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Is interactive ozone chemistry important to represent polar cap stratospheric temperature variability in Earth-System Models?

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Abstract

Considering the representation of the atmosphere, the current generation of Earth-System Models differs mainly in the representation of the stratospheric ozone layer and its variability and changes. So-called high-top models have a well resolved stratosphere and typically calculate ozone chemistry interactively, low-top models on the other hand rely on parameterized ozone chemistry or prescribed climatological ozone fields and have a model top below the stratopause. Here we investigate whether interactive ozone chemistry is important for representing temperature variability and extremes in the Arctic polar stratosphere. To this end we analyze a suite of two 200-year sensitivity simulations, one with interactive ozone chemistry and one without, performed with the Whole Atmosphere Community Climate Model version 4 (WACCM4), a stratosphere-resolving version of the National Center for Atmospheric Research Community Earth-System Model. We find a tight coupling between ozone and temperatures over the Arctic polar cap, manifesting in increased variability in stratospheric spring-time temperatures in simulations with interactive chemistry compared to simulations imposing climatological mean ozone abundances. Our results indicate that stratospheric temperature extremes regularly occurring in simulations with interactive chemistry are absent in uncoupled model simulations.

1. Introduction

Since the detection of the Antarctic ozone hole in the 1980s (e.g., Farman et al., 1985) the state of the stratospheric ozone layer has received increasing attention. Nowadays it is well understood that anthropogenic emissions of ozone depleting substances (ODSs) are the main driver of stratospheric ozone loss. ODS emissions have been phased out within the Montreal Protocol and subsequent amendments. Following the slow but steady decline in ODSs (e.g., Mäder et al., 2010; Montzka et al., 1999), simulations with state-of-the-art chemistry climate models (CCMs) performed within the Chemistry-Climate Model Initiative (CCMI) (Morgenstern et al., 2017) project a recovery of the ozone layer over the course of the 21st century, although in timing dependent on the latitude band (e.g. Dhomse et al., 2018).

Generally speaking climate models have become increasingly more complex over recent decades while evolving from high-end General Circulation Models to coupled Earth-System Models (ESMs). The Coupled Model Intercomparison Project Phase 5 (CMIP5) (Taylor et al., 2012) in support of the Intergovernmental Panel on Climate Change's Fifth Assessment Report (IPCC AR5) included both stratosphere resolving (high-top) models and models whose model top was below the stratopause (~ 50-60 km, low-top models) (IPCC, 2013). One major difference in high-top and low-top models is the consideration of the stratospheric ozone layer, its variability and changes. As the computational burden of coupled chemistry calculations is high, particularly for centennial integrations, most studies rely on low-top models or high-top models with a well-resolved stratospheric circulation but without interactive ozone chemistry (e.g., Charlton-Perez et al., 2013; Eyring et al., 2013).

A series of studies, utilizing high-top models, highlighted the role of ozone depletion, in addition to that of well-mixed greenhouse gases, as one of the key drivers of climate changes in recent decades in the Southern Hemisphere (e.g., Gillett and Thompson, 2003; Kang et al., 2011; McLandress et al., 2010; Polvani et al., 2011a; Polvani et al., 2011b; Son et al., 2009; Son et al., 2010). In addition, significant changes in the large-scale atmospheric circulation, such as the mean residual stratospheric circulation (i.e., the Brewer Dobson Circulation), have been attributed to ozone depletion (e.g., Oberländer-Hayn et al., 2015; Polvani et al., 2018) and several studies have addressed the role of ozone in driving stratospheric temperature changes (e.g., Ivy et al., 2016; Langematz et al., 2014; Shine et al., 2003). While the majority of research has focused on the Southern Hemisphere, several recent studies investigated the effects of ozone extremes on Northern Hemisphere climate (e.g., Calvo et al., 2015; Ivy et al., 2017).

