Reply to the comments from the reviewer (Mark Weber):

We thank Dr Weber for his useful comments and suggestions which have helped to improve the manuscript. The reviewer’s comments are given below in black text, followed by our responses in blue text.

This paper reports on ozone trends derived from observations (SWOOSH dataset) and three versions of the TOMCAT chemistry-transport-model (CTM). One of the CTMs (ML-TOMCAT) has been adjusted to satellite observations, while the other two used meteorological data from different reanalyses, ERA5 and its predecessor ERA Interim (up to 2019). Two types of regression models are used for ozone trend estimates before and after the peak of stratospheric halogens occurring in the middle 1990. The first is the ordinary-least-squares regression (OLS), the second is the ridge regression. The main idea behind the ridge regression is to introduce an additional constraint in the cost function that minimises the fit coefficients. Such a regression is generally recommended to avoid overfitting. In general the ridge regression reduces the (absolute) trends (and all other fit coefficients) and on the other hand reduces the variances (and correlation) between regression model and the underlying data. The trends after 1998 in the upper stratosphere are positive and significant in agreement with other studies (~2%/decade, e.g. Godin-Beekmann et al., 2022). The ridge regression roughly halves these trends. Overall the paper is well written. Some issues still need to be addressed before acceptance of the paper.

Discussion points:

1. 30, l. 34 and other places: Differences in ozone trends at 100 hPa from OLS and ridge are larger than 4%/decade (7%/decade in the tropics), but the trend uncertainties are on the order of 24%. This means that these differences are not significantly different from zero. More relevant is the difference in the upper stratosphere (~1%/decade vs ~2%/decade), both significant. This should be mentioned here.

Reply: According to the reviewer’s suggestion, we have updated our results with AR1 correction applied to the OLS regression. As mentioned by the reviewer, the trend coefficients do not change much but the uncertainties increase to some extent with this correction. Detailed figures are updated and shown in the revised manuscript.

We have modified the sentences in the abstract (Lines 29-38) based on the updated results:

“For 1984-1997, we observe smaller negative trends in the SWOOSH stratospheric ozone profile using Ridge regression compared to OLS. Except for the tropical lower stratosphere, the largest differences arise in the mid-latitude lowermost stratosphere (>4% per decade difference at 100 hPa). Since 1998, and the onset of ozone recovery in the upper stratosphere, the positive trends estimated using the Ridge regression model (~1% per decade near 2 hPa) are smaller than those in OLS (~2% per decade). In the lower stratosphere, post-1998 negative trends with large uncertainties are observed and Ridge-based trend estimates are somewhat smaller and less variable in magnitude compared to the OLS regression. Aside
from the tropical lower stratosphere, the largest difference is around 2% per decade at 100 hPa (with ~3% per decade uncertainties for individual trends) in northern midlatitudes. For both time periods the SWOOSH data produces large negative trends in the tropical lower stratosphere with a correspondingly large difference between the two trend methods. In both cases the Ridge method produces a smaller trend."

We also added the related information in the main text (Lines 290-295): "The largest difference between OLS and Ridge regression methods occurs in the tropical lowermost stratosphere with a difference of ~9% per decade at 100 hPa (but with larger uncertainties >10% per decade for both regression methods), followed by the NH mid-latitudes with >2% per decade difference at 100 hPa (~3% per decade uncertainties). Note that, despite the large differences between OLS and Ridge-based trends, they are still within the uncertainties of the individual trends."

1. 37: It is not surprising that ML-TOMCAT agrees better with SWOOSH than the other models. Satellite corrections are derived from the same data that are also part of SWOOSH (e.g. MLS). This should be mentioned here and also in the main text.

Reply: Yes. ML-TOMCAT agrees better with SWOOSH than the other models though it is adjusted with SWOOSH data only for the Microwave Limb Sounder (MLS) measurement period (UARS-MLS and AURA-MLS). We have added this information in the revised manuscript. For e.g., "Comparing the ML-TOMCAT-based trend estimates with the ERA5-forced model simulation, we find ML-TOMCAT shows significant improvements with much better consistency with the SWOOSH data set, despite the ML-TOMCAT training period overlapping with SWOOSH only for the Microwave Limb Sounder (MLS) measurement period." (Lines 44-46)

1. 102: A detailed comparison between ERAI-TOMCAT and ERA5-TOMCAT has been reported in Li et al. 2022. In this paper the model data have been extended to 2020, however, ERAI ends in 2019 and trends are only reported up to 2018 for the ERAI-driven model. As the differences between both models are not discussed in detail here but well covered in Li et al. 2022, it could be safely omitted from this paper.

