

Atmos. Meas. Tech. Discuss., referee comment RC1
<https://doi.org/10.5194/amt-2022-202-RC1>, 2022
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Comment on amt-2022-202

Anonymous Referee #1

Referee comment on "Correcting 3D cloud effects in X_{CO_2} retrievals from the Orbiting Carbon Observatory-2 (OCO-2)" by Steffen Mauceri et al., Atmos. Meas. Tech. Discuss., <https://doi.org/10.5194/amt-2022-202-RC1>, 2022

The authors develop a bias correction algorithm for the OCO-2 X_{CO_2} product using a (non-linear) random forest model with the aim to correct 3D cloud effects. The model is trained with bias derived from a "small area analysis" assuming no variation of X_{CO_2} at local scale (< 100 km). Variables from the OCO-2 CO_2 dataset and dedicated cloud features are considered as model features. A feature selection is conducted to identify 3 and 4 features for glint and nadir, respectively, that are used for training the final model. The dedicated cloud features are excluded at this step. The analysis of the model shows a reduction of biases in the validation dataset and compared to TCCON measurements.

The manuscript is well written and the topic is within the scope of AMT. A correction of 3D cloud effects in X_{CO_2} retrievals would be an important scientific progress, because it would increase the number of observations with good quality. Thus, it would make CO_2 satellites better suited for studying anthropogenic and natural sources. However, I am skeptical that the presented machine-learning model will correct only non-physical variability due to cloud effects. Based on the current description of the method, I suspect that the model also wrongly corrects true variability in X_{CO_2} , for example, from anthropogenic and natural sources (megacities, power plants, wildfires, etc.). My major concerns are the following:

Data filtering: The model is currently trained with $QF=0$ and $QF=1$ retrievals. The latter also includes retrievals where the quality is poor, for reasons other than (3D) cloud effects (e.g., high SZA, AOD, snow cover), which affects training, analysis and validation, because correlation coefficient and standard deviation are sensitive to outliers. I therefore think it is necessary to still apply some filtering to the $QF=1$ retrievals to remove poor-quality retrievals due to non-cloud effects.

Truth metric: The generation of the truth metric is described insufficiently. Apparently, a k-mean algorithm is used to divide OCO-2 orbits into small areas where X_{CO_2} does not vary strongly. The true bias is then defined as the deviation of the X_{CO_2} retrieval from the median in this area. I would like to see some examples for some orbits to better judge how well this method works. In particular, it is unclear what happens in proximity of CO_2

sources (megacities and power plants) where XCO₂ deviates from the mean due to local emissions. I assume that a filtering algorithm needs to be applied to remove these areas to avoid false (positive) biases in the training dataset, but such filtering is not mentioned in the manuscript.

Feature selection: The feature selection method ignores that some variables could correlate with the "truth metric", which is computed from the same dataset and might have some issues (see previous point). These variables cannot be used in the model. In particular, the presented model uses "xco2_strong_idp" as feature, which is XCO₂ retrieved from the IMAP-DOAS in pre-processing "normalized by subtracting the mean of each small area" (L155). This is extremely similar to the XCO₂ bias used for training, i.e. the difference between the XCO₂ retrieved from ACOS and the mean of each small area (L77). As a result, I strongly suspect that the bias correction correct not only cloud biases, but also any deviation from the local mean including enhancements due local sources (e.g. megacities and power plants). Applying this bias correction model to the OCO-2 CO₂ product, would make it impossible to estimate accurate CO₂ emissions from OCO-2 observations. To avoid this issue, the features used in the model need to be selected based on their correlation with cloud properties. The B10-cloud model shown in Section 4.3 is likely a good choice. It could be given more emphasis in the manuscript.

Model validation: The validation needs to be able show that true XCO₂ enhancements are not wrongly corrected by the model. Since TCCON is not well suited for this task as the instrument are generally not located downstream of a source, I suggest conducting some case studies near known CO₂ sources to show the effect of the bias correction in OCO-2 data. There is a large amount of literature on the use of OCO-2 to estimate power plant emissions with suitable cases (e.g., Nassar et al. 2017, Hakkarainen et al 2021). The validation should also be done for the B10-cloud model.

Specific comments

L17: Not clear if you find the bias in the XCO₂ product with or without (cloud) bias correction.

L33: The effect of 3D cloud effects on TROPOMI NO₂ was recently studied: Emde et al. 2022, Yu et al. 2021, Kylling et al. 2022.

L62ff: It would be nice to provide some more details on the 3D cloud effect features, so the reader does not need to check the cited citations.

L67: Since overpass time would matter for "CloudDistance", please specify if you use MODIS Aqua and/or Terra.

L95: Please provide reasoning why and how 3D cloud effects cause negative biases.

L101: Since OCO-2 might drift in time, please check if splitting by time affects your conclusions.

L143: Since the correlation coefficient is not sensitive to a bias in your model, it would be useful to use also other parameters (e.g. RMSE).

L180ff: The results here depend strongly on the definition of the truth metric, which might not contain only "non-physical variability" (see general point).

L299ff: The analysis here assumes that the truth metric is caused primarily caused by 3D cloud effect, which is likely a wrong assumption (see general points). I think that it is necessary that you describe quite clearly here why a feature would be effect by 3D cloud effects, e.g., why ACOS retrieves a wrong surface pressure (dp) in the proximity of clouds.

Technical corrections

L11 (and others): CO2 -> CO₂

L26: fraction -> fractions

L33 (and others): The citations style does not follow AMT requirements (here: "Massie et al. 2017")

L118: form -> from

References

- Emde et al. (2022) <https://doi.org/10.5194/amt-15-1587-2022>
- Hakkarainen et al. (2021) <https://doi.org/10.1016/j.aeaoa.2021.100110>
- Kylling et al. (2022) <https://doi.org/10.5194/amt-15-3481-2022>
- Nassar et al. (2017) <https://doi.org/10.1002/2017GL074702>
- Yu et al. (2021) <https://doi.org/10.5194/amt-2021-338>