

We thank the review for the insightful comments and suggestions. The responses to the reviewer are in red and modifications to the paper content are in *red and italic with indentation*. The equations, lines and sections in the comments are referred to the updated version of the manuscript.

I reviewed the manuscript years ago submitted to another journal + I did look forwarding to the revision which I did not see. Now I saw it in a different journal with significantly improvement in the experimental design and presentation style.

I recommended for publication as the study

- presented a novel way for medium resolution (Landsat-8 and Sentinel-2) satellite data atmospheric correction
- showed the presented method significantly improves the surface reflectance and aerosol property retrieval accuracy
- systematically validated the presented method using Landsat and Sentinel-2 data over globally distributed AERONET

Impressive work and I have to say this is a hard paper to review as there are many techniques used in the study. I appreciated the authors make the codes public available. I like many ideas in the paper but in particular the spatial smoothness prior and the validation of the uncertainty (many geostationary satellite Bayesian AOD estimation output uncertainty without validation). I really hope the authors later (not in this manuscript) can experimentally show that the proposed method is better than LaSRC and Sen2Cor – by running LaSRC and Sen2Cor software on the datasets used in this study (this maybe boring to the authors but I believe it is beneficial to the community and to the authors if the algorithm more convinced). Or simply participate ACIX and hope to see the algorithm will be an unambiguous winner in ACIX.

I have a few comments before the publication of the manuscript

SIAC has been part of the ACIX-II and comparisons will be published soon. The results from SIAC compared in the ACIX-II were submitted more than 2 years ago and many updates used in the current paper had not been implemented by that time.

Major issues

1, The readers may wonder what is the computational cost of the proposed method and the iteration nature of the gradient descent (L-BFGS-B algorithm) may boost the computation time rapidly. Add a paragraph for discussion.

We added a line at the end of Section 5.1:

The entire process (this includes state estimation, surface reflectance estimation, cloud masking and uncertainty quantification) of a single S2 or L8 scene on a standard workstation with a 3.1 GHz i7 CPU and 16 Gb RAM, takes between 20-30 minutes on a single process.

2, The authors omitted the deep blue bands for both Landsat-8 and Sentinel-2 and the band is most sensitive to aerosol among all the bands, any particular reason for doing so. MODIS does not have this band? use MODIS blue to replace not work ?

Discuss the possible shift from MODIS to VIIRS considering the dying of MODIS.

We added a comment on these two points in Sect. 5.3 ("Further developments"):

SIAC relies on the surface reflectance constrain from the MODIS MCD43 product, but the current MODIS satellites are approaching the end of their mission (Skakun et al., 2018; Xiong and Butler, 2020). VIIRS is designed to produce a continuity data record to MODIS, so it may be possible to use the VIIRS VNP43 product (Justice et al., 2013) as an alternative surface constraint, but this has not been tested. VIIRS land products additionally include bands within the deep blue spectral region (M1, M2), which are more sensitive to the aerosol variation. This information may be used to constrain the S2/L8 deep blue bands to retrieve AOT over bright surfaces (Hsu et al., 2013).

3, Spatial smoothness is interesting but unclear mostly related to how D matrix is derived. Is the spatial difference applied to the intermediate AOD and WV results derived for each iteration of L-BFGS-B algorithm. If so, Cxb is changing with iterations? The spatial difference is calculated over neighbor 8 pixels or over an entire 40 km window? How the row and column direction are averaged? Simply give an example of deriving D would solve my concern. After the line of 775, "over the whole of Gc" or of sub-40 km? Looks like the sub-40 km is used as a block to solve the equation which means the solution of each sub-40 km is independent to the neighbor sub-40 km block (but I am not sure).

We have tried to clarify the concept prior spatial correlation by rewriting parts of Section 2.4. We hope it is clearer (after L166):

This gives a constraint based on a background (a priori) estimate of atmospheric state, Xb . In SIAC, the prior mean comes from the European Centre for Medium-Range Weather Forecasts (ECMWF) CAMS Near-real-time services (Morcrette et al., 2009; Benedetti et al., 2009) for estimates of atmospheric composition parameters AOT at 550 nm, total column water vapour and total column of Ozone in Xb and Xac . These are at a coarse spatial resolution on a 40 km grid, but we need Xb on a 500m grid to match with rb , so the data are interpolated to 500 m resolution.

The role of Cxb is to encode the prior expectation of variance and spatial correlation of the AOT and TCWV fields. AOT and TCWV variances are reported in the CAMS global validation report (see Sect. B2 for a detailed derivation).