Recent work has also highlighted significant differences in model simulations with interactive and specified ozone chemistry (e.g., Gillett et al., 2009; Waugh et al., 2009) and biases in Southern Hemisphere climate trends resulting from coarsely specifying stratospheric ozone (Neely et al., 2014). However, the question whether interactive ozone chemistry is important for representing temperature variability in the Arctic polar stratosphere remains unanswered: here we aim on bridging this gap. Previous work has highlighted the coupling between ozone concentrations and stratospheric temperatures over the Arctic polar cap. In short, years with greater ozone depletion are expected to display greater cooling, and vice versa (e.g., Calvo et al., 2015; Rieder et al., 2014). Given the coupling of ozone and temperature our study seeks to answer the question whether Arctic polar cap temperature variability is equally represented in simulations with and without interactive ozone chemistry. We focus on daily and monthly mean temperatures in the lower (50 hPa) and middle stratosphere (30 hPa), the atmospheric layers with largest ozone abundances in the Arctic. While the bulk of the temperature distribution in both sets of simulations agrees well with the observational record our results below indicate substantial differences in stratospheric spring-time polar cap temperature variability between simulations with and without interactive ozone chemistry. Effects are particularly pronounced for the low tail of the temperature distribution and for probabilistic temperature extremes. Our results indicate that extreme temperatures that arise regularly in simulations with interactive ozone chemistry are absent in model simulations with prescribed ozone fields. Hence, our results argue for caution in estimating stratospheric temperature variability using simulations without interactive ozone chemistry

2. Methods

To investigate the role of interactive ozone chemistry on temperature variability over the northern polar cap (60-90º N) we analyze two long time-slice simulations performed with the Whole Atmosphere Community Climate Model version 4 (WACCM4), the stratosphere-resolving version of the National Center for Atmospheric Research Community Earth-System Model. The underlying model is well documented in Marsh et al. (2013) and Smith et al.

(2014). WACCM4 is fully coupled to interactive ocean, land, and sea ice components and includes an interactive atmospheric chemistry scheme (Kinnison et al., 2007). The models horizontal resolution is 1.9º in latitude and 2.5º in longitude; its vertical resolution ranges between about 1.2 km near the tropopause to about 2 km near the stratopause, the model top is located at 140 km and the model comprises a total of 66 levels.

We performed two 200-year long simulations with this model. Both simulations are performed with perpetual year 2000 forcings (including greenhouse gases, halogen concentrations, aerosols and total spectral irradiance) as specified by the Climate Model Intercomparison Project, Phase 5. The difference in the two simulations lies in ozone chemistry: one integration is performed with interactive ozone chemistry (INTER) one without (PRESC). In the PRESC integration we specify stratospheric ozone concentrations as the long-term zonal mean, monthly mean, obtained from INTER. The climatological mean state in INTER and PRESC is nearly identical (Smith et al., 2014).

Neely et al. (2014) highlighted significant biases in Southern Hemisphere climate, resulting from coarsely specified ozone concentrations due to under sampling of sub-monthly temporal changes in ozone during the seasonal evolution of the Antarctic ozone hole. Although sub-monthly ozone changes are also under sampled during Northern Hemisphere spring, this does not affect the robustness of our result given the overall much weaker amplitude (about a factor of 5; see Fig. S1) compared to the Southern Hemisphere (see Fig. 1 in Neely et al. (2014)).

3. Results

In Figs. 1a-b we illustrate the variability in daily ozone mixing ratios from INTER in the lower (LS; 50 hPa) and middle stratosphere (MS; 30 hPa) on monthly basis. While daily LS and MS ozone variability can be as large as 1 ppmv in late winter and spring, it is strongly reduced during summer season. We note that a general good agreement of ozone concentrations for this model version with radiosonde observations was illustrated in previous work (Calvo et al., 2015). For each month, we also illustrate the mean ozone mixing ratio specified in PRESC in Figs. 1a-b.

Since by design the only difference between INTER and PRESC lies in the modeled ozone chemistry (interactive or not) and thus the ability of ozone to vary inter-annually in one case (INTER) but not in the other (PRESC), we attribute temperature differences between the two integrations to radiative effects. We quantify the internal variability in these simulations by the frequency of Sudden-Stratospheric Warmings (SSWs), computed as in Charlton and Polvani (2007), for the extended winter season (NDJFM). Our results show that the number of SSWs is very similar in INTER (5.55 SSWs per decade) and PRESC (5.45 SSWs per decade). In Fig. 1c-d we show the spread of daily LS and MS temperatures on monthly basis for the two simulations. The bulk of the temperature distribution in INTER and PRESC is similar from June to March, which is consistent with the expectation based on the use of the climatological mean ozone from INTER in PRESC. While substantial overlap also exists in April and May, significant differences (at the 95% level, identified by a Kolmogorov-Smirnov (KS) test) emerge in the distributions. We thus ask whether a cleaner way exists to unravel the influence of ozone chemistry on temperature variability in the LS and MS.

