

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

2
3 We thank Dr Weber for his useful comments and suggestions which have helped to improve
4 the manuscript. The reviewer's comments are given below in black text, followed by our
5 responses in blue text.

6
7 This paper reports on ozone trends derived from observations (SWOOSH dataset) and three
8 versions of the TOMCAT chemistry-transport-model (CTM). One of the CTMs
9 (ML-TOMCAT) has been adjusted to satellite observations, while the other two used
10 meteorological data from different reanalyses, ERA5 and its predecessor ERA Interim (up to
11 2019). Two types of regression models are used for ozone trend estimates before and after the
12 peak of stratospheric halogens occurring in the middle 1990. The first is the
13 ordinary-least-squares regression (OLS), the second is the ridge regression. The main idea
14 behind the ridge regression is to introduce an additional constraint in the cost function that
15 minimises the fit coefficients. Such a regression is generally recommended to avoid
16 overfitting. In general the ridge regression reduces the (absolute) trends (and all other fit
17 coefficients) and on the other hand reduces the variances (and correlation) between regression
18 model and the underlying data. The trends after 1998 in the upper stratosphere are positive
19 and significant in agreement with other studies (~2%/decade, e.g. Godin-Beekmann et al.,
20 2022). The ridge regression roughly halves these trends. Overall the paper is well written.
21 Some issues still need to be addressed before acceptance of the paper.

22
23 Discussion points:

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

29
30 Reply: According to the reviewer's suggestion, we have updated our results with ARI
31 correction applied to the OLS regression. As mentioned by the reviewer, the trend coefficients
32 do not change much but the uncertainties increase to some extent with this correction.
33 Detailed figures are updated and shown in the revised manuscript.

34
35 We have modified the sentences in the abstract (Lines 29-38) based on the updated results:
36 "For 1984-1997, we observe smaller negative trends in the SWOOSH stratospheric ozone
37 profile using Ridge regression compared to OLS. Except for the tropical lower stratosphere,
38 the largest differences arise in the mid-latitude lowermost stratosphere (>4% per decade
39 difference at 100 hPa). Since 1998, and the onset of ozone recovery in the upper stratosphere,
40 the positive trends estimated using the Ridge regression model (~1% per decade near 2 hPa)
41 are smaller than those in OLS (~2% per decade). In the lower stratosphere, post-1998
42 negative trends with large uncertainties are observed and Ridge-based trend estimates are
43 somewhat smaller and less variable in magnitude compared to the OLS regression. Aside

44 from the tropical lower stratosphere, the largest difference is around 2% per decade at 100
45 hPa (with ~3% per decade uncertainties for individual trends) in northern midlatitudes. For
46 both time periods the SWOOSH data produces large negative trends in the tropical lower
47 stratosphere with a correspondingly large difference between the two trend methods. In both
48 cases the Ridge method produces a smaller trend."

49
50 We also added the related information in the main text (Lines 290-295): "The largest
51 difference between OLS and Ridge regression methods occurs in the tropical lowermost
52 stratosphere with a difference of ~9% per decade at 100 hPa (but with larger
53 uncertainties >10% per decade for both regression methods), followed by the NH
54 mid-latitudes with >2% per decade difference at 100 hPa (~3% per decade uncertainties).
55 Note that, despite the large differences between OLS and Ridge-based trends, they are still
56 within the uncertainties of the individual trends."

57
58 l. 37: It is not surprising that ML-TOMCAT agrees better with SWOOSH than the other
59 models. Satellite corrections are derived from the same data that are also part of SWOOSH
60 (e.g. MLS). This should be mentioned here and also in the main text.

61
62 Reply: Yes. ML-TOMCAT agrees better with SWOOSH than the other models though it is
63 adjusted with SWOOSH data only for the Microwave Limb Sounder (MLS) measurement
64 period (UARS-MLS and AURA-MLS). We have added this information in the revised
65 manuscript. For e.g., "Comparing the ML-TOMCAT-based trend estimates with the
66 ERA5-forced model simulation, we find ML-TOMCAT shows significant improvements with
67 much better consistency with the SWOOSH data set, despite the ML-TOMCAT training
68 period overlapping with SWOOSH only for the Microwave Limb Sounder (MLS)
69 measurement period." (Lines 44-46)

70
71 l. 102: A detailed comparison between ERAI-TOMCAT and ERA5-TOMCAT has been
72 reported in Li et al. 2022. In this paper the model data have been extended to 2020, however,
73 ERAI ends in 2019 and trends are only reported up to 2018 for the ERAI-driven model. As
74 the differences between both models are not discussed in detail here but well covered in Li et
75 al. 2022, it could be safely omitted from this paper.

