Dear Jesse,

We appreciate your comments and suggestions on this paper. We have worked to clarify any unclear descriptions in the manuscript and to address each of your questions. Your insights on cloud base height and the aerosol layer are especially valuable to our research. In response, we conducted additional simulations regarding cloud base height and aerosol top layer placement, which we discuss in detail in the responses below.

We also thank you for your suggestion on considering effective cloud distance with respect to vertical cloud base height and reflectance. Our main concern is that cloud-based information is not always readily available, introducing significant uncertainty in cloud distance calculations. We will continue exploring different effective cloud distances that incorporate various factors, including cloud reflectance, surface albedo, inhomogeneity, and, when possible, cloud base height.

Below, we provide our responses to each of your comments and suggestions. We have marked your comments in red, our responses in blue, and the original paper content in black.

Comment on egusphere-2024-1936:

This manuscript develops a method for the mitigation of 3D radiative transfer effects on retrievals of carbon dioxide concentration from the Orbiting Carbon Observatory satellites. The novelty of this work is that it provides a pathway for physics-based mitigation of 3D radiative transfer effects using parameterizations that can be applied operationally.

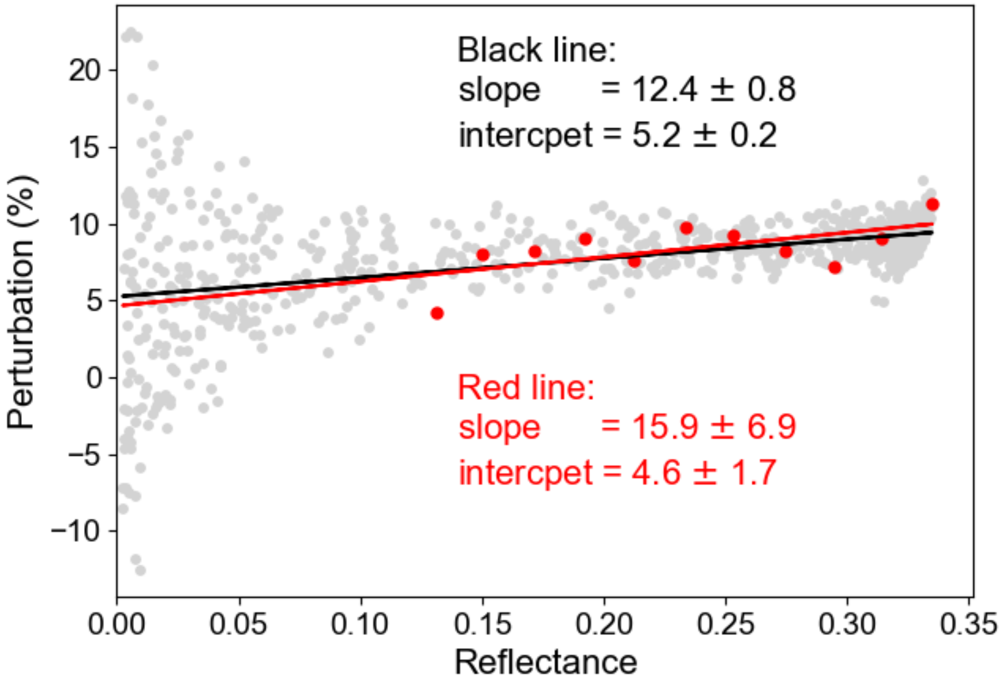
Thank you for summarizing the paper. We appreciate your comments on our research.

I enjoyed reading this paper, and I have several comments and suggestions detailed below:

As I understand it, all of the forward modelling of the OCO bands in this paper utilizes the linear approximation suggested by Schmidt et al. (in prep). For this paper, it is important that we know how the error in the linear approximation propagates into uncertainty in the relationship between ΔX_{CO2} and the radiances i.e., how accurate is the reference calculation?

> Thank you for the question. As shown in Fig. R1 (an edited version of Fig. 1), the perturbation at low reflectance spreads largely due to the high uncertainty of Monte Carlo radiance simulations at extremely low transmittance. To avoid high uncertainty and heavy computation, we define a minimum transmittance threshold for each band, set as the lower of either (1) 40% of the band's maximum transmittance or (2) the band's minimum transmittance. This threshold reduces the potential for linear approximation errors. Additionally, increasing the number of wavelengths and photons in the simulation further stabilizes the linear approximation. These steps ensure that the linear approximation accurately represents the perturbation across the entire

reflectance range within an acceptable level of uncertainty. However, to better quantify the impact of the linear approximation error, we will explore incorporating a detailed uncertainty analysis in future work, specifically assessing how deviations in the linear model propagate into ΔX_{CO2} estimates. A glimpse of this work is shown in the Figure below. It illustrates the difference in slopes and intercept values when using just a few representative wavelengths in a channel vs. all/many of them.