As we hypothesize that the presence of inter-annual variability in ozone results in increased temperature variability in INTER, we compare the tails of the polar cap temperature distributions obtained from INTER and PRESC. For each simulation, we select data from 20 years (10% of the simulation days). To allow for a targeted comparison, we select for INTER those years with lowest/highest April (May) mean ozone and for PRESC those with coldest/warmest mean April (May) temperatures. Figs. 1e-h illustrate the difference between the monthly springtime average of the extremes for the INTER and PRESC sub-sets. Low/ high ozone in INTER results in significantly colder/warmer mean LS and MS temperatures than reached, on average, in the coldest/warmest springs in the PRESC subset. Results are significant at a 95% level (assessed with a KS test) for the low ozone – coldest temperature pairs. If interactive ozone chemistry is not a necessary ingredient to capture the extremes, one would expect no significant difference in the distributions of the two sets or cooler conditions for the PRESC subset as it was selected based on temperature itself. For the high ozone – warmest temperature pairs the difference in the distribution is less robust and is altitude dependent (indicated by dashed distribution curves in the MS in April and LS in May). We assess the importance of interactive ozone chemistry further by comparing the shortwave (SW) radiative heating rates of the INTER and PRES simulations. The PDF of SW radiative heating rates is substantially wider in INTER than PRESC (see Fig. S2) and the two PDFs are significantly different at the 95% level (assessed with a KS test). This indicates that enhanced temperature extremes in INTER emerge largely due to the (direct) radiative effect of ozone.

This result confirms the tight coupling of temperature and ozone. However, it does not address the main question of interest here, namely whether one can detect a significant difference in stratospheric temperature variability between the INTER and PRESC simulations. To answer that question we next repeat the analysis considering the distribution of *daily* data contained in these 20 year subsets: this provides a more detailed insight into the temperature variability in INTER and its drivers.

First, we turn to the coupling between ozone and temperatures in the LS and MS. In Figs. 2a,b we illustrate the seasonal cycle of daily ozone in the LS and MS in INTER. Then, we sample the daily data based on April (for completeness we show results for May in the supplemental material, Figure S3) monthly mean ozone. It can be seen that ozone rich/poor springs are preceded by generally ozone rich/poor conditions throughout the winter season. This 'persistence' of the ozone field, which integrates the chemical and dynamical conditions of the polar cap, has been subject of interest also in our recent work (Rieder et al., 2018). Figures 2c,d show the temporal evolution of temperatures in the LS and MS. Comparing Figs. 2a,b and 2c,d one sees that the evolution in ozone (Figs. 2a,b) is reflected in the temperatures in the LS and MS. In addition we have performed a lagged correlation analysis on monthly time scales which reveals (i) a tight correlation between springtime mean ozone mixing ratios and temperature in spring and preceding months and (ii) a linear correlation (increasing with decreasing lag) between springtime mean temperature and ozone mixing ratios.

Next we focus on the spread of daily ozone in the low/high ozone samples on monthly basis (Figs. 2e,g). Here a clear separation of the bulk (the color-coded box) and overall significant difference at 95% level in the tails (represented through the whiskers) is present from January to May. This is also seen in the PDF of daily temperatures (Figs. 2f,h), particularly in the LS. Thus we conclude that ozone variability clearly affects daily temperature variability in INTER.

To investigate whether the ozone is indeed the driver of temperature extremes, we turn again to the comparison of the INTER and PRESC simulations. In Fig. 3 we compare the cumulative probability function (CDF) of daily April temperatures in the LS and MS in INTER and PRESC (brown and green curves respectively; for completeness we show results for May in Fig. S4). The CDFs are significantly different (at the 95% level according to a KS test), with generally higher probabilities for cold temperatures in INTER (Fig. 3a,b). As the temperature subset in INTER has been chosen based on springtime mean ozone, we can parse apart the contribution of ozone to this difference in Figs. 3c-d. First we turn back to temperatures in INTER, sub-sampled based on April mean ozone. The PDFs for neutral ozone (grey curve, containing data from 160 years) and ozone poor/rich conditions in INTER (red and blue curves respectively, each containing data from 20 years) are clearly offset and significantly different (at the 95% level according to a KS test). In INTER, extremely cold daily temperatures are unlikely to be reached in ozone rich (given in red) or neutral years (given in grey), while extremely warm temperatures require such conditions.