Reply: OK. We thank the reviewer for this insightful suggestion. We have removed the ERAI-TOMCAT simulation and used only ERA5-TOMCAT to make the plots and main text clearer and easier to read. Thus, all the data sets now have the same time period (1984-2020). We also updated all the related text and figures in the revised manuscript as well as in the supplement. Modifications are marked in red in the "track-changed" version of the revised manuscript. (Note: The ERA5-TOMCAT simulation data used in the revised manuscript are updated with the same latitude bins and pressure levels as SWOOSH and ML-TOMCAT data)
1. 161: The MLR setup is very different from Li et al. 2022. For instance, now twelve (monthly) trend terms are used instead of one (annual) and more proxies are used (e.g. EP flux). Please motivate why you added more terms into the regression.

Reply: Yes, the MLR setup used here is different from Li et al. (2022). It is a modified version of that used in Dhomse et al. (2022). We use twelve (monthly) trend terms instead of one (annual) as it is better at capturing seasonal patterns, and has better sensitivity to short-term fluctuations and improved flexibility that means better goodness of fit ($R^2$). We also use more proxies (e.g. EP flux) to account for the dynamical variability of stratospheric ozone and to separate the influence of individual processes (e.g. Dhomse et al., 2022; Weber et al., 2022). Additionally, although the inclusion of the dynamical proxies will generally improve the MLR fit, the various atmospheric-dynamics-related proxies are partially correlated which makes the attribution with a MLR a little tricky. So here we focus on using Ridge regression to avoid the over-fitting issue when more proxies are added into the regression. We also added a few sentences in the revised manuscript to motivate why we added more terms into the regression (See Lines 179-182).

1. 165: Here you mention the use of the EP flux proxy, but its contribution to ozone changes is not discussed in the paper. Its contribution needs to be added in Fig. 10.

Reply: We have added the contribution from the EP flux proxy (the vertical component $F_z$ at 50 hPa) in Figure 10 and the supplementary Figure S7. We also added discussion about its contribution to ozone changes in the revised manuscript (Lines 463-470): "Changes in the vertical component ($F_z$) of the stratospheric EP flux represents the ozone transport due to variations in planetary wave driving from the troposphere into the stratosphere (Fusco and Salby, 1999; Weber et al., 2003; Dhomse et al., 2006). In the tropics, the strengthened upward transport is linked to an upward shift of the maximum ozone mixing ratio in the middle stratosphere, as a result there are two cells of opposite ozone pattern near 10 hPa. A similar pattern appears at mid-latitudes due to enhanced transport by the stratospheric residual circulation. The out-of-phase between the tropics and mid-latitudes reflects the overturning Brewer-Dobson circulation (Randel et al., 2002). In the lower stratosphere, the hemispherical asymmetric ozone pattern could potentially result from the combination of changes in chemical and dynamical processes (Banerjee et al., 2016; Abalos et al., 2017)."
Figure 10: Latitude-pressure cross sections of the natural ozone variations (%) associated with (a-c) ENSO, (d-f) AO, (g-i) AAO and (j-l) EP flux (Fz50) derived from SWOOSH, ML-TOMCAT and simulation ERA5 based on the Ridge regression method. The stippling indicates regions that are significant at the 95% level.

l. 170: Only years 1991 and 1992 have been removed to avoid the use of an aerosol proxy, but Pinatubo eruption affected more years, e.g. end of 1990, 1993 and 1994. Please comment.