(edited version of Fig. 1) Figure R1. Example of the linear relationship between perturbation and reflectance. The grey dots represent the complete wavelength range, while the red dots indicate the subset selected for the O_2-A band simulation. The black and red lines represent the linear fit of the grey and red dots, respectively,

At the moment, Section 2 states the result of Schmidt et al. (in prep) but doesn't provide much physical justification for the linear approximation itself.

Thank you for the comment. We describe the physical meaning of the linear parameters in lines 140-147: "The slope and intercept are indicative of distinct physical phenomena: a non-zero slope corresponds to wavelength-dependent variations and differences in 1D and 3D radiances, photon path lengths, and absorption. Increased photon path lengths from multiple scattering in 3D-RT produce non-zero perturbations (percentage differences in 1D and 3D radiances) expressed in Eq. (1). Since wavelengths with higher absorption are attenuated more than those with lower absorption, the Eq. (1) perturbations are a function of reflectance (line absorption depth), referred to later as spectral distortion. The intercept is related to the oftenreported increase of reflectance near clouds, or decrease in shadows, whereas the slope accounts for spectroscopic effects.”

When we first found this remarkable linearity (Schmidt et al., 2019), we were somewhat surprised by it, and to this day there is no rigorous physical explanation. We only have empirical evidence that 3D perturbations are linear over the *relevant* dynamic range of reflectance, which arise from extra illumination of the surface mediated by multiple scattering in clouds. The photons causing this extra illumination have a history of photon path length *different* from the directly surface-reflected radiation. Specifically, absorption is enhanced for those photons experiencing longer photon path length.

We recognize that low-reflectance wavelengths do not always align well with the fitting lines due to their much lower intensities. Therefore, we focus our analysis on higher reflectance wavelengths, where the linear approximation is more robust and provides better accuracy in the relationship between ΔX_{CO2} and radiances.

Linearity actually breaks down for the very highest absorption optical depth (reflectance, transmittance ~0). At this point, the perturbation is close to zero. This can be shown with SHDOM calculations. However, this only happens at the very highest optical thickness, which relates to wavelengths where OCO-2 does not pick up a signal. For practical purposes, the assumption of linearity seems to be valid. For the future, it would be desirable to come up with a semi-analytic explanation for the transition from linear to non-linear range as the absorption optical thickness increases.

I think this section would benefit from a short paragraph discussing approximate acceleration methods for 3D RT such as (Partain et al., 2000; Doicu et al, 2020) in comparison to exact calculations like Emde et al. (2011), so that the strengths/weaknesses (accuracy vs. speed) of the linear approximation can be contextualized.

Thank you for the suggestion. We have included a few studies that have progress on accelerating multi-wavelength 3D-RT calculation. These two papers can make the introduction more comprehensive. We will add a summary of both papers in the introduction as below:

- Original text (Lines 80-88):

“Schmidt et al. (2024) explain that lateral photon transport can be understood as missing physics in the operational OCO algorithm, and any adjustments for discrepancies between 1D-RT and 3D-RT could introduce additional inaccuracies in X_{CO2} retrieval. Although advances have been made in expediting high-resolution 3D-RT simulations by using the same photon paths for various wavelengths (Emde et al., 2011; Iwabuchi and Okamura, 2017), the computational demands of such models have still hindered their operational application. Schmidt et al. (2019) introduced the 3D-RT radiance perturbation as the percentage difference between the 3D and 1D radiance simulations. This radiance perturbation is found to be linear over the relevant dynamic range of reflectance, which allows a simple representation of the perturbation as slope and intercept for each of the three OCO-2 bands. The details will be described in Section 2."