The PDFs for neutral years in INTER (i.e., the grey curve, including neither ozone rich/poor years in Figs. 3c-d) and the PRESC simulation (dashed green curve Figs. 3c-d) are very close together and agree with the available reanalysis record (see purple dashed curve for the MERRA-2 reanalysis (data for January 1980 to April 2018) in Fig. 3c-d). Thus we conclude that INTER and PRESC do not differ much in the mean state, again consistent with the use of a mean ozone climatology in PRESC, which is taken as a long-term average of INTER.

Temperature extremes as found in the low/high ozone subsamples of INTER have not emerged in the past observational record; our results however indicate that such extremes might be possible under the present ODS burden dependent on dynamic (pre)conditioning. The increased variability in stratospheric temperatures in INTER is represented in generally longer tails. This is further illustrated in Figs. 3e-f, where we summarize data from Figs. 3a-d in box-whisker plots. These confirm that temperatures in the bulk (colored boxes, with colors as described above) agree well between INTER and PRESC and with the available observational record from reanalysis. However, the overall variability amplitude (i.e. the full range encompassed by the whiskers) is unmatched between the two integrations, indicating that interactive chemistry is needed to capture the tails and overall variability of temperatures in the LS and MS.

Last we focus on the difference in the tails of MS and LS temperatures in INTER and PRESC. To this aim we apply extreme value theory (e.g., Coles, 2001). Specifically, we fit a Generalized Pareto Distribution to subsets of daily temperatures in INTER and PRESC representing extreme conditions and derive probabilistic return periods for stratospheric temperatures in both sub-sets. We do so for the low (temperatures below the 1%-quantile) and high tail (temperatures above the 99% quantile) of both simulations as well as the daily temperatures of the on average 20 coldest (warmest) Aprils in PRESC and on average 20 ozone poorest (richest) Aprils in INTER. The corresponding return periods are given in Fig. 4 (results for May are given in Fig. S5).

First, let us consider return periods based on the low and high tail of the temperature data in both INTER and PRESC (Figs. 4a-d). For these subsets the return period analysis shows that extreme LS and MS temperatures that are regularly occurring in INTER (i.e., with return period below 3 years) are rarely reached in PRESC. Temperatures with decadal occurrence frequency in INTER never occur in PRESC: this holds for both cold (Fig. 4a-b) and warm extremes (Fig. 4c-d). Overall return periods for extremes are clearly separated for INTER and PRESC as illustrated by the corresponding 95% confidence bound (dotted curves).

Next we derive probabilistic temperature return periods based on data from the on average 20 coldest (warmest) Aprils in PRESC and on average 20 ozone poorest (richest) Aprils in INTER (Figs. 4e-h). Contrasting Figs. 4e-h with Figs. 4a-d highlights that these differences in temperature extremes can be attributed to ozone variability between the two simulations. For INTER return periods derived from GPD fits to data sampled based on April mean ozone match closely those derived from the low tail of the entire 200-year simulation. These return periods are substantially shorter for both cold and warm extremes compared to those derived from data of the 20 coldest/warmest Aprils in PRESC. These results indicate that the inclusion of interactive ozone chemistry in ESMs is important to capture the temperature extremes in the polar stratosphere.

4. Discussion and Conclusions

The modeling capabilities of the scientific community have steadily expanded in recent years, leading to the development of fully coupled Earth System Models (ESMs). Despite growing computational resources, interactive stratospheric ozone chemistry is still expensive, particularly for centennial integrations, and is therefore not regularly included in ESMs. Several studies have highlighted substantial differences between results of models in the IPCC-AR5 (e.g., Gillett et al., 2009; Waugh et al., 2009) and the tight coupling between the stratosphere and troposphere has received attention (e.g., Charlton-Perez et al., 2013).

Motivated by this, here we assess the importance of interactive ozone chemistry for the representation of polar stratospheric temperature variability in ESMs. We do so by contrasting two multi-decadal (200-year) integrations with perpetual year 2000 forcings, one with interactive ozone chemistry and one without (which means that ozone mixing ratios are prescribed). Our results show a tight coupling between ozone and temperatures over the Arctic polar cap and a statistically significant difference in stratospheric spring-time temperatures for simulations with prescribed ozone vs. those with interactive chemistry.

Effects are particularly pronounced for the low tail of the temperature distribution and probabilistic temperature extremes. Applying return level analysis we show that temperatures that occur regularly in simulations with interactive chemistry are rarely or never reached when climatological ozone is prescribed. Given the tight stratosphere-troposphere coupling, studies exploring consequences for Northern Hemispheric surface climate are suggested for future research.