Reply: We agree with the reviewer, hence we have revised the regression models. To exclude the effect from Mt. Pinatubo eruption (1991), we removed the years of data from 1991 to 1994 in the updated regression models. The updated results with two more years (1993-1994) removed show very consistent results with previous results (1991-1992), except for some minor differences (e.g. ozone trends in the tropical lower stratosphere increase slightly during 1984-1997).

l. 175: Detrending means that the long-term trends in the proxies are moved to the linear trend terms. In Weber et al. 2022 we argued that the long-term dynamic trends are largely removed by the trends in the proxies, so that linear trends are then approximating the ODS related trends. In your case, the linear trends are combining dynamic and chemical trends. That should be mentioned here.
Reply: OK. We thank the reviewer for this reminder. We have added a sentence in the revised manuscript to make it clear that the linear trends in our case are the combination of dynamic and chemical trends (See Lines 187-188): "By de-trending, the long-term trends in various proxies are moved to the linear trend terms, that is, the independent linear trends in the MLR combine both the dynamic and the ODS-related chemical trends (Weber et al., 2022)."

1. 178: Collinearity means that both vectors (or time series) are 100% correlated, which is not the case here. What you mean is that many proxies are highly correlated with each other. It is suggested to avoid the term collinear throughout the text.

Reply: We thank the reviewer for the correction and suggestion. We have checked throughout the text and revised the term "multi-collinearity" to "over-fitting/highly correlated".

1. 187: "OLS will be not robust and will result in inaccurate model." I think this is not correct. The OLS regression model will yield the same (overall) results after orthogonalising all proxies, so OLS remains robust (as also your results show). The ridge regression is another representation with different constraints, but not necessarily better than OLS. Ridge and OLS derived trends in nearly all cases agree to within the uncertainties of the trends (Figs 2 and 3). Suggest to omit this sentence.

Reply: We apologise for this incorrect statement. We have omitted this sentence in the revised manuscript. We totally agree that "The ridge regression is another representation with different constraints, but not necessarily better than OLS".

1. 202: What is the training dataset? Suggest omit "to the training data"

Reply: We have omitted "to the training data".

1. 203: Omit "when the MSE reaches the minimum"; reference to Pedregosa et al. suffices.

Reply: We have omitted "when the MSE reaches the minimum".

1. 207: "cross-validated MSE" needs to be explained in the text. One may also want to state the drawback of ridge regression: the fit residuals (correlation between model and regression) will be larger (smaller) than that from OLS.

Reply: We have added the explanation of the "cross-validated MSE" in the revised manuscript (Lines 215-216): "The cross-validated MSE (the average of all of the test MSEs calculated from different training and testing sets) and coefficients for the Ridge regression model are also shown as the α value grows from 0.01 to 100."

Cross-validation is a way of studying how a specific sampled data set influences the mean squared error/model fit, and provides a less sample-specific estimate of the MSE. In our case, the fit residuals (correlation between model and regression) from Ridge regression are to
some extent larger (smaller) than that from OLS. The reason is probably that the original OLS
regression is somewhat over-fitting and this leads to smaller errors.

l. 239: different period is used for ERAI. Does that have an effect on the trends. Shouldn't
ERAI be compared with other data using the same period. see also comment earlier.

Reply: As replied earlier, we have removed ERAI-TOMCAT simulation from the manuscript
and used only ERA5-TOMCAT simulation in the revised version.

l. 241: readability of numbers in the tables will be improved if only one digit is only shown,
e.g. -3.4(2.5) instead of -3-39(2.47).

Reply: Thank you. To improve the readability, we have modified the numbers in the tables as
well as in the main text with only one digit.

l. 249: Within the uncertainties of both regressions the trend results (ridge and OLS) are not
different from each other! I think this should be mentioned in the main text as well (see earlier
comment). Is the annual mean the average of the twelve monthly means? Is the uncertainty of
the annual trend the standard deviation from taking the mean from the monthly values or are
the uncertainties from the individual months are error-propagated into the annual mean?
Please explain.

Reply: As replied earlier, we have modified the sentences in the abstract as well as in the
main text. Please find them in the revised manuscript.

Yes, the annual mean is the average of the twelve monthly means, and the uncertainty of the
annual trend is the standard deviation from taking the mean from the monthly values. We
have added the explanation in the main text (Lines 251-253).

l. 265: mention here that the large differences in trends are within the uncertainties of the
individual trends (see above).

