Response to Referee #2:

We appreciate the very helpful feedback from the referee. The referee's comments are listed in *italics*, followed by our response in blue. New/modified text in the manuscript is in **bold**.

This was a straightforward, well written paper that I enjoyed reading. For the most part, the methodology and results were clearly presented, although clarification is needed in a few spots (as listed below). After properly addressing the following (mostly minor) issues, I'd recommend the paper for publication.

"1Δ" should be "$^1Δ$" throughout the manuscript

Revised as suggested.

line 8 – I'm not sure I've ever heard the term "loading" before in the context of airglow. If this is a common term and I just haven't been paying attention, then it's fine, but otherwise I would suggest the word "density" or "concentration" instead.

Revised to "density" as suggested.

line 35 – Please briefly explain in the text what is meant by "confounds the retrieval algorithm"

This sentence is expanded to

"**The O_2 *A* band also overlaps with strong terrestrial solar-induced fluorescence that provides valuable information on plant photosynthesis but perturbs the O_2 absorption features and, if not properly accounted for, leads to systematically biased greenhouse gas retrievals (Frankenberg et al. 2012).**"

36 – "As an alternative" confused me, as you've already talked about the 1Δ band. I'd suggest you don't need an introductory remark for this sentence

Removed as suggested.

40-41 – Please be specific about what there is a "lack of assessment" of

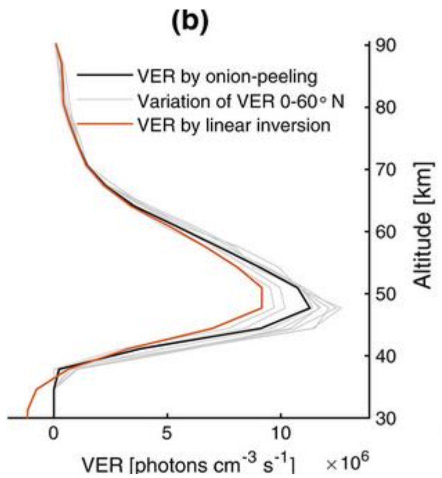
Revised to "… **but there is a lack of quantitative assessment of how the *A* band airglow impacts greenhouse gas retrieval.**"

42 – I think "chemically" should be "photochemically"

Revised as suggested.

53 – Please specify what is meant by "subject to errors"

"Errors" is replaced by "**systematic biases in the retrieved airglow VER**", and the reference to Sun et al. (2018) GRL is added. The bias is illustrated by Figure 2b in that paper (note the negative VER bias from linear inversion below 60 km):



70 – Based on your discussion of the results I don't think "degrees of freedom of signal" is the correct term. As per Rodgers, DOFS is trace(A), which is a single value. It looks to me like what you're calling DOFS is what is more commonly referred to as the retrieval response, i.e. the sum of the rows of A. Please clear this up.

Thanks for the comment. We use the DOFS as the sum of diagonal elements of the averaging kernel (AK) matrix, but not necessarily the entire AK. For example, an algorithm could retrieve a 50-element state vector where 10 elements are from a profile. It is not uncommon to sum the diagonal elements of that 10 state vector elements and report the DOFS of the profile retrieval. Sometimes DOFS in sub profiles is reported. For example, Kulawik et al. (2017, https://acp.copernicus.org/articles/17/5407/2017/acp-17-5407-2017.pdf) separated the GOSAT CO_2 retrieval of 1.6 DOFS into two partial columns with 0.8 DOFS each. The individual diagonal elements of AK may be referred to as "averaging kernel sensitivity" (e.g., Lu et al. 2022, https://acp.copernicus.org/articles/22/395/2022/acp-22-395-2022.html), but we prefer not introducing a new term when the concept of DOFS can be made inclusive. This is also consistent with the ozone profile work by Liu et al. (2010, https://acp.copernicus.org/articles/10/2521/2010/acp-10-2521-2010.pdf).