- Revised text, with the main changes underlined:

  "Schmidt et al. (2019) explain that lateral photon transport represents missing physics in the operational OCO algorithm, and any adjustments for discrepancies between 1D-RT and 3D-RT could introduce additional inaccuracies in X_{CO2} retrieval. To evaluate the differences between 1D-RT and 3D-RT, a high-resolution, multi-wavelength 3D-RT model is essential. Recent advancements have accelerated high-resolution 3D-RT simulations for multi-wavelength applications. For instance, Partain et al. (2000) introduced an enhanced implementation of the equivalence theorem, which decouples scattering and absorption calculations, allowing for accurate spectral integration without repeated multiple-scattering computations for Monte-Carlo models. Emde et al. (2011) developed the Absorption Lines Importance Sampling (ALIS) technique, which efficiently computes high-resolution polarized spectra by leveraging Monte Carlo photon tracing across multiple wavelengths simultaneously. Iwabuchi and Okamura (2017) also adopted a similar way of using the same photon paths for various wavelengths to accelerate multi-wavelength 3D-RT simulation. Doicu et al. (2020) accelerated the Spherical Harmonics Discrete Ordinate Method (SHDOM) 3D-RT model, which is different from Monte-Carlo-based 3D radiative transfer models, by combining the correlated k-distribution method with dimensionality reduction techniques, such as principal component analysis.

  While each of these acceleration methods has the potential to improve the accuracy of trace gas retrievals by taking into account missing physics (horizontal photon transport), current operational retrievals still do not use true 3D-RT in trace gas retrieval processes. Consequently, we adopt the approach introduced by Schmidt et al. (2019) as a practical method to approximate the 1D-RT and 3D-RT differences. They proposed the concept of a 3D-RT radiance *perturbation*, defined as the spectral percentage difference between 3D and 1D radiance simulations. This perturbation, plotted as a function of the radiance (or reflectance) itself, was shown to be linear across the relevant dynamic range of reflectance, which simplified its represenation significantly, and allowing it to be represented by a simple slope and intercept for each of the three OCO-2 bands. Building on these findings, this study applies the linear representation to real-world data to mitigate 3D cloud biases, with further details provided in Section 2."

The mitigation parameterization is based on simulated scenes derived from observations. Due to weak atmospheric scattering, the 3D enhancement effect studied here depends primarily on cloud-surface interactions. These will strongly depend on the geometric distance between cloud and surface (i.e., cloud base height and thickness). At the moment, the methodology doesn't state how the cloud base height is retrieved from the MODIS observations to form a synthetic cloud field, or its uncertainty. This procedure's uncertainty will feed into the simulations and affect how the intercept and slope parameters scale with effective distance. It would be good to address this within the manuscript as it will affect both the baseline and bypass approaches.

> Indeed, this is a problem that injects uncertainty. Unfortunately, it is not easy to address since MODIS retrievals only provide cloud top height. Attempts have been made (not by our team, but other OCO-2/3 team members) to retrieve cloud geometric thickness in addition to optical thickness from the OCO-2/3 observations *themselves*, but even if this were always successful, these retrievals would only be available for OCO-2 footprint locations, and not for the wider scene context. In this study, we therefore assume a fixed geometric thickness for clouds, specifically 1 km for cloud top heights smaller than 4 km, and a cloud base height of 3 km for cloud top heights greater than 4 km. This is a starting point for illustration of the general approach. The subjective assumption can be changed once more detailed cloud information does become available.
>
> We believe that your opinion is partially correct. A fraction of the enhanced surface illumination causing the observed perturbations does indeed stem from multiple reflections between the cloud base and the surface, especially when the cloud fraction is very low. However, the primary path of enhanced illumination does stem from multiple scattering, when considering a clear-sky patch in the *vicinity* of a cloud. For the alternate path suggested by the review (which does factor into the extra illumination to some degree), the photon path length distribution is much more comparable to direct illumination than the radiation traveling through the cloud because even multiple reflections between the cloud (base) and the surface do not enhance the photon path nearly as much as multiple scattering in an extended cloud layer. That said, the photon path length distribution change mediated by the cloud itself does depend on the thickness of the cloud, so our approximation of a fixed geometric thickness is not ideal in either event. We will add a statement to this effect in the revised paper.
>
> Inspired by your comment, we decided to look into this issue a little deeper than we initially had. We performed a simulation that reduced the geometric cloud thickness to 0.5 km for low clouds, as shown in Table R1. Compared to the simulation of a geometric cloud thickness of 1 km in Table R2 (same as Table 2 in the manuscript),

the amplitude of slope (a_s) decreases notably when clouds have smaller geometric thickness. This indicates that the cloud base height or geometric cloud thickness could impact the 3D effect magnitude for the same COT. It is, however, unclear whether this is caused by reflections between the surface and the cloud, or simply by changes of the multiple scattering photon paths *inside* the cloud, which we believe are the more important pathway. The relative importance of the multi-scattering within clouds and multiple reflections between the cloud base and the surface needs further studies. The good news is that with the advent of Oxygen A-Band measurements from space, cloud geometric thickness in addition to cloud top height should become more widely available than it is now.

