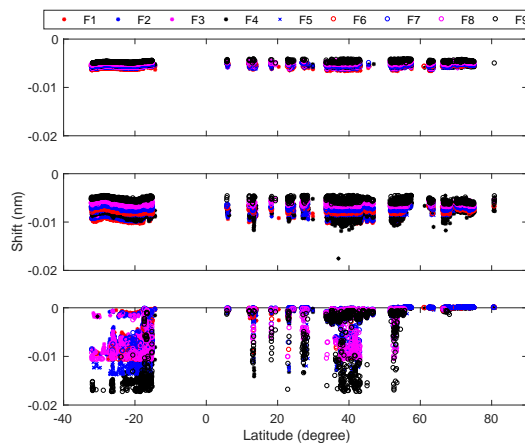
Fig. 2. Another case for wavelength changes derived from the second method on 5 April 2017. The top panel is for O2A, the middle is for WCO2 and the bottom is for SCO2.