76
77 Reply: OK. We thank the reviewer for this insightful suggestion. We have removed the
78 ERAI-TOMCAT simulation and used only ERA5-TOMCAT to make the plots and main text
79 clearer and easier to read. Thus, all the data sets now have the same time period (1984-2020).
80 We also updated all the related text and figures in the revised manuscript as well as in the
81 supplement. Modifications are marked in red in the "track-changed" version of the revised
82 manuscript. (Note: The ERA5-TOMCAT simulation data used in the revised manuscript are
83 updated with the same latitude bins and pressure levels as SWOOSH and ML-TOMCAT
84 data)

86 l. 161: The MLR setup is very different from Li et al. 2022. For instance, now twelve
87 (monthly) trend terms are used instead of one (annual) and more proxies are used (e.g. EP
88 flux). Please motivate why you added more terms into the regression.

89

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

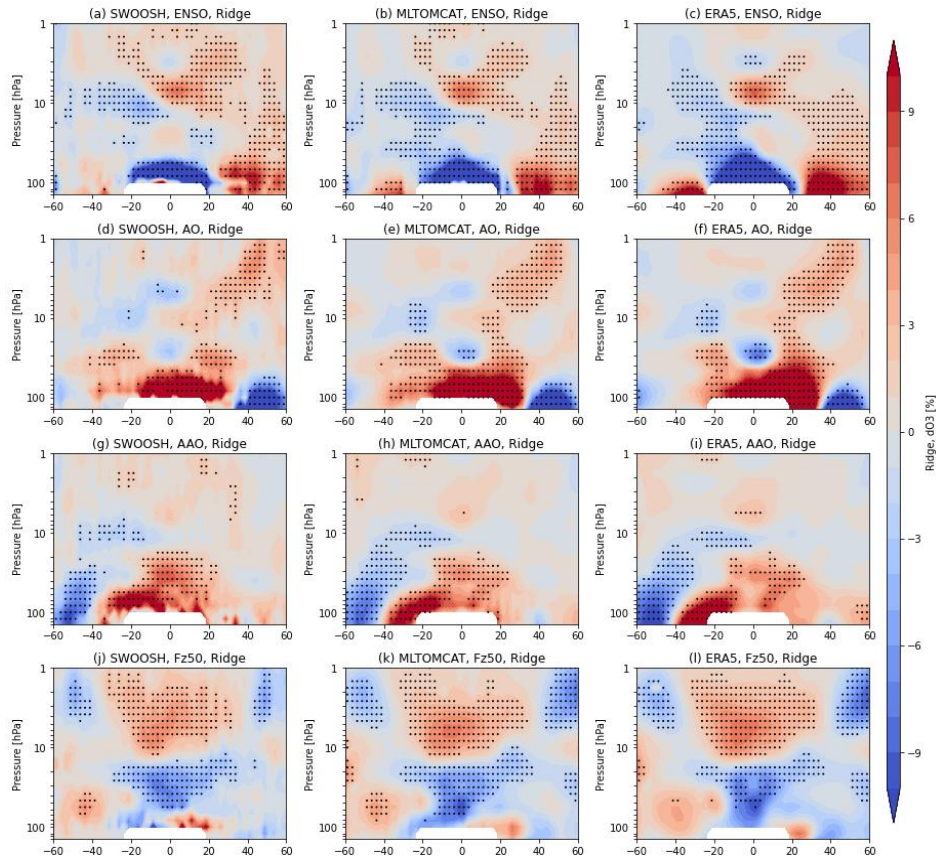
102

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

105

106 Reply: We have added the contribution from the EP flux proxy (the vertical component Fz at
107 50 hPa) in Figure 10 and the supplementary Figure S7. We also added discussion about its
108 contribution to ozone changes in the revised manuscript (Lines 463-470): "Changes in the
109 vertical component (Fz) of the stratospheric EP flux represents the ozone transport due to
110 variations in planetary wave driving from the troposphere into the stratosphere (Fusco and
111 Salby, 1999; Weber et al., 2003; Dhomse et al., 2006). In the tropics, the strengthened upward
112 transport is linked to an upward shift of the maximum ozone mixing ratio in the middle
113 stratosphere, as a result there are two cells of opposite ozone pattern near 10 hPa. A similar
114 pattern appears at mid-latitudes due to enhanced transport by the stratospheric residual
115 circulation. The out-of-phase between the tropics and mid-latitudes reflects the overturning
116 Brewer-Dobson circulation (Randel et al., 2002). In the lower stratosphere, the hemispherical
117 asymmetric ozone pattern could potentially result from the combination of changes in
118 chemical and dynamical processes (Banerjee et al., 2016; Abalos et al., 2017)."

119



120
 121 **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.

122
 123
 124
 125
 126
 127 l. 170: Only years 1991 and 1992 have been removed to avoid the use of an aerosol proxy, but
 128 Pinatubo eruption affected more years, e.g. end of 1990, 1993 and 1994. Please comment.