We expect the AOT and TCWV fields to have long correlation lengths (Anderson et al., 2003), which result in non-zero off-diagonal elements in Cxb . This spatial correlation structure is defined using a Markov process covariance after Rodgers (2000). This has two free parameters, the variance σ^2_{xb} and relative length scale. Since the covariance appears in the constraint Eq. (5) in inverse form, we use a fast approximation this is derived from Rodgers (2000) and implemented as a first-order spatial difference constraint defined in matrix D .

We have also added a small summary towards the end of the Section describing the effect of these choices, as well as a definition of the D matrix:

The matrix D is given as an example for a variable length of n : (7)

$$\begin{bmatrix} -1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & \cdots & 0 \\ 0 & 0 & -1 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix}_{(n-1) \times n}$$

Having this prior inverse covariance matrix allows a flow of information from regions in the scene that are well constrained by observations, to areas that are poorly constrained or missing.

The study need a consistent check of the writing style. For example, lines 102-103.

Line 105, how to treat b09. Is MODIS band 2 reflectance (after D2 transformation) used as a prior for b09 reflectance?

Changed the text to accommodate both comments:

The output of the spectral mapping provides an estimate of reflectance from 400 to 2400 every 1. This provides a surface reflectance estimation for S2 B09, a band strongly sensitive to TCWV, even though MCD43 does not include this spectral region. Uncertainty from the spectral mapping is explicitly treated in the SIAC framework.

Line 675, there is another MCD43 PSF estimation paper worth citing (Che et al. 2021).

Che, X., Zhang, H. K., & Liu, J. (2021). Making Landsat 5, 7 and 8 reflectance consistent using MODIS nadir-BRDF adjusted reflectance as reference. *Remote Sensing of Environment*, 262, 112517.

Added.

Line 130, not quite familiar with the L-BFGS-B algorithm. But does the L-BFGS-B algorithm have its own way to calculate the gradient or the authors really used the back propagation of ANN to calculate ANN (ANN uses an automatic differentiation method) to feed into L-BFGS-B algorithm. Or back propagation gradient is only used in B4 for RBF uncertainty but not used in L-BFGS-B?

We have added some text to describe the use of emulators as providers of the Jacobian of the cost function:

The cost function and its partial derivatives exploit the ability of the emulators to provide accurate approximations to the atmospheric RT model and its partial derivatives (Gómez-Dans et al., 2016).

Line 140, the LaSRC cannot be considered as DDV method anymore as each single pixel on the global have a visible/SWIR ratio (not just DDV pixels) see Vermote et al. 2016.

Yes, LaSRC is a variant of it, but strictly speaking it cannot be treated as DDV. So, we have removed it from the list.

Line 155, the framework can tolerate incomplete coverage of Y^A , how? If incomplete Y^A , then the incomplete inversion of aod and wv will be spatially interpolated? Or get value using spatial smooth prior.

This is the role of the spatial correlation in the prior pdf (Sect 2.4). We have already expanded on this as a response to another comment, and hope it is clearer now.

Line 200, “a estimates” – grammar

Changed

Line 260, how the σ_{xaero} is set

We have added a reference to Sect. 3.2, where these magnitudes are defined.

Line 310, which TOA band, the blue band should definitely greater than 10% mostly

We disagree with this comment. The filter is applied to each band of the 6 compared bands. Those two sensors agree better than 5% for most of the time even the blue and deep blue bands, please refer to paper mentioned in the previous line (309). Another paper by Helder, et al., (2020):

<https://doi.org/10.3390/rs10091340>

Line 330 we are already in Section 4.3

Removed this line

Please label and re-arrange figures 10-12 correctly. Some are clearly surface but labelled as TOA. Check the labels of the plots. Rearrange them so that the TOA spectra and TOA plot are at the same row.

After checking figures 10-12 (11-13 in the new version), they are in the correct order. You may say that the surface reflectance cannot have a better statistic than the TOA, but it can happen as the surface reflectance has a better contrast and stretches the reflectance values to a wider range than the TOA reflectance. We have added some clarification on this:

The fact that sometimes the BOA statistics are better than the TOA is probably due to the better dynamic range of the surface reflectance signal compared to the TOA one.

Line 470, yes, in many Landsat calibration literature, the calibration accuracy is 3%. Should this linked to appendix H?

Yes, this has been linked to Appendix H.

Line 580. There is no Schaff 2021 in reference list

It is in Line 1110.