Reply: We have modified the sentence and added the information as follows: "The largest
difference between OLS and Ridge regression methods occurs in the tropical lowermost
stratosphere with a difference of ~9% per decade at 100 hPa (but with larger
uncertainties >10% per decade for both regression methods), followed by the NH
mid-latitudes with >2% per decade difference at 100 hPa (~3% per decade uncertainties).
Note that, despite the large differences between OLS and Ridge-based trends, they are still
within the uncertainties of the individual trends." (Lines 290-295).

l. 335: In the lower stratosphere ridge and OLS are not reliable and fail to capture the large
variability. In addition, the data quality of satellites is lower in this region. So the "linear
relationship" is not the issue here
Reply: We apologise for the incorrect statement. We have modified this sentence in the revised manuscript (Lines 373-376) as follows: "The considerable differences suggest that there is a large degree of uncertainty in the estimates of seasonal ozone trends, particularly in the lower stratosphere, where dynamical processes dominate, in addition there is larger uncertainties in the satellite data. Therefore, caution is needed when discussing the results for this region, as neither regression method can reliably capture the large variability."

1. 340: "These differences between OLS- and ridge- based ozone profile trends imply that Ridge regression to some extent has improved the reliability of the model in the presence of multi-collinearity." This is not generally true as discussed above. Again: Differences between OLS and ridge-based trends are within the uncertainties of the individual trends.

Reply: We have modified this sentence as follows: "Despite these differences between OLS- and Ridge-based ozone profile trends, the even larger uncertainties e.g. in the lower stratosphere (Figure S3), indicate the ozone trends from two regression models are not different from each other." (Lines 382-384)

1. 346: "Considering the nonlinear effect, the monthly terms of QBO proxies are used for regression analyses" I do not understand what is meant to be said here. Statement can be omitted.

Reply: OK. We have omitted this statement to avoid misinterpretation.

1. 355: "corresponds to the more positive ozone trends in both simulations". To me it is not clear how long-term ozone trends can be associated with QBO (contains only periodic changes after detrending)

1. 358: "... may account for the more positive ozone trends", see previous comment

Reply: We apologize for the misleading statements. We have omitted these sentences in the revised manuscript.

1. 363: How is the anomaly defined (amplitude, i.e. max minus minimum response relative to the long term zonal mean ozone times the sign of the fit coefficient?). Please specify.

Reply: The ozone anomaly (in %) is calculated by referencing the monthly mean ozone to the climatological mean for each calendar month. As all the explanatory proxies in the regression models are normalised between 0 and 1, the contribution of the natural processes (QBO, solar, ENSO, AO, AAO and EP flux) to the percentage ozone changes can be directly denoted by the fit coefficients (also equivalent to the max minus minimum response relative to the long-term zonal mean ozone times the sign of the fit coefficient).

1. 388: ozone trends are only shown below 60degs, but solar response up to 90degs. Ozone is not well sampled above 50-60degs in the early period by SWOOSH. Is the solar response a
result from a fit solely limited to the late period after 1998? Why are ozone trends above 60degs not shown?

Reply: The solar response (Fig. 8), as well as the response from other natural processes (Fig. 10), is a result from a regression fit over the whole time period 1984-2020, not solely limited to the late period after 1998. To avoid the not-well-sampled data above 50-60° in the early period by SWOOSH, we have adjusted the latitude region in Figs 8 and 10 from 80°S-80°N to 60°S-60°N, at the same time to have consistent latitude regions as shown in the ozone trend results (Figs 2-5).

1. 395: use only single digits (see earlier comments). Is the table needed as the numbers can be derived from Fig. 9?

Reply: We have checked throughout the main text and changed the numbers to one digit. As the table here is derived from Fig. 9, we removed it in the revised version.

1. 409: see comments to l. 388. Please add the results of the EP flux proxy (I guess it is the vertical component of the EP flux).

Reply: As replied earlier, we have added the results and discussion about the contribution from the EP flux proxy (the vertical component of the EP flux), as shown in the revised Figure 10 and Figure S7, and the main text (Lines 463-470)

1. 425: "The negative AO (AAO) indices in the extratropics ...". This is evident in the models and ML-TOMCAT above 60 degs but not in SWOOSH. Can this be explained? Are the regressions above 60degs problematic?

Reply: As replied earlier (l. 388), the AO/AAO response is derived from a regression fit over the whole time period 1984-2020. To avoid the not-well-sampled data above 60° by SWOOSH, we have adjusted the latitude region from 80°S-80°N to 60°S-60°N.