129
 130 Reply: We agree with the reviewer, hence we have revised the regression models. To exclude
 131 the effect from Mt. Pinatubo eruption (1991), we removed the years of data from 1991 to
 132 1994 in the updated regression models. The updated results with two more years (1993-1994)
 133 removed show very consistent results with previous results (1991-1992), except for some
 134 minor differences (e.g. ozone trends in the tropical lower stratosphere increase slightly during
 135 1984-1997).

136
 137 l. 175: Detrending means that the long-term trends in the proxies are moved to the linear trend
 138 terms. In Weber et al. 2022 we argued that the long-term dynamic trends are largely removed
 139 by the trends in the proxies, so that linear trends are then approximating the ODS related
 140 trends. In your case, the linear trends are combining dynamic and chemical trends. That
 141 should be mentioned here.

143 Reply: OK. We thank the reviewer for this reminder. We have added a sentence in the revised
144 manuscript to make it clear that the linear trends in our case are the combination of dynamic
145 and chemical trends (See Lines 187-188): "By de-trending, the long-term trends in various
146 proxies are moved to the linear trend terms, that is, the independent linear trends in the MLR
147 combine both the dynamic and the ODS-related chemical trends (Weber et al., 2022)."

148

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

152

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

155

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

162

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

166

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

168

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

170

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

172

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

174

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

178

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

183

184 Cross-validation is a way of studying how a specific sampled data set influences the mean
185 squared error/model fit, and provides a less sample-specific estimate of the MSE. In our case,
186 the fit residuals (correlation between model and regression) from Ridge regression are to

187 some extent larger (smaller) than that from OLS. The reason is probably that the original OLS
188 regression is somewhat over-fitting and this leads to smaller errors.

189

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

192

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

195

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

198

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

201

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

208

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

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

214

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

217

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

225

226 l. 335: In the lower stratosphere ridge and OLS are not reliable and fail to capture the large
227 variability. In addition, the data quality of satellites is lower in this region. So the "linear
228 relationship" is not the issue here

229

230 Reply: We apologise for the incorrect statement. We have modified this sentence in the
231 revised manuscript (Lines 373-376) as follows: "The considerable differences suggest that
232 there is a large degree of uncertainty in the estimates of seasonal ozone trends, particularly in
233 the lower stratosphere, where dynamical processes dominate, in addition there is larger
234 uncertainties in the satellite data. Therefore, caution is needed when discussing the results for
235 this region, as neither regression method can reliably capture the large variability."
236

237

238 l. 340: "These differences between OLS- and ridge- based ozone profile trends imply that
239 Ridge regression to some extent has improved the reliability of the model in the presence of
240 multi-collinearity." This is not generally true as discussed above. Again: Differences between
241 OLS and ridge-based trends are within the uncertainties of the individual trends.
242

243 Reply: We have modified this sentence as follows: "Despite these differences between OLS-
244 and Ridge-based ozone profile trends, the even larger uncertainties e.g. in the lower
245 stratosphere (Figure S3), indicate the ozone trends from two regression models are not
246 different from each other." (Lines 382-384)
247

248 l. 346: "Considering the nonlinear effect, the monthly terms of QBO proxies are used for
249 regression analyses" I do not understand what is meant to be said here. Statement can be
250 omitted.
251

252 Reply: OK. We have omitted this statement to avoid misinterpretation.
253

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

257 l. 358: "... may account for the more positive ozone trends", see previous comment
258

259 Reply: We apologize for the misleading statements. We have omitted these sentences in the
260 revised manuscript.
261

262 l. 363: How is the anomaly defined (amplitude, i.e. max minus minimum response relative to
263 the long term zonal mean ozone times the sign of the fit coefficient?). Please specify.
264

265 Reply: The ozone anomaly (in %) is calculated by referencing the monthly mean ozone to the
266 climatological mean for each calendar month. As all the explanatory proxies in the regression
267 models are normalised between 0 and 1, the contribution of the natural processes (QBO, solar,
268 ENSO, AO, AAO and EP flux) to the percentage ozone changes can be directly denoted by
269 the fit coefficients (also equivalent to the max minus minimum response relative to the
270 long-term zonal mean ozone times the sign of the fit coefficient).
271

272 l. 388: ozone trends are only shown below 60degs, but solar response up to 90degs. Ozone is
273 not well sampled above 50-60degs in the early period by SWOOSH. Is the solar response a

274 result from a fit solely limited to the late period after 1998? Why are ozone trends above
275 60degs not shown?

276

277 Reply: The solar response (Fig. 8), as well as the response from other natural processes (Fig.
278 10), is a result from a regression fit over the whole time period 1984-2020, not solely limited
279 to the late period after 1998. To avoid the not-well-sampled data above 50-60° in the early
280 period by SWOOSH, we have adjusted the latitude region in Figs 8 and 10 from 80°S-80°N to
281 60°S-60°N, at the same time to have consistent latitude regions as shown in the ozone trend
282 results (Figs 2-5).