In summary our results argue for caution, as they indicate that extreme temperatures that arise regularly in simulations with interactive ozone chemistry are absent in model simulations with prescribed ozone. These findings imply that interactive chemistry needs to be included in ESM simulations, and argue for caution in quantifying stratospheric temperature variability in simulations with prescribed ozone fields in upcoming CMIP 6 activities. In closing, we note that the question whether the stratospheric temperature extremes analyzed here are also able to affect the surface climate will be carefully addressed in follow up work.

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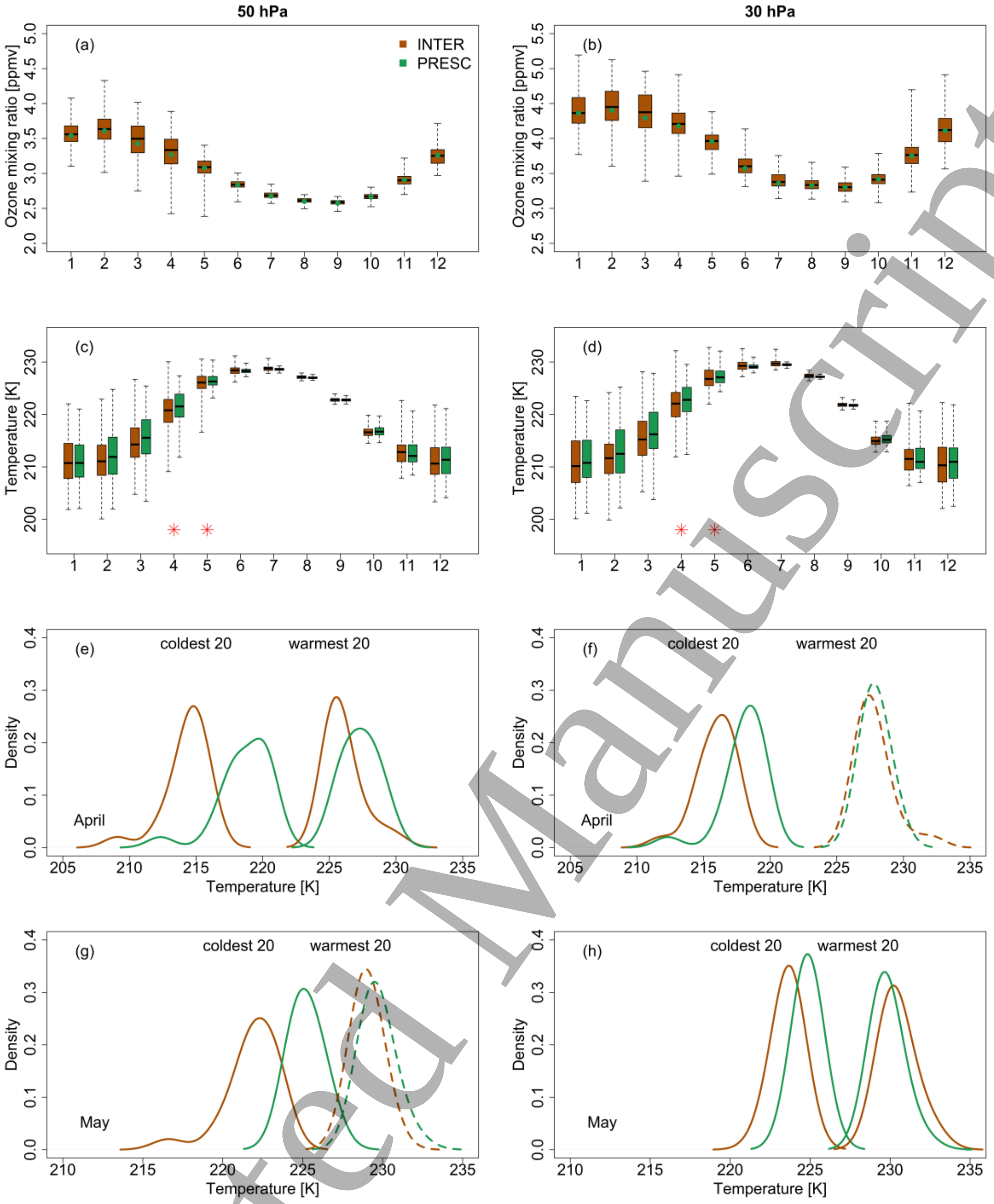