Table R1. Amplitude and e-folding distances for ***s*** and ***i*** fittings of the simulation with a homogeneous aerosol layer in the O_2-A, WCO_2, and SCO_2 bands for 0.5 km geometric cloud thickness of low clouds.

	Slope			Intercept		
	s_{O_2-A}	s_{WCO_2}	s_{SCO_2}	i_{O_2-A}	i_{WCO_2}	i_{SCO_2}
a_s or a_i	0.214 ± 0.059	0.094 ± 0.032	0.150 ± 0.052	1.033 ± 0.349	1.069 ± 0.405	0.811 ± 0.383
d_s or d_i (km)	7.13 ± 1.34	6.86 ± 1.52	6.31 ± 1.41	2.83 ± 0.32	2.65 ± 0.39	2.49 ± 0.45

Table R2. The same table as Table 2 in the manuscript. Amplitude and e-folding distances for ***s*** and ***i*** fittings of the simulation with a homogeneous aerosol layer in the O_2-A, WCO_2, and SCO_2 bands for 1.0 km geometric cloud thickness of low clouds.

	Slope			Intercept		
	s_{O_2-A}	s_{WCO_2}	s_{SCO_2}	i_{O_2-A}	i_{WCO_2}	i_{SCO_2}
a_s or a_i	0.457 ± 0.094	0.123 ± 0.037	0.250 ± 0.041	0.755 ± 0.327	0.648 ± 0.227	0.847 ± 0.406
d_s or d_i (km)	3.82 ± 0.44	5.04 ± 0.89	4.58 ± 0.78	2.69 ± 0.32	2.91 ± 0.31	2.35 ± 0.33

We will add the following statement in Section 4.2.3 of the manuscript to clarify our views (we may shorten the exact wording, depending on your feedback):

- Additional text to be added:

“By necessity, this study makes the assumption of a fixed cloud geometric thickness (1 km for cloud top height smaller than 4 km and cloud base at 3 km for cloud top height greater than 4 km). The additional photon path caused by multiple scattering within clouds influences the magnitude of the 3D cloud effect, so the slopes are sensitive to the choice of geometric cloud thickness. But unfortunately, this parameter is not readily available from operational products. Some attempts are being made to exploit the O_2-A channel of OCO-2. Once these are mature, the information will be

> used by our algorithm. Generally, since the vertical cloud properties can influence the magnitude and distribution of the 3D cloud effect, further investigation of the impact of cloud properties, including COT, CTH, and cloud base height, on the 3D cloud effect is recommended for future research."

For the parameterization, it might be beneficial to have a generalized distance that doesn't just take into account horizontal distance but rather the 3D distance of a surface point from cloud base (or side). For isotropic scatterers, the downwelling flux impinging on a point on the surface would scale with the inverse square of this distance, so square distance weighting seems like a good choice as used in the study.

> Thanks for the suggestion. We have considered incorporating vertical distance into our parameterization; however, the lack of reliable cloud base height data poses a challenge. The variation in slope and intercept parameters at the same effective cloud distance may arise from differences in vertical heights, which we currently cannot accurately quantify due to this data limitation. We will explore this approach further when more comprehensive cloud height data becomes available. That said, it remains to be resolved whether the most significant effect is cloud-surface reflections (as suggested by you) or by multiple scattering within the cloud itself (as favored by us). Most likely, it is a combination. If multiple scattering were the sole source, the vertical dimension should not matter as much in future parameterization as the horizontal. Of course, this will depend on other factors as well, for example the solar zenith angle and the surface reflectance.

Along with that, not all clouds are equally bright, and their 3D enhancement should increase with overall cloud brightness. It might be useful to have a generalized distance that includes weighting by cloud reflectance. This might help the parameterization/bypass approach generalize more effectively.

> This is an interesting thought. We appreciate this idea and agree that the parameterization can be done better by considering more factors, such as cloud brightness. It remains to be seen, however, whether the enhanced surface illumination stemming from clouds does scale with brightness. Our impression is that what matters more is the general cloud context (i.e., the geometric distribution), but this is, again, somewhat subjective and will be studied more systematically in the future. Using cloud brightness as one of the input parameters for future bypass methods will be a good line of investigation. Our approach is merely an initial attempt to bypass 3D-RT.

The vertical distribution of aerosol will also influence the distance scaling of the slope and intercept parameters. Currently, the study examines aerosol within the cloud layer and states that it localizes enhancements to regions closer to cloud due to reduced free paths. The effect of an elevated aerosol layer may differ. Higher-altitude scattering layers tend to increase the horizontal distance over which 'adjacency' effects occur (Minomura et al., 2001). I think it would be worthwhile to discuss the role of the vertical distribution of the aerosol.

> Thank you for this insightful comment. In response, we have provided an additional simulation with the aerosol top layer set at 2 km, which is lower than the case discussed in Section 5.3 (3.1 km), while keeping other conditions consistent with the setup in Section 5.3. Table R3 presents the resulting slope and intercept values. Compared to Table R1 (above) and Table 1 in the manuscript (which did not include surface aerosols), a_s decreases and d_s across all three bands. This suggests that the relative height between the aerosol top layer and cloud base and top heights can influence slope parameterization.

Table R3. Amplitude and e-folding distances for ***s*** and ***i*** fittings of the simulation with a homogeneous aerosol layer in the O_2-A, WCO_2, and SCO_2 bands for the top of aerosol layer at 2 km. Consider this table relative to Table R1.

	Slope			Intercept		
	s_{O_2-A}	s_{WCO_2}	s_{SCO_2}	i_{O_2-A}	i_{WCO_2}	i_{SCO_2}
a_s or a_i	0.106 ± 0.051	0.072 ± 0.022	0.114 ± 0.040	0.933 ± 0.424	0.531 ± 0.192	0.574 ± 0.316
d_s or d_i (km)	8.90 ± 2.72	8.14 ± 1.61	7.76 ± 1.68	2.43 ± 0.38	3.03 ± 0.42	2.48 ± 0.48

> We will add a paragraph in Section 5.3 discussing the potential impact of aerosol vertical distribution on the 3D cloud effect:

- Additional text to be added:

  "Currently, we assume an even distribution of aerosols in the boundary layer in our radiance simulations. However, as Minomura et al. (2001) demonstrate, the effect of aerosols on radiance scattering can vary significantly depending on vertical distribution—particularly when surface albedo differences are pronounced, or the aerosol layer is low. In contrast, elevated aerosol layers can extend the horizontal range of adjacency effects, potentially altering the scaling of slope and intercept parameters. This is also applicable to spectroscopy. Consequently, non-uniform vertical aerosol distributions or uncertainties in boundary layer height could introduce variability in evaluating 3D cloud effects. Vertical aerosol and cloud distribution information, such as the data from CALIPSO on the A-train, could be beneficial for improving the accuracy of simulations, but they are not implemented in the initial software release. "

The issues of cloud base height and aerosol don't seem insurmountable at least for measurements acquired in vicinity of A-train sensors. I think it would be beneficial to provide a sketch of how these additional measurements can be used to constrain these other factors and develop an operational parameterization.

Indeed! As stated above, CALIPSO could be used to constrain the vertical distribution of aerosols, whereas the oxygen A-Band on OCO-2 itself could be used to estimate geometric cloud thickness, the two greatest 'caveats' of this study that you pointed out, and that we fully acknowledge. However, this is only the initial software release and the first associated paper. Reconstructing the real cloud, aerosol, and surface fields at the level of detail suggested by you and other reviewers have been beyond the scope of this initial step. It is also important to note that LIDAR data are not always available for every satellite track; for instance, there was no CALIPSO data available for the same track in the case examined in this study.

We will add the following text in Section 5.3 (with the previous response):

- Added text:

"Vertical aerosol and cloud distribution information, such as the data from CALIPSO on the A-train and from the Oxygen A-Band of OCO-2 will be considered in future releases of the algorithm. They are expected to improve the predictions of the slope and intercept parameters, and thus make the mitigation of cloud vicinity effects more accurate and powerful."

References:

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