We modify this sentence to

"**The use of Bayesian inversion enables incorporation of *a priori* knowledge, balancing of measurement error and prior error, and detailed posterior error analysis including the averaging kernel matrix and degrees of freedom for signal (DOFS) (Rodgers, 2000, Brasseur and Jacob, 2017).**"

The definition of DOFS is given at line 274

"**In this study, the DOFS of each state vector element refers to the corresponding diagonal element in the averaging kernel (Liu et al., 2010).**"

71 – please specify what is meant by "the formula"

It refers to equations 3-6 in this manuscript. We modify this sentence and leave detailed explanation to section 3:

“**The airglow emission spectra are simulated based on the spectral model for the O_2 $^1\Delta$ band proposed by Sun et al. (2018), which we demonstrate can be extended to the O_2 *A* band with simple generalization.**”

84 – “tangentially” is not needed

Removed as suggested.

87 – file format details are unnecessary

Due to the complexity of SCIAMACHY native file format, this is actually a significant amount of work that is crucial for the following retrieval. The file formats and the usage of the SciaL1C command-line tool are frequently mentioned in SCIMACHY retrieval papers. Our customized algorithm converted the L1B files to a much more user-friendly NetCDF format, and more importantly, enabled separation of 8 across track positions instead of always averaging them. Therefore, we would prefer keeping these sentences.

99-104 – I would assume that a proper background correction would be critical in altitude regions far from the emission profile peak, so I think this requires a bit more discussion. It would also be interesting to see a plot of typical or averaged background signals. Whether or not you include a plot of the background signals, I would appreciate at least a brief discussion on the shape of the background signals, and the assumptions/limitations that go in to using a scaled thermospheric signal.

The background correction follows Zarboo et al. (2018). Figure 2 of that paper, copied below, shows uncorrected and corrected limb radiance for both bands. The spectrum at 142 km is a typical background signal for the *A* band, whereas the background for the $^1\Delta$ band is simply a linear fit using out-of-band radiances.

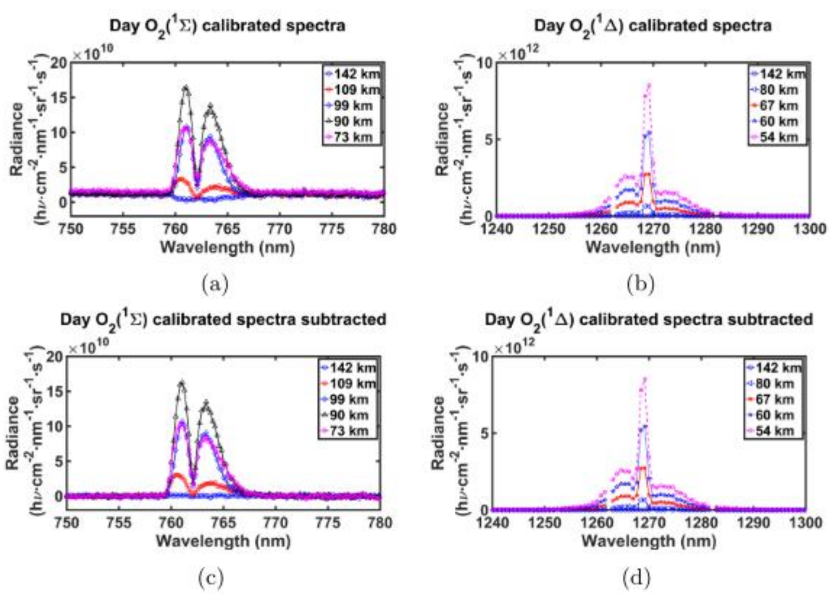


Figure 2. Examples of the daytime-calibrated spectra and the background-corrected spectra. **(a)** $O_2(^1\Sigma)$ on 3 February 2010; orbit 41 455; mean latitude 17.3° N, mean longitude 94.3° E. **(b)** as **(a)** but for the $O_2(^1\Delta)$ band. **(c)** as **(a)** but with background correction applied. **(d)** as **(b)** but with background correction applied.