1. 444: "it is inappropriate to use the same regression model for all locations" Not clear what is meant here, you mean you cannot use a ridge regression with a constant tuning parameter or you mean OLS. As discussed earlier I do not think that the use of OLS is inappropriate.

Reply: What we want to say here is that for Ridge regression we cannot use a constant tuning parameter for all locations. We agree with the reviewer that the OLS regression will yield robust results when the atmospheric-dynamics-related proxies are orthogonalised (Weber et al., 2022), and the Ridge regression we use here is another representation with different constraints, but it is not necessarily better than OLS.

1. 456: "The largest difference between OLS and Ridge regression methods appears in the tropical lower stratosphere (with ~7% per decade difference at 100 hPa).", but do not forget the trend uncertainties for both regression are very high (~23%/decade).
Reply: Yes. As replied earlier, we have revised this sentence and also checked throughout the paper to make relevant modifications. These modifications can be found in the revised manuscript (Lines 290-295, 506-508).

Technical (selected):

1. 37: change to "the SWOOSH dataset" Done.
1. 58: "controlled by transport and" (omit "the") Done.
1. 150: add Snow et al. 2014 (doi:10.1051/swsc/2014001) as reference for the MgII index
   The reference has been added.
1. 183: I am not sure if "objective function" is the right term, suggest "cost function" instead.

Thanks. We have changed it to "cost function".
1. 194: "as described in Hastie" (add "as described in") Done.
1. 204: "the Python scikit module" (add "the") Done.
1. 220: better: "where MSE is minimum" Done.
1. 226: "fit residuals". I guess you mean trends Yes. We have changed it to “trends”.
1. 231: Reword: You probably mean less variability in the ridge model and lower absolute fit coefficients in the ridge regression. Please reword.

Yes. We have modified this sentence to "Compared with the trend profiles derived from OLS regression, the Ridge regression model has less variability and lower absolute fit coefficients." (Lines 256-258)
1. 233: "insignificant due to large uncertainties) up to 24-24%/decade" (replace "with" with "due to" and remove "up to")

Thanks. We have modified this sentence to "The largest ozone decreases appear in the tropical lower stratosphere (with about -30 % per decade for OLS and -12 % per decade for Ridge regression) although there are large uncertainties (>20 % per decade)." (Lines 259-260)
1. 233: "These large uncertainties" (remove "decreases and") Done.
1. 239: "We note" (remove "should") Done.
1. 249: change "compared between" to "derived from" Done.
1. 256: "across all three" (remove "the") Done.
1. 257: change "relatively" to "slightly" Done.
1. 262: change "in the NH" to "at NH" Done.
1. 280: "; and ERA5 shows". remove "and" and start a new sentence here Done.
1. 281: remove "more overestimated" Done.
1. 289: change "monthly mean variations" to "seasonal variations" Done.
1. 302: change ",, to some extent with smaller coefficients" to "absolute ridge-based trends and fit coefficients are smaller" Done.
1. 310: "based on the ridge regression" (add "the") Done.
1. 312: change "minimal" to "minimum" Done.
1. 363: "QBO response on ozone" (add "response") Done.
1. 373: change "there is a minimal solar cycle signal (negative and statistically significant) at ~10 hPa" to "there is a negative and statistically significant solar cycle response at ~10 hPa" Thanks. As we have updated the results for OLS regression, we have changed this sentence and added more information in the revised manuscript (Lines 410-439).
References:


Reply to the supplementary comment from Mark Weber:

There was one point I missed in my review. For trends from monthly mean ozone time series a correction is applied in the regression to account for autoregression (AR1). This correction does not change trends so much but increases the uncertainties due to the reduction of degree-of-freedom associated with AR. It can be applied to both OLS and Ridge regression and should be done. If not, at least a good reason should be given why it is not needed here.

Reply: We thank the reviewer for his comments and suggestions about applying a correction in the regression to account for the autoregression (AR1) for the trends from monthly mean ozone time series.

We have updated our results by including a lag-1 autocorrelation correction process in the OLS regression model with the Cochrane-Orcutt method (1949). The Cochrane-Orcutt method is a popular approach used to correct for first-order autocorrelation (AR1) in the residuals of a regression model with ordinary least squares (OLS) method (e.g. Dhomse et al., 2006; Ball et al., 2019; Petropavlovskikh et al., 2019; Bognar et al., 2022; Godin-Beekmann et al., 2022). The procedure is performed iteratively with the covariance matrix updated for each iteration until the autocorrelation coefficient has converged sufficiently (Cochrane-Orcutt, 1949; Prais and Winsten, 1954).