283

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

286

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

289

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

292

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

296

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

300

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

304

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

308

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

314

315 l. 456: "The largest difference between OLS and Ridge regression methods appears in the
316 tropical lower stratosphere (with ~7 % per decade difference at 100 hPa).", but do not forget
317 the trend uncertainties for both regression are very high (~23%/decade).

318

319 Reply: Yes. As replied earlier, we have revised this sentence and also checked throughout the
320 paper to make relevant modifications. These modifications can be found in the revised
321 manuscript (Lines 290-295, 506-508).

322

323 Technical (selected):

324 l. 37: change to "the SWOOSH dataset" Done.

325 l. 58: "controlled by transport and" (omit "the") Done.

326 l. 150: add Snow et al. 2014 (doi:10.1051/swsc/2014001) as reference for the MgII index

327 The reference has been added.

328 l. 183: I am not sure if "objective function" is the right term, suggest "cost function" instead.

329 Thanks. We have changed it to "cost function".

330 l. 194: "as described in Hastie" (add "as described in") Done.

331 l. 204: "the Python scikrit module" (add "the") Done.

332 l. 220: better: "where MSE is minimum" Done.

333 l. 226: "fit residuals", I guess you mean trends Yes. We have changed it to "trends".

334 l. 231: Reword: You probably mean less variability in the ridge model and lower absolute fit
335 coefficients in the ridge regression. Please reword.

336 Yes. We have modified this sentence to "Compared with the trend profiles derived from OLS
337 regression, the Ridge regression model has less variability and lower absolute fit
338 coefficients." (Lines 256-258)

339 l. 233: "insignificant due to large uncertainties) up to 24-24%/decade" (replace "with" with
340 "due to" and remove "up to")

341 Thanks. We have modified this sentence to "The largest ozone decreases appear in the
342 tropical lower stratosphere (with about -30 % per decade for OLS and -12 % per decade for
343 Ridge regression) although there are large uncertainties (>20 % per decade)." (Lines 259-260)

344 l. 233: "These large uncertainties" (remove "decreases and") Done.

345 l. 239: "We note" (remove "should") Done.

346 l. 249: change "compared between" to "derived from" Done.

347 l. 256: "across all three" (remove "the") Done.

348 l. 257: change "relatively" to "slightly" Done.

349 l. 262: change "in the NH" to "at NH" Done.

350 l. 280: "and ERA5 shows". remove "and" and start a new sentence here Done.

351 l. 281: remove "more overestimated" Done.

352 l. 289: change "monthly mean variations" to "seasonal variations" Done.

353 l. 302: change "... to some extent with smaller coefficients" to "absolute ridge-based trends
354 and fit coefficients are smaller" Done.

355 l. 310: "based on the ridge regression" (add "the") Done.

356 l. 312: change "minimal" to "minimum" Done.

357 l. 363: "QBO response on ozone" (add "response") Done.

358 l. 373: change "there is a minimal solar cycle signal (negative and statistically significant) at
359 ~10 hPa" to "there is a negative and statistically significant solar cycle response at ~10 hPa"

360 Thanks. As we have updated the results for OLS regression, we have changed this sentence
361 and added more information in the revised manuscript (Lines 410-439).

362 l. 403: "being about twice larger" (add "being") Done.
363 l. 468: change "The negative AO/AAO coefficients" to "The negative phase of AO/AAO"
364 Done.

365

366 *PS: Some references are added according to the updated content in the revised manuscript.*

367

368 **References:**

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400 *to ozone-depleting substance (ODS) changes derived from five merged ozone datasets,*
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402 **Reply to the supplementary comment from Mark Weber:**

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

408
409 Reply: We thank the reviewer for his comments and suggestions about applying a correction
410 in the regression to account for the autoregression (AR1) for the trends from monthly mean
411 ozone time series.

412
413 We have updated our results by including a lag-1 autocorrelation correction process in the
414 OLS regression model with the Cochrane-Orcutt method (1949). The Cochrane-Orcutt
415 method is a popular approach used to correct for first-order autocorrelation (AR1) in the
416 residuals of a regression model with ordinary least squares (OLS) method (e.g. Dhomse et al.,
417 2006; Ball et al., 2019; Petropavlovskikh et al., 2019; Bognar et al., 2022; Godin-Beekmann
418 et al., 2022). The procedure is performed iteratively with the covariance matrix updated for
419 each iteration until the autocorrelation coefficient has converged sufficiently
420 (Cochrane-Orcutt, 1949; Prais and Winsten, 1954).

421
422 As mentioned by the reviewer, the trend coefficients do not change much but the uncertainties
423 increase to some extent with this correction. It should be noted that the residuals in some
424 region of the tropical mid-lower stratosphere are still large and auto-correlated after the AR1
425 correction with the Cochrane-Orcutt method. Hence, some limitations and assumptions of the
426 Cochrane-Orcutt method should be noted, e.g.:

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

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

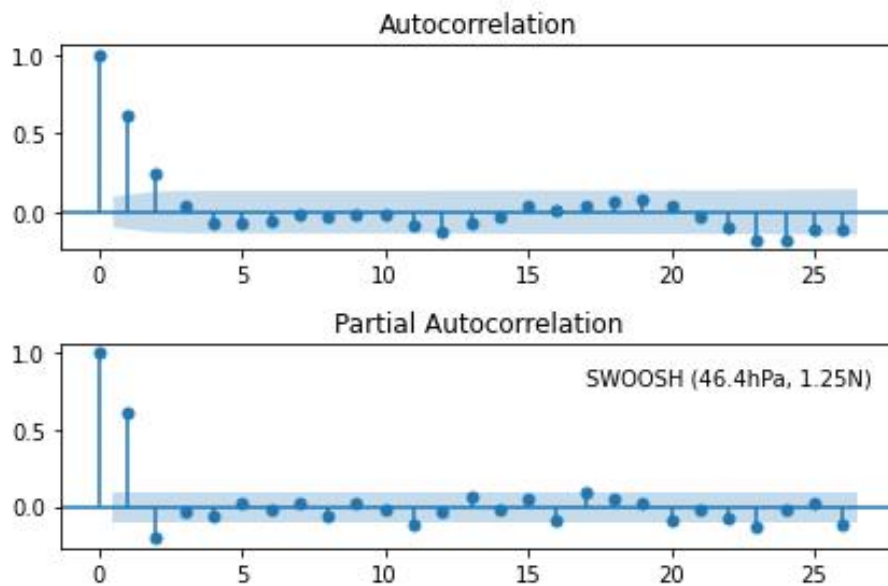
434 (3) Parameter Interpretation: After applying the Cochrane-Orcutt correction, the
435 estimated regression coefficients and their interpretation can be affected. The coefficients of
436 the corrected model may not have a direct interpretation in the same way as those from the
437 original model.

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

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

444 (6) Data Transformation: The method involves transforming the data and iteratively

445 estimating parameters, which may lead to additional complexities and computational burden,
446 especially for large datasets.



447

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

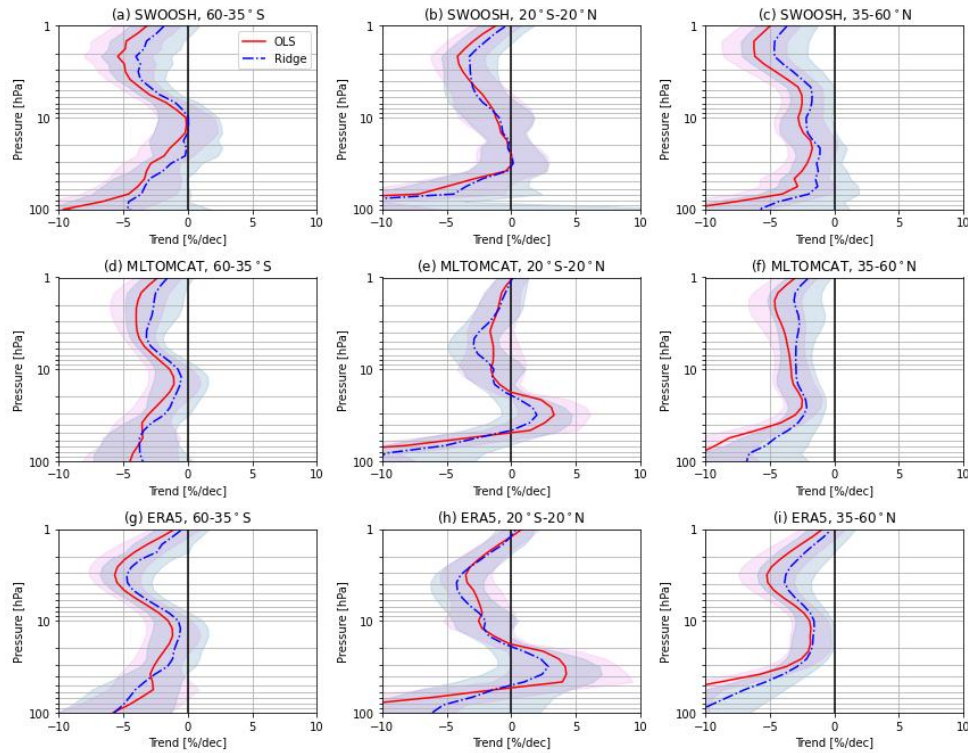
450 Figure RC1 shows a case of the AR2 structure estimated by the autocorrelation and partial
451 autocorrelation function of the residuals. Despite the limitations of the Cochrane-Orcutt
452 method, the method of the usual least squares can still yield the best linear unbiased estimates
453 of the regression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

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

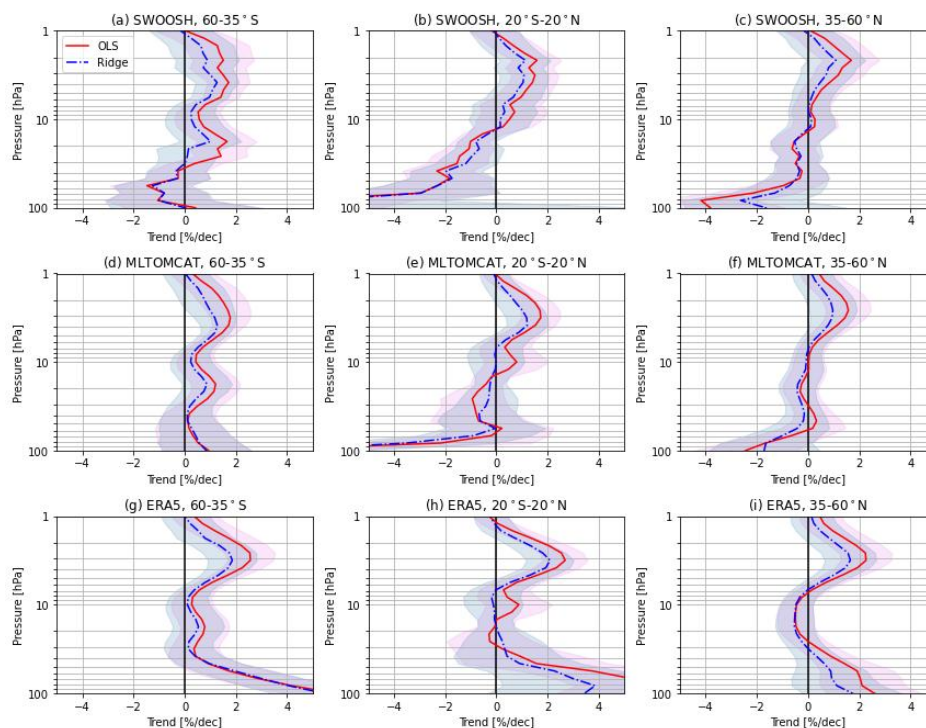
467 We have added a paragraph in the revised manuscript to clarify the differences using OLS and
468 Ridge regression models (Lines 231-245). In Figures RC2-3, the updated ozone trend profiles
469 with AR1 correction applied to the OLS regression are shown and compared with Ridge
470 regression results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

472 We also updated the other figures with corrected OLS regression and more detailed

473 modifications of the updated results are marked in red in the revised manuscript. The related
474 code and data files are uploaded on github ([https://github.com/AmyLee07/
475 Data-and-code-for-OLS-and-Ridge-regression.git](https://github.com/AmyLee07/Data-and-code-for-OLS-and-Ridge-regression.git)).
476



477
478 **Figure RC2:** Profiles of annual mean stratospheric ozone trends (% per decade) compared
479 between OLS and Ridge regression methods for three latitude bands (60-35°S, 20°S-20°N and
480 35-60°N) from (a-c) SWOOSH, (d-f) ML-TOMCAT, and (g-i) ERA5 model simulation over
481 the period 1984-1997. Shaded regions are 2- σ uncertainties. (Data during 1991-1994 are
482 removed).



483

484 **Figure RC3:** Same as Figure RC2 but for the post-1998 time periods (1998-2020) for
 485 SWOOSH, ML-TOMCAT and ERA5 model simulation.

486

487

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518

519 **Reply to the comments from the editor (Jens-Uwe Grooß):**

520

521 Editor Review of the Manuscript "Stratospheric ozone trends and attribution over 1984-2020
522 using ordinary and regularised multivariate regression models" by Li et al.

523 As one of the reviewers of this manuscript did not commit a review and the other review was
524 quite positive, I decided to base the decision of this manuscript on only one regular review
525 and this editor review. Although I am not an expert on regression methods, I find the paper
526 written clearly and understandable. Especially, the uncertainties of the derived ozone trends
527 depending on the regression methods seem important to me. Also the depiction of the
528 contribution of the natural processes to ozone changes is described well.

529 I would, however, suggest some more discussion of the results: To me it is not clear, in how
530 far the shown differences in regression methods are now explaining the discrepancy in the
531 lower stratosphere that was first pointed out by Ball et al. (2020). Besides the variability
532 induced by the regression method, is there a model improvement with respect to the
533 Multi-model-mean shown by Ball et al.? Or is this only the difference between free running
534 CCMs and the CTM shown here. What can be learned from the machine-learning results
535 (ML-TOMCAT)? Does the similarity with SWOOSH suggest that the basic mechanisms are
536 well understood or would you expect this similarity as it is constructed by machine-learning
537 using the observations? Why are the trends in the tropics so different between the two
538 re-analyses? Is this due to the vertical velocities?

539 Therefore I suggest minor revisions to include this discussion, that would potentially bring the
540 shown results better into the context of the present literature.

541

542 **Reply:** We thank the editor for his useful comments and suggestions about more discussion of
543 the results, which have helped to improve the manuscript. The editor's comments are given
544 below in black text, followed by our point-by-point responses in blue text.

545

546 (1) how far the shown differences in regression methods are now explaining the discrepancy
547 in the lower stratosphere that was first pointed out by Ball et al. (2020).

548

549 **Reply:** Indeed, regression model methodologies do play some role in the trend estimation.
550 Ball et al. (2020) used dynamical linear regression model (DLM) that attempts to determine
551 time varying trends. Basically, DLM takes into account the temporal relationship between the
552 dependent and independent variables, whereas OLS-type models assume that temporal
553 relationship between dependent and independent variables is not important. So, to some
554 extent somewhat larger negative trends shown in the study of Ball et al. (2020) are most
555 probably due to the regression methodology adopted in their study. On the other hand, even
556 with OLS/Ridge regression, models used here also show negative (though smaller in
557 magnitude) in the lower stratosphere and exact causes for those trends are still not well
558 understood. Although many recent studies (e.g., Chipperfield et al., 2018, Dietermüller et al.,
559 2021, Li et al., 2022) attribute negative ozone trends in the lower stratosphere to dynamical
560 changes, usage of reanalysis forcings (ERA1, ERA5, MERRA) are also not consistent, adding
561 uncertainty in our understanding about the dynamical changes (e.g. Davis et al., 2023).

562

563 We have added some discussion about the differences in regression methods and comparison
564 with the previous results (e.g. Ball et al., 2020) about the lower stratospheric ozone trends in
565 the revised manuscript: "Negative trends with larger uncertainties are observed in the lower
566 stratosphere, which are most pronounced in the tropics (-6.1 ± 12.0 % per decade at 100 hPa),
567 followed by the decrease at NH mid-latitudes (-1.6 ± 3.2 % per decade at 100 hPa). The largest
568 difference between OLS and Ridge regression methods occurs in the tropical lowermost
569 stratosphere with a difference of ~ 9 % per decade at 100 hPa (but with larger
570 uncertainties >10 % per decade for both regression methods), followed by the NH
571 mid-latitudes with >2 % per decade difference at 100 hPa (~ 3 % per decade uncertainties).
572 Note that, despite the large differences between OLS and Ridge-based trends, they are still
573 within the uncertainties of the individual trends. The observed ozone decreases in the lower
574 stratosphere are similar to recent records (e.g. Ball et al., 2019; 2020; Godin-Beekmann et al.,
575 2022), which could be explained by the increased tropical upwelling and mid-latitude mixing
576 (Wargan et al., 2018; Ball et al., 2020; Orbe et al., 2020; Davis et al., 2023). Nevertheless, the
577 modelled lower stratospheric trends do not match those derived from observations." (Lines
578 295-304)

579 "Compared to the trend estimates from simulation ERA5 in Figure 3, the ML-TOMCAT data
580 set shows more consistent results with the SWOOSH data, with negative ozone trends in the
581 tropical and NH mid-latitude lower stratosphere. Largest differences between SWOOSH- and
582 ML-TOMCAT-based ozone trends appear in the SH mid-latitude lower stratosphere where
583 ML-TOMCAT shows positive trends, and in the tropical mid- and lower stratosphere with
584 close to zero trends near 60 hPa (although these trends have large uncertainties). On the other
585 hand, trends from model simulation ERA5 show largest inconsistencies with respect to
586 SWOOSH-based trends in the lower stratosphere. Simulation ERA5 shows positive trends for
587 all three latitude bands that are more pronounced in the SH mid-latitudes (5.4 ± 2.0 % per
588 decade at 100 hPa for Ridge regression). These differences between satellite-based datasets
589 and model simulation suggest there are still large uncertainties in the lower stratosphere
590 where dynamical processes dominate (Dietmüller et al., 2021; Li et al., 2022). Ball et al.
591 (2020) reported significant discrepancies in observation-model lower stratospheric ozone
592 trends by using various satellite-based data sets and chemistry-climate models (CCMs).
593 Although the inconsistencies vary with various datasets and fit methods (Dietmüller et al.,
594 2021; Bogner et al., 2022), models generally do not reproduce the observations and the reason
595 remains an open question." (Lines 305-319)

596

597 (2) Besides the variability induced by the regression method, is there a model improvement
598 with respect to the Multi-model-mean (MMM) shown by Ball et al.? Or is this only the
599 difference between free running CCMs and the CTM shown here.

600

601 Reply: The TOMCAT 3-D off-line chemical transport model (CTM) shown here is forced
602 with meteorological fields from ECMWF ERA5 reanalyses (Hersbach et al., 2020) with a
603 coherent historical assimilation of observations and full stratospheric chemistry scheme to
604 reproduce the behaviour of ozone as closely as possible.

605

606 Objectively, there is no model improvement with respect to the Multi-model-mean (MMM)
607 shown by Ball et al. (2020). The inconsistencies in observation-model lower stratospheric
608 ozone trends shown in this study show some differences with those in previous study (Ball et
609 al., 2020), which results from the difference between free-running CCMs and the CTM shown
610 here. As replied above, we have added some discussion about the discrepancy of the ozone
611 trends in the lower stratosphere.

612

613 (3) What can be learned from the machine-learning results (ML-TOMCAT)? Does the
614 similarity with SWOOSH suggest that the basic mechanisms are well understood or would
615 you expect this similarity as it is constructed by machine-learning using the observations?

616

617 Reply: The ML-TOMCAT data set we use here is a long-term chemically (and dynamically)
618 consistent, satellite-data-based global gap-free stratospheric ozone profile data generated by
619 applying a supervised machine-learning (ML) algorithm to the random-forest (RF) regression
620 analysis (Dhomse et al., 2021).

621

622 The similarity or better agreement with SWOOSH is not surprising, as also mentioned by the
623 reviewer (Dr Mark Weber), since satellite corrections used for ML-TOMCAT are derived
624 from the same MLS data which are also part of SWOOSH, i.e. using 20 years of UARS-MLS
625 (1991–1998) and AURA-MLS (2005–2016) measurements as a training period. However, it is
626 also important that for the non-MLS time period, SWOOSH relies on limited (~30 profiles
627 per day) observations from SAGE II and HALOE solar occultation instruments. So, monthly
628 zonal means in SWOOSH data would have a limited set of observations but ML-TOMCAT
629 would have means from all the model grid points. Dhomse et al. (2021) have demonstrated
630 that ML-TOMCAT ozone concentrations are well within uncertainties of the observational
631 data sets at almost all stratospheric levels, and there are significant improvements compared
632 to the TOMCAT 3-D chemical transport model. Here we aim to illustrate that even with a
633 limited set of denser observations to construct machine-learning based data, it still shows
634 remarkable consistency with purely satellite measurement-based data in terms of ozone
635 trends.

636

637 We have also added some sentences and comments about the similarity/agreement of the
638 ML-TOMCAT data set with SWOOSH in the revised manuscript, e.g. "Comparing the
639 ML-TOMCAT-based trend estimates with the ERA5-forced model simulation, we find
640 ML-TOMCAT shows significant improvements with much better consistency with the
641 SWOOSH data set, despite the ML-TOMCAT training period overlapping with SWOOSH
642 only for the Microwave Limb Sounder (MLS) measurement period." (abstract, Lines 44-46)
643 & "The better agreement between ML-TOMCAT and SWOOSH, due to satellite corrections
644 derived from the same MLS measurements, show some improvements in this
645 machine-learning based data set compared to TOMCAT chemical transport model." (Lines
646 306-308).

647

648 (4) Why are the trends in the tropics so different between the two re-analyses? Is this due to
649 the vertical velocities?

650

651 Reply: Due to the differences existed between ERA5 and ERA-Interim reanalyses (e.g.
652 vertical and horizontal resolutions, radiative transfer models and measurements assimilated,
653 and changes in number and type of observations adopted), the differences of the trends in the
654 tropics between the two re-analyses can be attributed to many reasons, including the different
655 vertical velocities.

656

657 A detailed comparison between the model simulations forced by two re-analyses (ERA-Interim and
658 ERA5), including the difference of the stratospheric ozone profiles trends, has been reported
659 in Li et al. (2022). From the discussion about the differences in age-of-air (AoA) tracer
660 between two simulations, there exist some fundamental differences in the representation of
661 Brewer-Dobson circulations between two reanalysis data sets.

662

663 As for TOMCAT setup, simulation ERA5 shows improvements in the TCO biases in the
664 tropics compared to simulation ERA-Interim. A possible explanation is that the finer vertical
665 resolution in ERA5 alters vertical transport pathways that are critical for controlling ozone
666 concentration as, within a few kilometres in the stratosphere, the ozone lifetime changes from
667 days to a few years. Besides, simulation ERA5 shows increasing AoA trends in the whole
668 stratosphere, while simulation ERA-Interim shows a hemispheric dipole trend pattern with increasing
669 AoA in the NH and decreasing trend in the SH lower stratosphere.

670

671 As differences between TOMCAT simulation forced with ERA-Interim and ERA5 are already
672 discussed in Li et al., (2022), the reviewer (Dr Mark Weber) suggested to omit results and
673 discussion of ERA-Interim. Hence, all the related comparison between the two model simulations has
674 been removed from the revised manuscript.

675

676

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