Figure 1: (a) Lower stratospheric (50 hPa) monthly mean ozone mixing ratios for the INTER integration and climatological monthly mean values prescribed in the PRESC integration. (b) as (a) for the middle stratosphere (30 hPa). (c) monthly mean lower stratospheric temperatures for the INTER and PRESC integrations. (d) as (c) but for the middle stratosphere. Asterisks indicate months with significant difference between INTER and PRESC distributions, at the 95% level. PDFs of (e-f) April and (g-h) May mean temperature for the coldest and warmest 20 years in the INTER and PRESC integrations. Solid curves indicate a significant difference between the two integrations at the 95% level, while dashed curves indicate no significant difference.

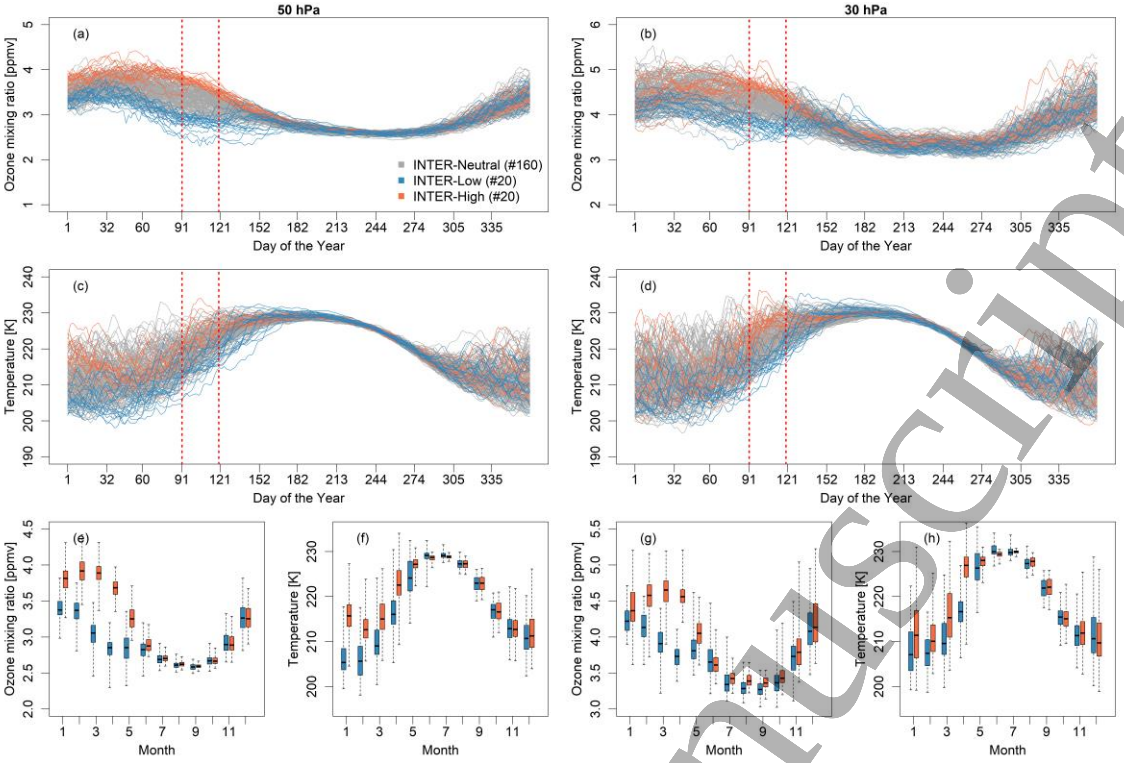

Figure 2: Temporal evolution of ozone mixing ratios in the (a) lower (50 hPa) and (b) middle stratosphere (30 hPa) for the INTER integration. (c-d) as (a-b) but for temperatures. (e-f) lower and middle stratospheric ozone mixing ratios and (g-h) temperatures, aggregated on monthly basis, during years with low/high ozone in April. Curves in (a-d) and boxplots in (e-h) are color coded based on April mean ozone mixing ratios (see legend in panel (a)).

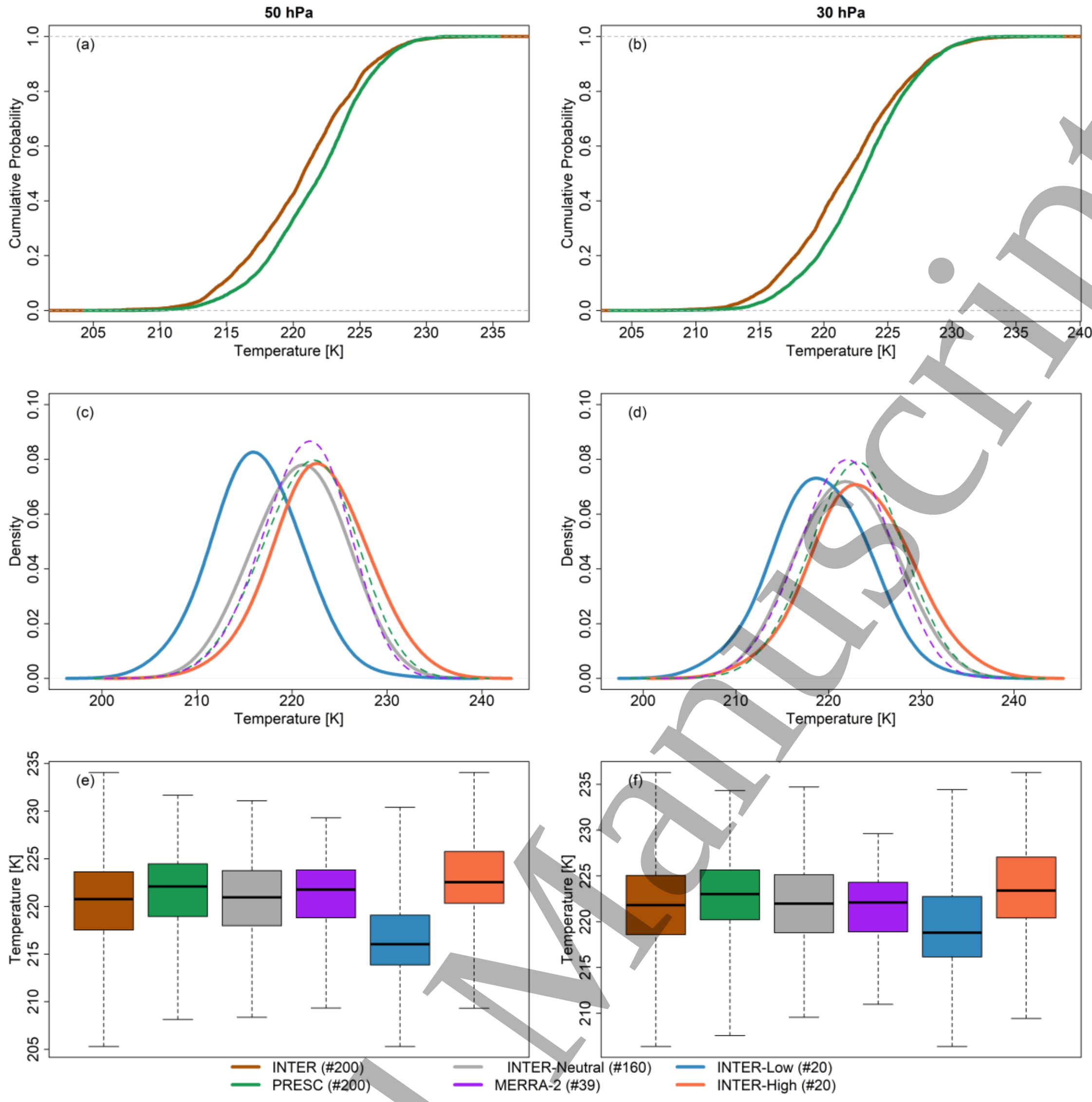

Figure 3: Cumulative probability function for April daily mean temperature in the INTER and PRESC integrations for the (a) lower (50 hPa) and (b) middle stratosphere (30 hPa). (c-d) PDFs of subsets of INTER (based on mean April ozone mixing ratios). For convenience, the PDF for the PRESC integration (dashed green curve) and MERRA-2 reanalysis data (dashed purple curve) is given, along INTER. (e-f) box and whisker illustration of subsets shown in (a-d); colored boxes mark the 25% to 75% quantile range, solid black lines the median value.

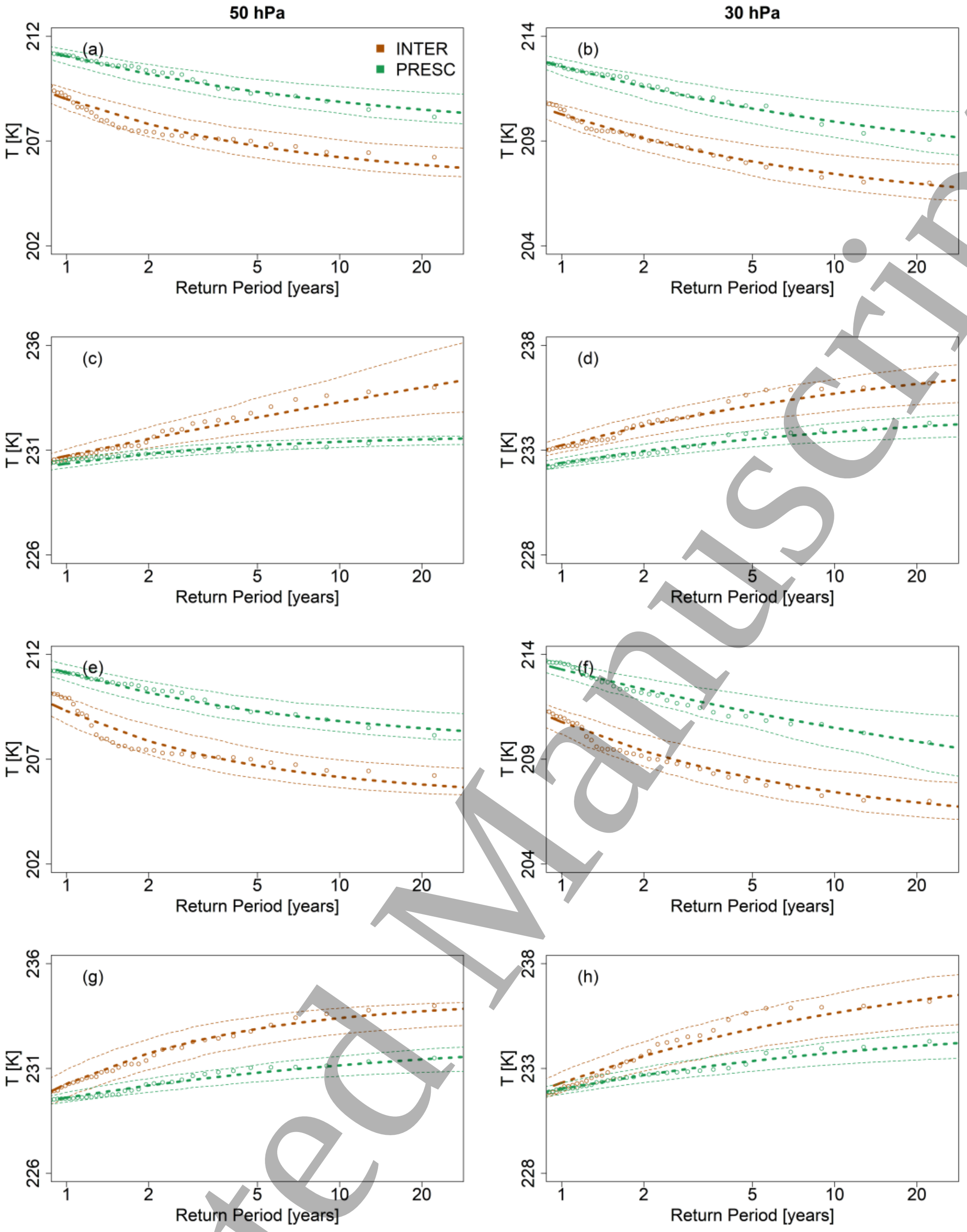

Figure 4: Probabilistic return period estimates (long dashed curves) for (left) lower (50 hPa) and (right) middle (30 hPa) stratospheric daily temperature extremes in April for the INTER and PRESC simulations. Panels (a,b) show return periods for cold and panels (c,d) for warm temperature extremes; defined as the 1% and 99% quantile, respectively. Panels (e-h) show return level estimates based on 20-year subsets with lowest (e,f) / highest (g,h) monthly mean ozone (INTER) and coldest (e,f) / warmest (g,h) monthly mean temperature (PRESC). The dotted lines in (a-h) provide the 95% confidence bounds for return period estimates.