We expand the discussion:

"**In addition to airglow emissions, the observed radiance spectra contain photons from Rayleigh scattering and multiple scattering by the atmosphere and the surface. The scattering signal can be approximated by limb views at maximum tangent heights and contains O_2 absorption feature for the *A* band. No O_2 absorption is observed for the $^1\Delta$ band due to much weaker atmospheric scattering and lower O_2 absorption. To account for the scattered light, a background signal consisting of averaged *A* band spectra at high tangent heights (130-150 km) from the same sounding is subtracted from each limb spectrum (Zarboo et al., 2018). Before each subtraction, the background signal is scaled to match its out-of-band radiance with the out-of-band radiance of the limb spectrum to be corrected for. This step assures the out-of-band radiance centers at zero after correction. This correction assumes the spectral shape of scattered light is the same for all tangent heights and may leads to systematic errors at low tangent heights from the *A* band, where airglow emission is low, and scattering path may differ significantly from the thermosphere. Following Zarboo et al. (2018), we consider 750-759 nm and 767-780 nm to be out of band.**"

Section 2.2 – MSIS v2 is now the most recent version, https://doi.org/10.1029/2020EA001321. I don't necessarily think you need to update to this version (although it would definitely strengthen the paper), but, if you don't, you at least need to discuss the limitations of MSIS-E-00 (especially in polar MLT regions) as is done in some of your references.

Thanks for the information. We rely on a third-party Python package to interface MSIS, and there seems to be no easy way to update. We referred to the MSIS v2 paper in the last paragraph as a future direction:

"**A recent development improved the MSIS model especially at the MLT regions (Emmert et al., 2020), and future adoption of the new MSIS profiles will improve the *a priori* estimates.**"

118 – "into two high and low altitude regimes" should just be "into two altitude regimes"

Revised as suggested.

Section 2.3 – temperatures from ACE-FTS have been used in multiple comparison studies (easily found at https://ace.scisat.ca/publications/). Please briefly discuss the results of these studies so readers have an idea of the quality of the ACE-FTS temperatures in the upper atmosphere.

The following sentences are added to Section 2.3:

"**The ACE-FTS temperature profiles have been extensively used in the validation of profiles from other instruments such as SOFIE (Marshall et al., 2011), MIPAS (García-Comas et al., 2014), and OSIRIS (Sheese et al., 2012).**"

Section 2.4 – same as ACE-FTS, please briefly discuss the quality of MIPAS temperature retrievals

We expand the discussion about MIPAS in Section 2.4. Specifically, the MA/UA/NLC modes are added according to a suggestion from referee#1:

"**The measurement modes of MIPAS used in this study include the nominal measurement mode with an altitude coverage of roughly 6-70 km, the middle atmosphere (MA) mode covering 18-102 km, the upper atmospheric (UA) mode covering 42-172 km, and the noctilucent cloud (NLC) mode covering 39-102 km. The nominal measurement mode makes up the bulk of MIPAS measurements, whereas the MA and UA modes were available every at least 10 days, and the NLC mode only happened on a few days in 2010. We use the nominal temperature profiles from version 8 of MIPAS Level 2 data retrieved by ESA (Dinelli et al., 2021). Version 8 data from the other modes are obtained through the Institute of Meteorology and Climate Research in cooperation with the Instituto de Astrofísica de Andalucía (IMK/IAA) retrieval algorithm (García-Comas et al., 2012; Kiefer et al., 2021). The typical total errors are 0.5-2 K below 70 km and 2-7 K above (for MA, UA, and NLC modes). The typical vertical resolutions in the comparison range of this study are 3-7 km.**"

132 – You use the line parameters from HITRAN to calculate absorption/emission spectra. Also, please indicate here what version(s) of HITRAN you're using

We used both HITRAN 2016 and 2020. The description can be found in Section 3.1, lines 153-158.

142 – should be "coefficients" as they are different for the two bands

Revised as suggested.

142 and after – the "n" in "n[x]" is not necessary as the square brackets already (typically) indicate number density

Thanks for the suggestion. They have been revised.

140-150 – It seems odd that you're discussing this in terms of density of "emitting" O2 instead of excited O2 in the specific state. The math is fairly straight forward, and all you need to add to the equation is a branching ratio, e.g. the Franck-Condon factor for the A-band.

Thanks for the suggestion. The main reason we wanted "emitting" rather than "excited" is that there is another emission channel from $b^1\Sigma_g^+$ state to the $a^1\Delta_g$ state (i.e., the Noxon band). Since this work only focus on emissions at 0.76 and 1.27 μm, we think it is more appropriate to use "emitting".

151 and after – please use the more standard variables λ and v_bar (nu with a bar over it) to represent wavelength and wavenumber

We replace w with λ for wavelength, but we prefer keeping wavenumber as v to be consistent with HITRAN (https://hitran.org/docs/definitions-and-units/).

Figure 1 – could use a dashed vertical line in the middle to indicate the center of the line-of-sight/location of tangent height. Also, the description indicates that the tangent height is in the

middle of a layer, whereas here it looks like it is at the bottom of a layer. Please make it consistent.

The tangent height is at the bottom of a layer. We clarify this by modifying lines 137-139 to

"**An atmospheric layer bounded by two tangent heights of SCIAMACHY limb observations is the basic spatial resolving unit of this study. We create an additional layer above the outermost tangent height by assuming a layer thickness equal to the average difference between adjacent tangent heights.**"

A dashed vertical line is added to the figure as suggested.

Section 3.3 – In optimal estimation, the measurement vector is typically represented by y (the retrieval function is typically R), so it's a bit odd having the measurement vector as r

We see that point, but since the measurement vector elements are radiances, we would rather keep the same symbol (*r*) and just use bold symbol to indicate it is a vector.

238 – I would suggest using something like "retrieval system" instead of "forward model" in order to be more encompassing

Revised as suggested.

250 – I would assume that results of the linear inversion would be prone to large, unrealistic oscillations that could lead to convergence issues. Is that the case? And if so, could some type of heavy regularization (smoothing) be applied to the result to get the profiles closer to a realistic estimate?

Regularization will likely improve the linear inversion but it seems unnecessary. We did not use the full profile from linear inversion but rather take the mean value of this profile as a uniform a priori. The a priori error is 100 times of this value to guarantee the posterior is dominated by observation. To clarify, lines 251-252 are revised to

"**The corresponding prior error is set to be 100 times the prior, a constant value for all altitudes. This effectively gives no prior constraint to the [O_2*] profile and assures its information all comes from observations through near-unity DOFS of retrieved [O_2*].**"

258 – was it mentioned earlier that this is performed in log space? If not, please explicitly state this prior to here and discuss the trade off of retrieving log values.

Only the ground-state O_2 number density is retrieved in log space. This is because it's more natural to formulate the error of prior O_2 profile (from MSIS) as a percentage, instead of absolute O_2 number density. That sentence is updated to

"**In the state vector, we also include changes of the O_2 profile relative to the *a priori* from MSIS, which is equivalent to retrieving the natural log of [O_2].**"

265 – why does the xi+1 variable have a "d" in front of it?

Because this is the update of the state vector for the iteration.

280 – The "airglow retrieval" is not attempted

Revised as suggested.

338 – What is meant by "over and above the mesopause region"?

Revised to "**The emitting O_2 number density ($[O_2(b^1\Sigma_g^+)]$) can be retrieved with high precision above ~90 km.**"

343 – I get what you're saying about the profile being "W" shaped, but it's not exactly intuitive what that means. If you want to describe it in that way, I'd say it's more "ε" shaped, but I'd suggest simply describing it as an inversion layer or a possible double mesopause.

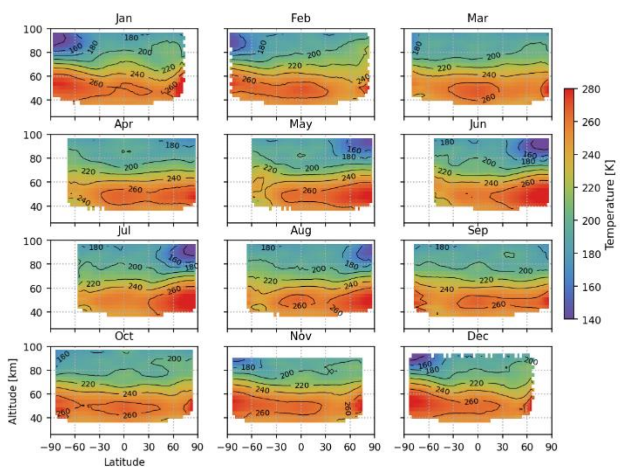
This sentence is revised to "**Both SCIAMACHY-based temperature profiles capture the double mesopause feature observed by ACE-FTS and agree well between each other at 80--95 km, where both airglow are strong and less interfered.**"

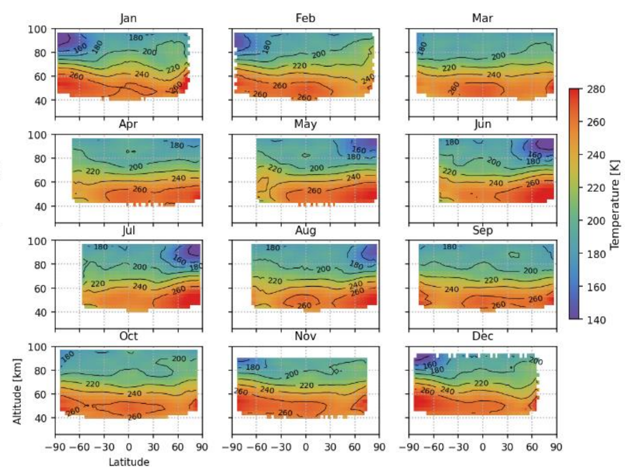
382-383 – The secondary ozone peak has been studied for multiple decades now, so the Li et al. 2020 reference is not appropriate on its own.

Thanks for the suggestion. We add a reference to Smith and Marsh, (2005, doi:10.1029/2005JD006298).

393 – a value of 0.5 seems relatively low, as I usually expect ~0.7-0.8 as a cut-off point. Can you please discuss the distribution of "DOFS" values (what I would call "response" values) for the retrievals (e.g., what percentage of retrievals are rejected if you use 0.5, 0.75, etc., like what is done later in section 5)

See the previous response about the DOFS. These are diagonal values of the averaging kernel, i.e., $\frac{\partial \hat{x}_i}{\partial x_i}$, not sum of rows. As shown by Figure 3c, the DOFS for temperature is a strong function of altitude and close to unity above ~50 km. It drops rapidly in the stratosphere due to stronger a priori constraint and diminishing airglow signal. Increasing the DOFS threshold will just slightly move up the lowest altitude of temperature profiles. The following two figures compare thresholds of 0.5 and 0.8 side-by-side:





We will keep the threshold as 0.5 as it shows the stratopause better. This sentence is modified to

"**Only temperature retrievals with DOFS greater than 0.5 are included in the averaging, and only grid cells with more than 5 measurements averaged are shown, which limits the temperature profiles to above ~40 km.**"

409 – Please explain what you mean by "due to horizontal heterogeneity at large SZA". Are you saying at larger SZAs there is more diurnal variation along the line-of-sight? If so, wouldn't it be for SZAs closer to 90° (i.e. sunset or sunrise), not necessarily larger?

Yes, at these altitudes the sunset and sunrise happen at SZA slightly larger than 90°. We remove the ascending portion of an orbit and SZA above 100° when averaging individual orbits into the climatology. The sentence at line 409 is revised to

"**We believe those are retrieval artifacts potentially due to horizontal gradient of airglow intensity at sunrise or sunset conditions.**"

Figure 13 – please include the 1:1 lines

The 1:1 lines are already there as the red dashed lines.

436 – What is meant by "very consistent"? because that's not how I would necessarily describe those results.

This sentence is revised to "**Overall, the correlation coefficients of mesopause temperatures from the two bands ranges from 0.75 to 0.90, with the *A* band temperature colder than the $^{1}\Delta$ band temperature by 5-8 K.**"

440 – coincidence criteria

Revised as suggested.

Figure 14 – a color bar is needed to indicate altitude.

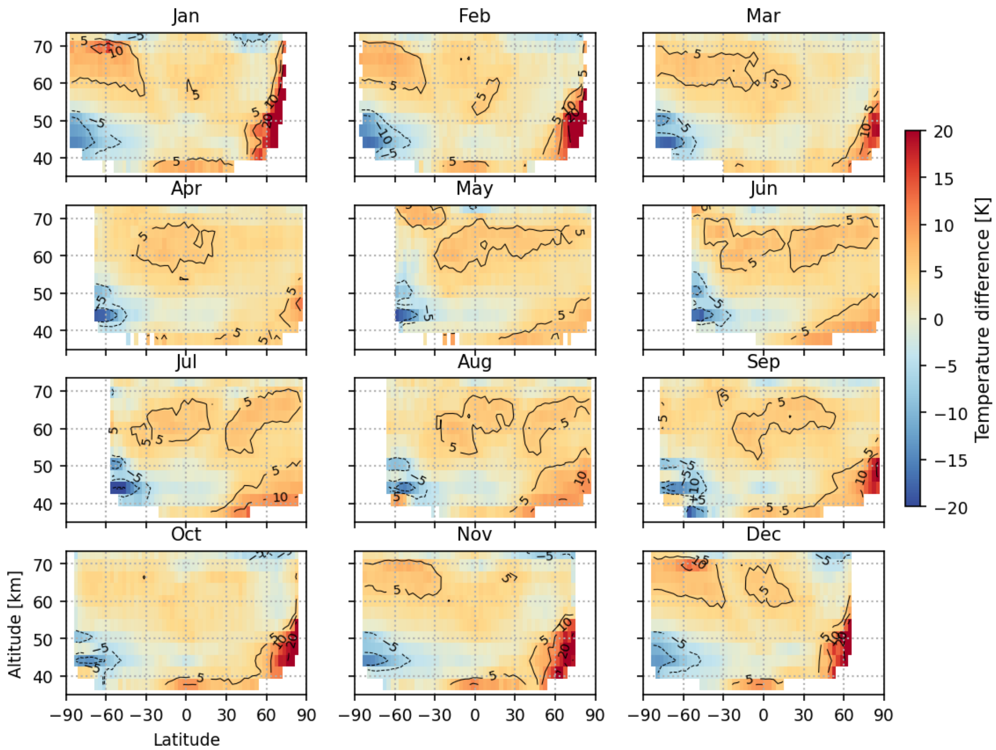
Revised as suggested.

478 – please quantify the findings of previous MIPAS temperature comparisons

This sentence is revised to "**Garcia-Comas et al. (2014) compared MIPAS with a range of satellite and ground-based temperature observations and found that MIPAS temperature differs from others by 2 K at 50-80 km in spring, autumn and winter at all latitudes, and summer at low to mid-latitudes. Differences between MIPAS and the other instruments in the summer high latitudes are typically smaller than 2 K at 50-65 km and 5 K at 65-80 km. MIPAS in general shows colder temperatures in the mid-mesosphere.**"

Figure 16 – Please use either a dashed line or maybe shading to indicate areas where the MIPAS data is from climatology

We change the vertical ranges to only show the recommended vertical range of MIPAS nominal data (below 70 km). The updated Figure 16 is included here:



500 – It's unclear what is meant by "due to horizontal heterogeneity of airglow"

It is revised to

"… **strong warm bias at winter polar stratopause region likely due to horizontal gradient of airglow intensity that violates the homogeneous layer assumption for the retrieval algorithm.**"

Math is not my thing, so I did not check the equations in the appendices. In my opinion, the appendices aren't necessary, but I'm not opposed to them.

We hope to keep Appendices A and B as a formal documentation of the forward model and jacobians. The derivation of the emitting layer optical depth was an essential step, as otherwise the layers with strong self-absorption would be subject to unacceptable temperature biases. Appendix C is removed.