As mentioned by the reviewer, the trend coefficients do not change much but the uncertainties increase to some extent with this correction. It should be noted that the residuals in some region of the tropical mid-lower stratosphere are still large and auto-correlated after the AR1 correction with the Cochrane-Orcutt method. Hence, some limitations and assumptions of the Cochrane-Orcutt method should be noted, e.g.:

1. Limited to AR1 Autocorrelation: The Cochrane-Orcutt method is specifically designed to handle first-order autocorrelation (AR1). If the autocorrelation in the residuals follows a higher-order AR process or a different pattern, this method may not be appropriate or effective.

2. Relying on AR1 Parameter Estimation: Estimating the AR1 parameter involves making assumptions about the structure of autocorrelation and may not be reliable, especially with small sample sizes or noisy data.

3. Parameter Interpretation: After applying the Cochrane-Orcutt correction, the estimated regression coefficients and their interpretation can be affected. The coefficients of the corrected model may not have a direct interpretation in the same way as those from the original model.

4. Efficiency Loss: Correcting for autocorrelation may lead to a loss of statistical efficiency in parameter estimates, potentially resulting in wider confidence intervals and reduced power to detect significant effects.

5. Diagnostics: Assessing the adequacy of the correction and the presence of any remaining autocorrelation may be challenging. Model diagnostics become essential to ensure the correction's appropriateness and to identify any model misspecification issues.

6. Data Transformation: The method involves transforming the data and iteratively
estimating parameters, which may lead to additional complexities and computational burden, especially for large datasets.

**Figure RC1:** Estimates of a higher-order AR structure (AR2) of the residuals using autocorrelation and partial autocorrelation based on SWOOSH dataset.

Figure RC1 shows a case of the AR2 structure estimated by the autocorrelation and partial autocorrelation function of the residuals. Despite the limitations of the Cochrane-Orcutt method, the method of the usual least squares can still yield the best linear unbiased estimates of the regression coefficients provided the autocorrelated error terms are taken into account (Cochrane-Orcutt, 1949).

In the Ridge regression, an additional constraint (an L2 penalty) in the cost function is introduced to constrain the magnitudes and fluctuations of the coefficient estimates. This constraint helps to reduce the variance of the model at the expense of no longer being unbiased. For our current MLR setup, we choose not to apply the AR1 correction to Ridge regression. If we still apply the AR1 correction to Ridge regression as for the OLS regression, the estimated regression coefficients can be affected as the correlation between the regression model and underlying data becomes very poor after "correction", and the regression in this case is in an "under-fitting" state with a very large tuning parameter. Besides, when applying the AR1 correction to Ridge regression, the autocorrelation coefficient does not always converge during iteration which makes it impossible to obtain the covariance matrix as in OLS regression. Hence, care is needed when applying the AR1 correction to Ridge regression and more detailed work can be carried out in future studies.

We have added a paragraph in the revised manuscript to clarify the differences using OLS and Ridge regression models (Lines 231-245). In Figures RC2-3, the updated ozone trend profiles with AR1 correction applied to the OLS regression are shown and compared with Ridge regression results (with no AR1 correction). Please also see Figures 2-3 in the revised manuscript.

We also updated the other figures with corrected OLS regression and more detailed
modifications of the updated results are marked in red in the revised manuscript. The related code and data files are uploaded on github (https://github.com/AmyLee07/Data-and-code-for-OLS-and-Ridge-regression.git).

**Figure RC2:** Profiles of annual mean stratospheric ozone trends (\% per decade) compared between OLS and Ridge regression methods for three latitude bands (60-35°S, 20°S-20°N and 35-60°N) from (a-c) SWOOSH, (d-f) ML-TOMCAT, and (g-i) ERA5 model simulation over the period 1984-1997. Shaded regions are 2-σ uncertainties. (Data during 1991-1994 are removed).
Figure RC3: Same as Figure RC2 but for the post-1998 time periods (1998-2020) for SWOOSH, ML-TOMCAT and ERA5 model simulation.

References:


