Stratospheric Age-of-Air: Sensitivity to Finite Volume Remapping Algorithm

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Key Points:

- In GEOS-5 the stratospheric mean age-of-air is sensitive to the remapping scheme used within the finite-volume dynamical core that controls how individual material surfaces are vertically interpolated back to standard pressure levels after each horizontal advection time step.
- This sensitivity in the age-of-air imprints not only on other idealized tracers, but also on several long-lived chemical trace gases (e.g., N_2O, CH_4).
- The age-of-air differences primarily reflect changes in resolved wave convergence over the Northern Hemisphere midlatitude stratosphere, which impact the strength of upwelling within the tropical lower stratosphere.

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Abstract

Accurately modeling the large-scale transport of trace gases and aerosols is important for interpreting past (and projecting future) changes in atmospheric composition. Simulations of the stratospheric mean age-of-air continue to show persistent biases among chemistry climate models although the drivers of these biases are not well understood. Here we identify one key driver of simulated transport differences among various NASA Goddard Earth Observing System Version 5 (GEOS-5) candidate model versions that have been considered for the upcoming GEOS-5 Retrospective analysis for the 21st Century (GEOS-R21C). In particular, we use targeted model experiments aimed at disentangling the influence of recent model development updates, to show that the age-of-air is sensitive to the so-called "remapping" algorithm used within the finite-volume dynamical core that controls how individual material surfaces are vertically interpolated back to standard pressure levels after each horizontal advection time step. Differences in the age-of-air within the middle stratosphere (50 hPa) approach $\sim$ 1 year over high latitudes - or about 30% climatological mean values – and imprint on a broad range of trace gases, including methane (CH_4) and nitrous oxide (N_2O). These transport sensitivities reflect, to first order, changes in the strength of tropical upwelling which are driven by changes in resolved wave convergence over northern midlatitudes as (critical lines of) wave propagation shift in latitude. Furthermore, we show that degradations in the performance of the age-of-air, stratospheric upwelling and zonal wind climate statistics derived from 30-year-long atmosphere-only (AMIP) experiments, also translate to degraded skill in the analysis states used within data assimilation experiments. Our results strongly support continued examination of the role of numerics in contributing to transport biases in composition modeling.

Plain Language Summary

TBD

1 Introduction

The chemical and radiative properties of the troposphere and lower stratosphere are strongly influenced by the stratosphere-troposphere exchange of mass and tracers (e.g., Morgenstern and Carver (2001); Hegglin et al. (2006); Pan et al. (2007)). Properly simulating the stratospheric circulation and its influence on atmospheric composition in earth system models is important for capturing past decadal trends in surface climate, particularly in response to changes in Southern Hemisphere ozone depletion (e.g., Son et al. (2009); Polvani et al. (2011)). In the Northern Hemisphere (NH), the stratospheric circulation's coupling to ozone could represent an important feedback on the climate's response to future increases in greenhouse gases (GHGs), especially over the North Atlantic (e.g., Chiodo and Polvani (2019)). On shorter subseasonal timescales, stratospheric ozone changes associated with strong polar vortex states may also modulate Arctic sea level pressure and surface temperatures (e.g., Ivy et al. (2017); Oehrlein et al. (2020)), so much so that seasonal forecast systems employing prognostic ozone show increased signal-to-noise ratio in predictions of the North Atlantic Oscillation (B. M. Monge-Sanz et al. (2022)).

Key to properly ensuring a consistent and accurate representation of coupling between the stratospheric dynamical circulation and atmospheric composition is ensuring that a model's underlying transport circulation is well represented. To this end, much effort has been paid to developing and refining so-called "tracer-independent" metrics of transport (Holzer and Hall (2000)) such as the mean age-of-air (Hall and Plumb (1994)) and to applying these measures to rigorously evaluate model transport characteristics in chemistry climate models (CCMs) (e.g., Hall et al. (1999); Orbe et al. (2018); Dietmüller et al. (2018); Abalos et al. (2020)).

While the assessment of CCMs participating in the SPARC Chemistry Climate Model Validation (SPARC CCMVal) effort showed a marked improvement in simulated transport characteristics relative to previous intercomparisons (J. Neu et al. (2010)), more recent analysis of models participating in the SPARC Chemistry Climate Modeling Initiative (CCMI) (Eyring et al. (2013)) do not demonstrate any improvement (Dietmüller et al. (2018), see their Figure 3). In particular, although some models produce mean age values that agree well with observational estimates, the CCMI intermodel spread is $\sim$50%, with models generally simulating transport that is too vigorous, relative to observations. While documenting these transport differences among models is straightforward, understanding the drivers of this spread remains a key challenge and to this point there is no consensus identifying a clear driver of simulated age biases among the current generation of CCMs.

A key challenge in identifying the drivers of age-of-air – and other stratospheric transport – biases is that they reflect the time-integrated effects of advection by the residual mean circulation and eddy diffusive mixing, or the quasi-random transport due to the breaking of Rossby waves (e.g., Holton et al. (1995); Plumb (2002)). Given that the influences of mixing and advection are not easily separable, studies have come to different conclusions about the drivers of age biases in models. In particular, the analysis of the CCMVal models showed a strong correlation between the intermodel spread in the age-of-air and lower stratospheric tropical upwelling, whereas Dietmüller et al. (2018) argued that the age spread among the CCMI models was driven by differences in mixing. While future attempts to further distinguish between these drivers of age biases using either simplified "leaky pipe" models (Plumb (1996); J. L. Neu and Plumb (1999)) or more complete measures of the transport circulation such as the "age spectrum" (e.g., Hall and Plumb (1994); Waugh and Hall (2002))) may prove enlightening, at present there is no consensus on what is driving biases in the mean age in models.

A potential limitation of using multi-model intercomparisons to understand drivers of age biases is that many aspects of model formulation can influence both stratospheric (advective) upwelling and mixing. Thus, while intercomparisons are useful for identifying common model biases, understanding the drivers of these biases is difficult absent single model-based process studies. Among these, several aspects of model formulation have been identified as influencing representations of the stratospheric mean age. As the mean age is sensitive to vertical motion in the lowermost stratosphere, these include large sensitivities to vertical resolution (Orbe et al. (2020)) and to spurious vertical mixing either introduced in vertical coordinate transformations in offline chemical transport models (B. Monge-Sanz et al. (2007)) or through use of assimilated winds performed either in offline (e.g., Legras et al. (2004)) or online data assimilation and "nudged" configurations (e.g., Pawson et al. (2007); Orbe et al. (2017); Davis et al. (2022)). These age sensitivities can be still further amplified, depending on whether or not parameterized gravity waves are included (Eichinger et al. (2020)).

By comparison, sensitivities of the mean age to underlying tracer numerics have been less well examined, although Eluszkiewicz et al. (2000) documented a large sensitivity in age-of-air calculations to the choice of advection scheme. More recently, Gupta et al. (2020) showed differences of $\sim$ 25% in the age-of-air across identical experiments performed using four different dynamical cores, especially between those using spectral versus finite-volume schemes. The experiments employed in that study, however, were highly idealized and it is not clear if the strong influence of tracer numerics that they identified is also realized in more comprehensive model simulations, especially in the context of model development as carried out in operational modeling centers.

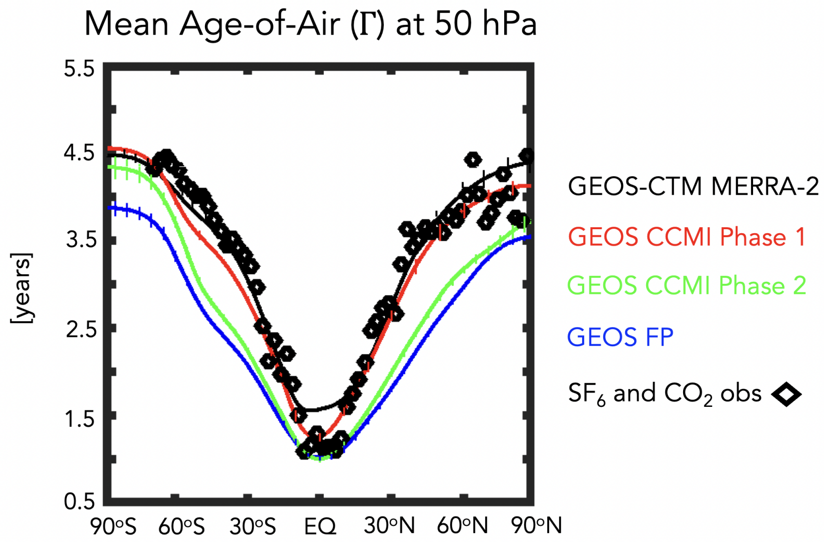

Figure 1. The 2000-2010 climatological annual mean meridional profile of the stratospheric mean age-of-air (Γ), evaluated at 50 hPa. Results from a GEOS-CTM integration constrained with MERRA-2 meteorological fields (black line) as well as free-running GEOS simulations using a model configuration for CCMI Phase 1 (red line), CCMI Phase 2 (green line) and a more recent GEOS-FP development tag (blue line) are shown. All simulations are constrained with the same (observed) historical sea surface temperatures. Diamonds correspond to SF_6 and CO_2 in situ based estimates of Γ from)boering1996stratospheric and Engel et al. (2009). Vertical dashed lines denote $\pm\sigma$, the standard deviation of Γ over 2000-2010, for each model simulation.

To this end, here we document the sensitivity of the stratospheric mean age in several recent versions of the NASA Goddard Earth Observing System Version 5 (GEOS-5) general circulation model (Molod et al., 2015) that represent different stages in model development since MERRA-2 (Gelaro et al. (2017)). Our focus on transport evaluation is in wake of the upcoming release of the GEOS-5 Retrospective analysis for the 21st Century (GEOS-R21C), which will serve as an intermediate reanalysis between MERRA-2 and MERRA-3 ($\sim$ 2025). As GEOS-R21C will be used to drive an off-line chemistry reanalysis (GEOS-R21C-Chem) it is imperative that it produces a credible representation of transport processes.

In particular, in the process of evaluating candidate systems for GEOS-R21C it was noted that the mean age was $\sim$ 1 younger than the values produced in the model version used to produce MERRA-2 (Figure 1). The model versions shown in Figure 1 reflect more than 10 years' worth of accumulated changes in model development, most notably changes in radiation, parameterized convection and, as we focus on here, changes in the algorithm used to transform advected fields from Lagrangian levels to fixed pressure levels after each horizontal advection time step. We show that slight modifications in this so-called "remapping" algorithm are the primary driver of the age-of-air degradation exhibited in recent GEOS-R21C candidate model versions, a result which may have broader implications for other general circulation models using finite volume (FV) dynamical cores. We begin by discussing methods in Section 2 and present key results and conclusions in Sections 3 and 4, respectively.

2 Methods

2.1 Model Configurations

Here we present results from several versions of GEOS-5 spanning MERRA-2 to more recent candidates for GEOS-R21C. Among these model versions, a subset are more "official" as they have been documented and/or employed in recent model intercomparisons and are highlighted in Figure 1. In particular, these include an intermediary model version that was used in Phase 1 of CCMI and documented in Orbe et al. (2017), marked in the red line. In addition, a later version that was used in the CCMI Phase 2 simulations (correspondence with Michael Manyin) is shown in the green line.

We begin by comparing 10-year (2000-2010) climatological mean zonally averaged age-of-air profiles at 50 hPa across this subset of model versions, derived from 30-year long atmosphere-only (AMIP) integrations constrained with observed sea surface temperatures (Figure 1). First, we note that the profiles for the CCMI Phase 1 version of the model (blue line) are very close to observations (black stars), consistent with the "GEOSCCM" documented age characteristics reported in Dietmüller et al. (2018) (see their Figure 3). In addition, while passive tracers were not integrated within MERRA-2, results using the GEOS chemistry transport model (GEOS-CTM, Kouatchou et al. (2015)) constrained with MERRA-2 meteorological fields (black line) also exhibits good agreement with observed values. This good agreement between the CTM-generated age-of-air and the observations is consistent with results from a previous GEOS-CTM simulation (constrained with MERRA) that was documented in Orbe et al. (2017).

Moving to more recent development versions of the model (green and blue lines), however, reveals a reduction in the mean age by $\sim$ 1 year over both southern and northern high extratropical latitudes, or a decrease of $\sim$ 20-30% relative to MERRA-2. As discussed earlier, the green line refers to the CCMI Phase 2 model version, whereas the blue line refers to an undocumented candidate version that corresponds best to a model configuration similar to what is used in the GEOS forward processing (FP) numerical weather prediction system (As of which date? Ask Amal.). Note that this decrease in the age in both model versions is statistically significant, relative to internal variability (vertical bars on solid lines).

As there were numerous development updates in the model that occurred since MERRA-2, after discussing the model configurations highlighted in Figure 1 in Section 3.1, we then perform targeted experiments oriented at successively undoing various changes that were made to the model since MERRA-2 (Section 3.2). Among those aspects most likely impacting the stratospheric transport circulation, these include updates to the radiation scheme, moving from Chou and Suarez (1994) in the shortwave and Chou (1990, 1992) in the longwave to the Rapid Radiative Transfer Model for GCMS (RRTGM; Iacono et al. (2008).

In addition to the radiation changes, another more consequential model development was made to the handling of the remapping algorithm within the model's finite-volume (FV) dynamical core. In particular, vertical motion is realized through the Lagrangian transport of the "floating" vertical coordinate such that after each horizontal advection step the individual material surfaces are vertically interpolated back to standard pressure levels through FV's so-called "REMAP" algorithm. There are various user-defined parameters and decisions that are made within this interpolation process.

First, the vertical remapping algorithm in its current implementation involves 1) computing total energy (TE = $C_pT + K + \Phi$) on the input grid; 2) fitting piecewise parabolic functions to layer-mean values of TE, u, v and tracers; 3) producing new layer-mean values by integrating functions between edges of the output grid and 4) constructing a "remapped" temperature profile via $T = (TE - K - \Phi)/C_p$. Note that T, u, v, C_p, K and Φ correspond to temperature, zonal wind, meridional wind, specific heat capacity and kinetic and po-

Table 1. Finite Volume Remapping Algorithm: The two versions examined in this study control how individual material surfaces are vertically interpolated back to standard pressure levels. REMAP Options 2 and 1 corresponds to the configurations used in more recent (green and blue lines, Figure 1) and older (red and black lines, Figure 1) model configurations, respectively. Here T, u, v, C_p, K and Φ correspond to temperature, zonal wind, meridional wind, specific heat capacity and kinetic and potential energy, respectively.

Step	REMAP Option 2 (CTRL)	REMAP Option 1 (MERRA-2)
1	compute TE = C_pT+K+Φ on input grid	compute TE = C_pT + K + Φ on input grid
2	Fit PPM functions to layer-mean TE u, v and tracers	Fit PPM functions to layer-mean u, v and tracers
3	Integrate functions between output grid edges to produce new layer-mean TE, u, v and tracers	Integrate functions between output grid edges to produce new layer-mean u, v and tracers
4	Construct "remapped" T via T = (TE - K -Φ)/C_p	Calculate TE at new mid-layer pressures using cubic interpolation and a-posteriori integral conservation
5	n/a	Construct "remapped" T via T = (TE - K - Φ)/C_p

tential energy, respectively. This implementation setup is consistent with what is currently being used in most recent model versions (i.e. blue and green lines, Figure 1) and hereafter is referred to as REMAP Option 2 (Table 1, left). The alternative version – which best mimics what was used in MERRA-2 – involves two changes to this procedure and is hereafter referred to as REMAP Option 1 (Table 1, right; red line in Figure 1). First step 2) is performed only for u, v and tracers (not TE). Second, an additional step between 3) and 4) is added which involves calculating TE at new mid-layer pressures using cubic interpolation and a posteriori ensuring integral conservation.

It is worth noting other important model development changes that occurred related to the parameterization of deep convection (Grell and Freitas (2014); Freitas et al. (2018)) which could, potentially, have an indirect impact on the stratospheric circulation through their influence on wave propagation into the stratosphere. As we show, however, while these have a substantial impacts upon their incorporation in a nonhydrostatic version of the model on characteristics like the diurnal cycle of precipitation (Arnold et al. (2020)) and on convective transport within the troposphere (Freitas et al. (2020)), their indirect influence on the stratosphere is less impactful.

To this end, in order to investigate the drivers of the differences illustrated in Figure 1 we perform targeted model experiments aimed at further disentangling all of these development changes (Table 2). First, we begin by defining a control experiment (CTRL; Table 2, row 1), which best corresponds to the blue line shown in Figure 1. Then we define three new experiments based off this control that are used to distinguish between the age changes resulting from changes in radiation versus changes in the handling of the REMAP algorithm (Section 3.2.1). Specifically, these include experiments in which we revert back from RRTMG to Chou and Suarez (1994) in the shortwave (CSRAD; Table 2, row 2), b) revert back to the MERRA-2 REMAP approach (i.e. REMAP Option 1) (M2REMAP; Table 2, row 3) and c) combine these two changes (CSRAD+M2REMAP; Table 2, row 4). Note that we have also have performed experiments in which RRTMG

Table 2. GEOS Model Experiments: Targeted GEOS-5 model experiments based off a control experiment (row 1) were carried out to identify the influence of radiation (row 2) and the FV remapping algorithm changes since MERRA-2 (row 3), as well as their combined influence (row 4). Sensitivities within the FV remapping algorithm were further explored with respect to the order of the interpolation to pressure levels (rows 5-9). Experiments in rows 1-7 are 30-year-long AMIPS used for climate statistic evaluation, whereas rows 8-9 are 1-year-long DAS runs used for evaluation of the analysis state.

Experiment Name	Configuration Change	Experiment Type
CTRL	Control, REMAP Option 2	AMIP (30 yrs.)
CSRAD	Chou-Suarez (1994) Shortwave (SW) Radiation	AMIP (30 yrs.)
M2REMAP	MERRA-2 REMAP Option 1 (cubic)	AMIP (30 yrs.)
CSRAD+M2REMAP	Chou-Suarez (1994) SW + REMAP Option 1 (cubic)	AMIP (30 yrs.)
LINEAR	MERRA-2 REMAP Option 1 (linear)	AMIP (30 yrs.)
QUADRATIC	MERRA-2 REMAP Option 1 (quadratic)	AMIP (30 yrs.)
CUBIC	MERRA-2 REMAP Option 1 (cubic)	AMIP (30 yrs.)
CTRL-DAS	Control, REMAP Option 2	DAS (1 yr.)
CUBIC-DAS	MERRA-2 REMAP Option 1 (cubic)	DAS (1 yr.)

is reverted back to Chou (1990); Chou and Suarez (1994) in the longwave (not shown), but these changes are less impactful, compared to the shortwave changes.

As we will show, the M2REMAP experiment produces the largest changes in age-of-air and we thus focus the remainder of our investigation (Section 3.2.2) on examining a clean set of experiments in which only the interpolation occurring between steps 3) and 4) within REMAP Option 1 is altered. Specifically, we perform three experiments that are all based off the CTRL configuration and revert back to the REMAP Option 1. The difference between them is that the calculation of TE at the mid-layer pressure levels is performed either using a linear (LINEAR; Table 1, row 5), quadratic (QUADRATIC; Table 1, row 6) or cubic interpolation (CUBIC; Table 1, row 7), with the latter corresponding to the approach that was used in MERRA-2. We note that, while the LINEAR and QUADRATIC experiments do not actually correspond to any of the development tags shown in Figure 1, they highlight the large sensitivity of the mean age to otherwise innocuous seeming changes in the interpolation scheme. We also show that they provide further support for the relationship between upwelling strength and stratospheric mean age as realized in GEOS.

Finally, in all experiments using REMAP Option 1 (i.e. M2REMAP, CSRAD+ M2REMAP, LINEAR, QUADRATIC, CUBIC) additional modifications to the divergence damping coefficients were used so as to ensure best consistency with what was used in MERRA-2. As they only differ in this single respect, these experiments are therefore useful for cleanly isolating the impacts of changes in the interpolation scheme. Specifically, these include changes to the number of layers for vertical subgrid mixing, the DAS coefficient for barotropic mode damping, the use of 2nd vs. 6th order divergence damping and the strength of the divergence damping coefficients.

2.2 Analysis Approach

2.2.1 Stratospheric Circulation and Transport Diagnostics

To diagnose the transport circulation we focus primarily on the age-of-air (Hall and Plumb (1994)). This is inferred from an idealized global "clock" or ideal age tracer (Γ) (Thiele and Sarmiento (1990)) that is defined with respect to all grid points in the first model level. Initially, the ideal age tracer is set to zero throughout the troposphere and thereafter held to zero over the entire Earth's surface, subject to a constant aging of 1 year/year throughout the atmosphere. We present here the statistically stationary (equilibrated) value of Γ(r), which is equal to the average time since the air at a location r in the stratosphere last contacted the Earth's surface. In addition to the mean age, we also show results from an idealized e90 tracer that is uniformly emitted over the entire surface layer and decays exponentially at a rate of 90 days^{-1} such that concentrations greater than 125 ppb and less than 50 ppb tend to reside in the lower troposphere and stratosphere, respectively (Prather et al. (2011)). As this tracer features strong near-tropopause gradients and takes significantly less time to equilibrate, compared to the mean age, it is useful for evaluating stratosphere-troposphere-exchange and transport within the upper troposphere/lower stratosphere (Abalos et al. (2017, 2020)).

In addition to the idealized tracers, we also evaluate the impacts of the age changes on real trace gas distributions. Two of the experiments shown here were run with full interactive chemistry and correspond to the two CCMI (Phase 1 and Phase 2) integrations (red and green lines, Figure 1), which both employed the same Global Modeling Initiative (GMI) chemical mechanism (Strahan et al. (2013)). Results from these experiments show the imprint of the age-of-air changes on nitrous oxide (N_2O) and methane (CH_4).

As we show in Section 3, the changes in age-of-air across the different model versions are strongly tethered to changes in the advective component of the circulation, which we quantify using the Transformed Eulerian Mean (TEM) framework. Thus, in addition to more standard Eulerian metrics of the circulation (e.g., zonal winds and temperatures), we also examine the TEM estimate of the Lagrangian transport of mass by the circulation, which is far more relevant to consituent transport. In particular, we focus on the vertical component of the TEM residual velocity, defined as $\overline{w}^* = \overline{w} + \frac{\partial(\psi cos\phi)}{acos\phi\partial\phi}$, where $\psi = \overline{v'\theta'}/\frac{\partial\overline{\theta}}{\partial p}$ is the eddy stream function, θ refers to potential temperature and overbars and primes denote zonal means and deviations therefrom, respectively (Andrews et al. (1987)). In addition, in order to interpret the response in w* we examine the Eliassen-Palm flux divergence ($\nabla \cdot$ F), whose horizontal (F(ϕ))and vertical (F(p)) components are respectively defined as F(ϕ)=acos$\phi[\frac{\partial u}{\partial p}\psi - \overline{u'v'}]$ and F(p)=acos$\phi([f - \frac{\partial \overline{ucos\phi}}{acos\phi\partial\phi}]\psi - \overline{u'\omega'})$.

2.2.2 Experimental Setup

We begin our analysis by interpreting the results shown in Figure 1, which are all based on AMIPs performed over the period Dec 1985 – Feb 2015 (Check with Larry exact years). As these runs represent more "official" model tags they are performed at different horizontal resolutions (indicated in the figure caption TO DO). A clean/meaningful analysis of this set of runs is therefore hampered not only by the model development differences between them, but also by resolution differences. Nonetheless, they present an important motivation for the experiments that follow. They also indirectly highlight how other development changes that occurred (to convection, for example) were less consequential in terms of their impacts on the stratospheric circulation.

Given the limitations of the experiments highlighted in Figure 1, we focus the bulk of our analysis on the model configurations listed in Table 2. For these model runs climatological AMIPS were carried at a cubed sphere C180 (approximately half-degree) resolution and used to infer the climate characteristics of the different model configurations. For a subset of these experiments (Table 2, rows 5-9) integrations were also carried out at C360 horizontal resolution. All integrations carry the same idealized passive tracer package (including the e90 and Γ tracers) that was described in Orbe et al. (2017).

In addition to AMIPS we also include results from so-called "EMIPs" which were also run at C180 and consist of performing ensembles of 3-month-long integrations initialized on December 1 of each year between 1985 and 2015 (Larry, is this correct?). As we show, the December-January-February (DJF) climatological mean statistics derived from EMIP experiments of various climate metrics converge to the statics of the corresponding AMIP runs using the same model configurations. In particular, we find excellent agreement between the vertical profile of w^*, averaged over 1985-2015 and between the tropical turnaround latitudes, deduced from AMIP and EMIP experiments run using one of the model tags described herein (corresponding to the blue line in Figure 1) (Appendix Figure 1). This somewhat incidental finding, represents, to the best of our knowledge, the first time that this result has been documented for the stratospheric metrics considered in this study. Furthermore, as EMIPs present a much more computationally efficient alternative to running AMIPs, this approach was used to quickly ascertain the impacts of the changes documented in Table 2. We note, however, that this approach is not appropriate for evaluating the time-integrated transport characteristics reflected in the age-of-air. To this end, we show results from both AMIP and EMIP experiments.

Finally, in addition to examining the climate statistics of the different model configurations we also inquire into implications for the analyzed atmospheric states from data assimilation for a subset of the experiments (Table 2, rows 8-9). Specifically, we examine the root-mean-square error of various climate fields (Amal, need description of relevant metrics/analysis). This evaluation is important given that in GEOS-R21C any underlying model biases will be partly ameliorated through replaying of the model state to the analysis. Assessing the impact of reduced biases from the free-running model for the analysis state, is therefore important for informing the development of GEOS-R21C.

2.3 Observations and Reanalyses

While our focus is on interpreting and understanding the behavior across the different model versions, we incorporate observations to provide context, although we do not present an exhaustive evaluation of the model's transport characteristics (for that see earlier studies including Orbe et al. (2017, 2018)). For the circulation diagnostics all comparisons are made relative to MERRA-2, although similar comparisons against ERA-5 have also been made (not shown) and reveal a similar picture.

As the tracers are not directly integrated in MERRA-2 (with the exception of ozone), we compare against independent observational estimates. For the mean age we first compare simulated meridional age profiles at 50 hPa with values derived from in situ aircraft measurements of carbon dioxide (CO_2), averaged in 2.5 degree latitude bins over the altitude range 19.5 to 21.5 km (Boering et al. (1996), see also Figure 5 in Hall et al. (1999)).

We also briefly evaluate impacts of transport biases on the simulated trace gas distributions for the CCMI Phase 1 and 2 experiments. The simulated fields of methane (CH_4) are compared with the climatologies derived for 1991–2002 from the Halogen Occultation Experiment (HALOE) on board the Upper Atmosphere Research Satellite (UARS) (Grooß and Russell III (2005)). Comparisons of simulated nitrous oxide (N_2O) are made against 2005–2015 climatologies derived from the Microwave Limb Sounder (MLS) on the Earth Observing System (EOS) Aura satellite. We use the 190-GHz retrieval from Version 4.2 because the 640-GHz data set ends in summer 2013 due to the failure of the N_2O primary band.

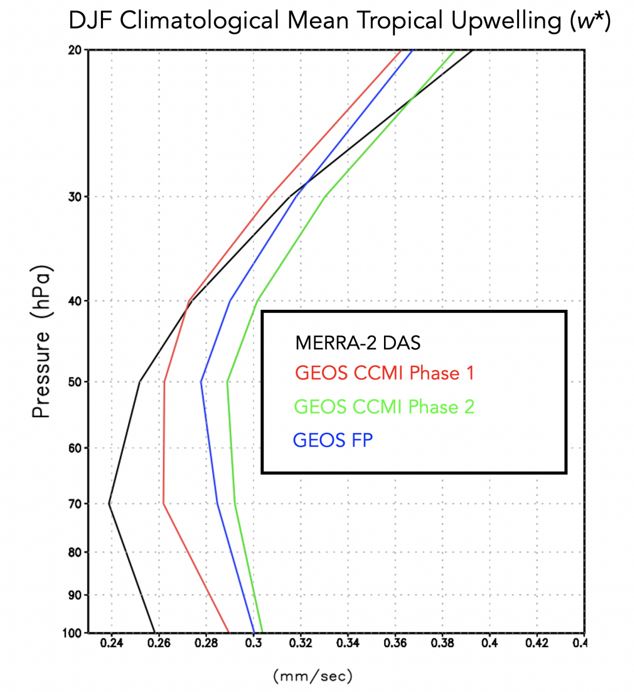

Figure 2. The DJF 1985-1994 (ideally would include years 1994-2015) climatological mean vertical residual mean velocity, w^*, averaged between the turnaround latitudes for GEOS model configurations corresponding to the CCMI Phase 1 (red) and Phase 2 (green) submissions and to GEOS-FP (blue). MERRA-2 is shown in black.

3 Results

3.1 Reduction in Stratospheric Mean Age Since MERRA-2

We begin by interpreting the reduction in mean age exhibited in more recent model versions in terms of changes in the strength of upwelling associated with the Brewer-Dobson circulation. In particular, we find that the reductions in Γ (Figure 1) are consistent with increases in the strength of lower stratospheric tropical upwelling, with w^* becoming progressively stronger in more recent model tags, relative to MERRA-2 (Figure 2). Though perhaps naive, this relationship between lower stratospheric upwelling and the mean age is consistent with the long-term behavior of Γ inferred from both historical and projected future climate simulations (Butchart et al. (2010); Abalos et al. (2021)). A strong relationship between the strength of lower stratospheric ascent and the mean age was also shown to hold in the CCMVal models (see Fig. 5.20 in J. Neu et al. (2010)). Nevertheless, it is important to note that a clear relationship between w^* and Γ is not a priori expected, as the age-of-air is also known to be very sensitive to mixing, which may be important in interpreting differences among the CCMI Phase 1 models (Dietmüller et al. (2018)).

The differences in w^* highlighted in Figure 2 are associated with enhanced Eliassen-Palm flux convergence over NH midlatitudes (Figure 3), relative to MERRA-2. Increased wave convergence is evident not only within the subtropical lower stratosphere ($<$ 30°N, 50-100 hPa) but also over higher latitudes and altitudes ($\sim$ 40°-70°N, 20-50 hPa). The fact that differences in extratropical wave convergence imprint on tropical upwelling is consistent with our understanding of the so-called "downward control" principal (Haynes

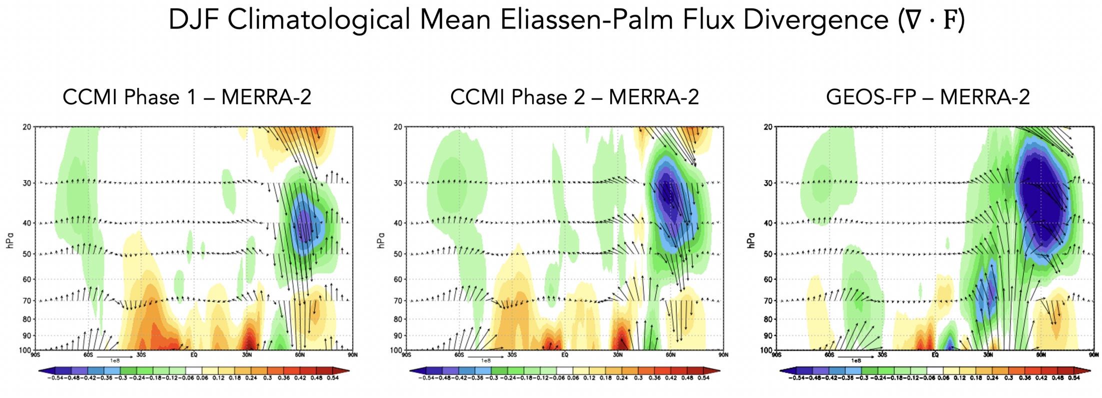

Figure 3. Colors shown anomalies in the DJF climatological mean Eliassen-Palm (EP) flux divergence between the CCMI Phase 1 (left), CCMI Phase 2 (middle) and GEOS-FP (right) model versions, relative to MERRA-2. Arrows denote anomalies in the vertical and meridional EP flux vectors (relative to MERRA-2).

et al. (1991)). In particular, the strength of the residual mean streamfunction (Ψ^*) is, via downward control, directly related to the vertically integrated eddy-induced total zonal force above that level and has contributions both from the (resolved wave) Eliassen-Palm flux divergence (Figure 3) as well as parameterized waves (not shown). The tropical upward mass flux – defined as Ψ^*_{max}-Ψ^*_{min} evaluated at the turnaround latitudes (e.g. Rosenlof (1995)) – is therefore directly dependent on the wave forcing aloft. Over extratropical latitudes, the zonal force associated with wave convergence will be associated with downwelling at high latitudes that will, through mass balance, necessarily be accompanied by enhanced upwelling in the tropics. This indirect impact of higher latitude wave drag can be seen in our simulations (Appendix Figure 2, Ask Lary to make), which show enhanced downwelling over the NH polar region that is consistent with enhanced upwelling over the tropics.

While the reduction in Γ (Figure 1) of $\sim 30\%$ at 50 hPa is significant, it is neither clear if this change is representative of other altitudes within the stratosphere nor how this age bias imprints on real chemical species. To this end, we begin by comparing the full latitude-pressure distribution of changes in Γ and another passive tracer (e90) (Figure 4) between the CCMI Phase 1 and Phase 2 model configurations (red and green lines, Figure 1). In particular, we find that the changes in both passive tracers – large reductions in Γ within both hemispheres (Fig. 4, top right) and increased values of e90 within the lower stratosphere (Fig. 4, bottom right) – are reflective of an overall increase in the strength of the transport circulation. This is highlighted in the CCMI Phase 2 – 1 model differences for the passive tracer distributions (Fig. 4, right panels) which are shown in the absence of robust observational constraints of Γ at higher altitudes (or any observational constraints for e90, for that matter). The reduced/increased stratospheric burdens of the age and e90 tracers are consistent with stronger upwelling in the CCMI Phase 2 model configuration (Figure 2).

While the observational constraints on Γ presented in Figure 1 and the departure of w^* away from MERRA-2 suggest that transport properties of the newer model configurations are moving in the wrong direction, it is relevant to ask whether or not the trace gas satellite measurements also support this conclusion. Indeed, comparisons with observations show larger biases in N_2O (Fig. 5, top panels) and CH_4 (Fig. 5, bottom panels), increasing from 10% to 30% in the CCMI Phase 2 model configuration, depending

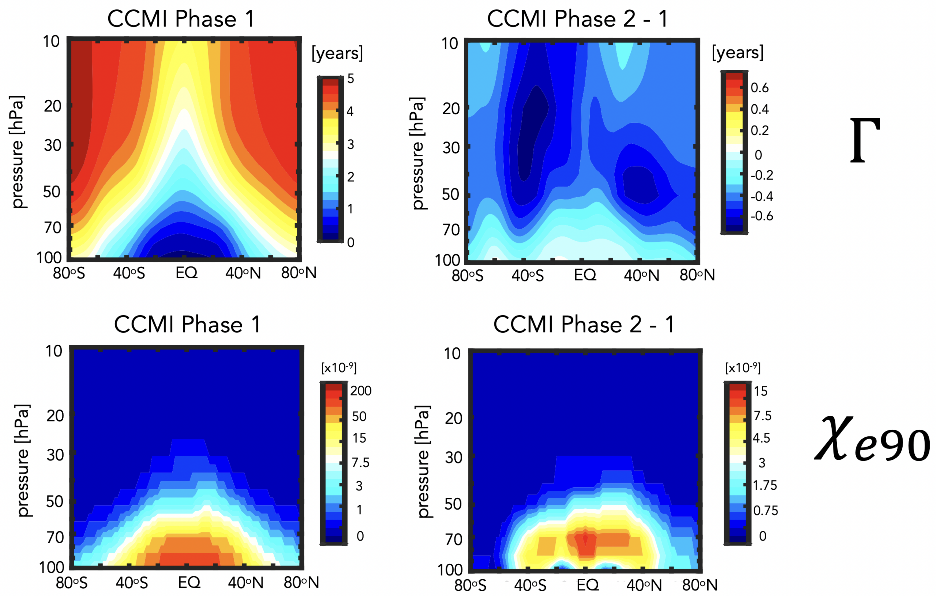

Figure 4. The climatological mean (2000-2010) distribution of the mean age-of-air (Γ) (left, top) and e90 idealized tracers (left, bottom) for the CCMI Phase 1 model configuration. Climatological differences between the CCMI Phase 2 and Phase 1 model configurations are shown in the left panels. Note that a nonlinear colorbar has been used in the e90 subplots.

on the species. The patterns of these biases are generally consistent with the biases in the mean age (Fig. 4), suggesting a strong link between the tracers. Recall that the same chemistry mechanism is used in both CCMI Phase 1 and 2 simulations.

The fact that the mean age changes have a significant imprint on the simulated trace gases is consequential for the GEOS-RC21 system. However, the configurations shown in Fig. 1-5 differ in many respects (physics, resolution, radiation, FV remapping algorithm) and it is difficult to meaningfully interpret what is driving the changes in w^* (and the tracers). We therefore move next to the targeted model experiments (Table 2) in order to interpret the model development steps that resulted in these transport circulation changes.

3.2 Identifying Drivers of Upwelling and Tracer Changes Since MERRA-2

3.2.1 Radiation versus REMAP Algorithm

As discussed in Section 2, among the model changes that were made since MERRA-2, the changes in radiation and the FV remapping algorithm are most likely to directly have impacted the stratospheric circulation. We therefore begin by assessing which of these changes dominates the decreases in Γ shown in Figure 1.

Figure 6 shows the distribution of Γ for experiments in which the shortwave radiation and REMAP updates since MERRA-2 have successively been undone. Relative to the control experiment (CTRL; Table 2, row 1), the reversion back to Chou (1992) in the shortwave results in an increase in the mean age of ~ 0.5 years throughout the stratosphere (CSRAD; Table 2, row 2). Though significant, this change in Γ is smaller than the change that results from reverting back to REMAP Option 1 (M2REMAP; Table

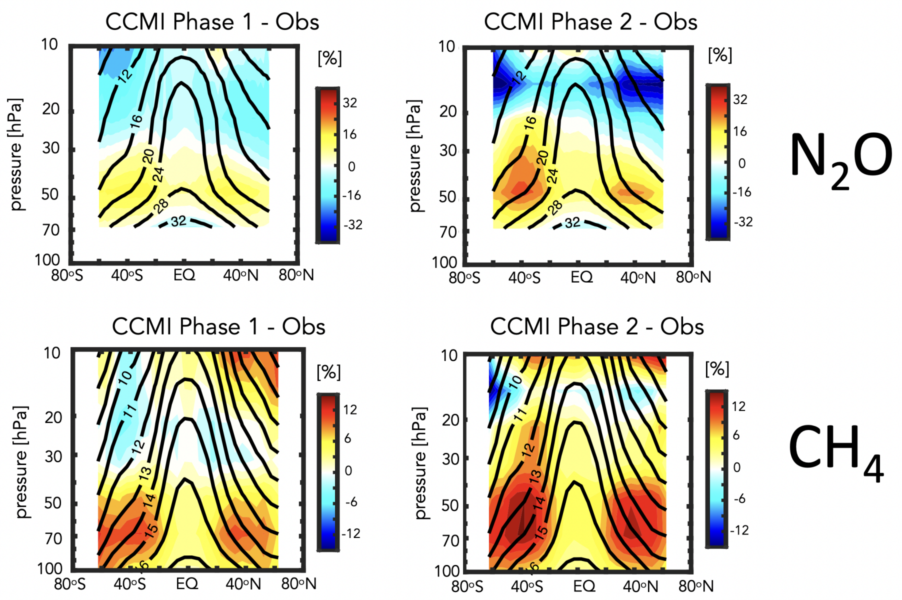

Figure 5. Colors shown anomalies in the simulated distributions of nitrous oxide (N_2O) (top) and methane (CH_4) (bottom), relative to the MLS and HALOE observed values, respectively, for the CCMI Phase 1 (left) and Phase 2 (right) GEOS model configurations. Climatological mean observed values are shown in the black contours.

1; row 3), in which the mean age increases by $\sim$ 1 year. The combined impacts of both changes (CSRAD+M2REMAP; Table 1 row 4) is roughly linear, with age values of $\sim$ 5.5 years over high latitudes at 50 hPa, consistent with the values simulated by the GEOS-CTM MERRA-2 integration (black line in Figure 1) and with the CCMI Phase-1 version of the model (red line, Figure 1).

Next we ask if the behavior of Γ exhibited in Figure 6 can be interpreted in terms of changes in the strength of lower stratospheric tropical upwelling and extratropical wave convergence, as our previous analysis of the CCMI experiments suggested. Indeed, Figure 7 shows that values of upwelling decrease in the CSRAD and M2REMAP experiments, with larger decreases in the latter, relative to the CTRL integration. The increase in upwelling resulting from both changes (CSRAD+M2REMAP) is still larger, consistent with the larger age decreases in that experiment. This change in the behavior of w^* within the tropical stratosphere can be interpreted in terms of changes in the Eliassen Palm flux convergence over NH midlatitudes (not shown, should consider adding this as a figure), which features smaller values in the CSRAD, M2REMAP (and CSRAD+MSREMAP) experiments. Note that our examination of the changes in w^* are derived from EMIP integrations, which we showed previously converge (for DJF) to the statistics derived from corresponding AMIP experiments.

3.2.2 FV REMAP Algorithm: Sensitivity of Climate Statistics

Having shown in the previous section that the largest changes in the mean age and lower stratospheric upwelling were realized through the reversion back to REMAP Option 1, we now investigate further the sensitivity of the transport circulation to the choice of remapping interpolation scheme. In particular, we compare simulations in which total energy is calculated at new mid-layer pressures using cubic, quadratic and linear in-

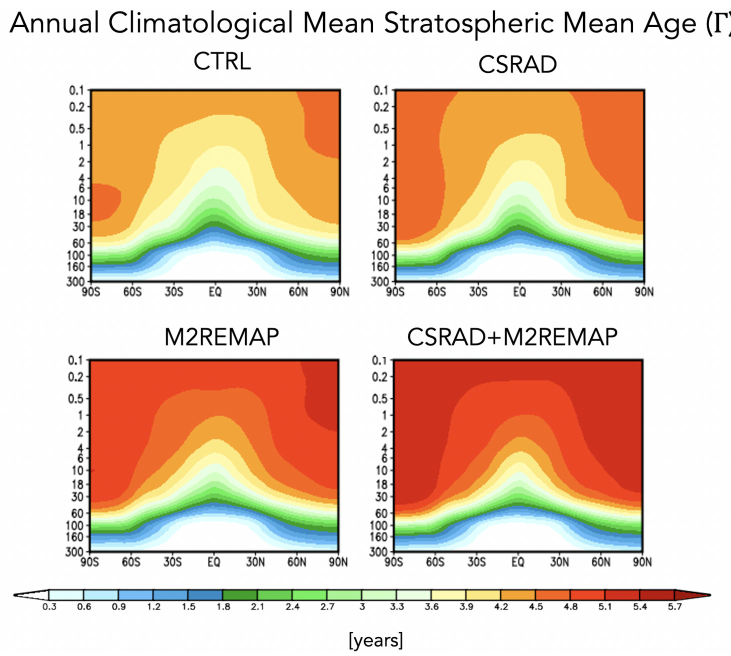

Figure 6. Colors show the simulated 2000-2010 climatological annual mean distributions of the mean age-of-air (Γ) for the CTRL (top left; Table 1, row 1), CSRAD (top right; Table 1, row 2), M2REMAP (bottom left; Table 1, row 3) and combined CSRAD+M2REMAP (bottom right; Table 1, row 4) experiments.

terpolation prior to the aposterior integral conservation (Table 2, rows 5-7). In addition, in this section we seek to understand how the changes in the Eliassen-Palm flux convergence over NH midlatitudes arise via analysis of the large-scale wind structure.

Figure 8 (left panels) shows a clear sensitivity in tropical upwelling to the choice of interpolation scheme, with w^* progressively increasing in strength moving from the CUBIC to QUADRATIC to LINEAR schemes. This sensitivity is robust across horizontal resolutions as the same suite of experiments performed at C360 exhibit the same sensitivity (Fig. 8, right panels). While no current model tag actually employs a linear scheme (the control simulation, rather uses a piecewise parabolic method and is delineated in the cyan line), this suite of experiments highlights the strong sensitivity to choice of interpolation scheme within the remapping algorithm, heretofore unreported in the literature. Furthermore, as we show next, this clean set of experiments allow us to inquire mechanistically into the processes that are driving the changes in wave convergence over midlatitudes, unencumbered by differences in horizontal resolution, physics, etc.

Consistent with our expectations based on the analysis of the previous experiments, the drivers of the changes in w^* are related to increased wave convergence moving from the CUBIC to QUADRATIC to LINEAR schemes (Figure 9). Unlike in the previous sections, however, we exploit the fact that these experiments only differ with respect to the interpolation scheme to further inquire into the drivers of the wave convergence changes. To this end, Figure 10 compares profiles of the zonal mean zonal wind between the CUBIC, QUADRATIC and LINEAR experiments, averaged over the region of enhanced wave convergence (i.e. 20°N-60°N). The experiments featuring stronger wave convergence (LINEAR and QUADRATIC) are also simulations with stronger zonal winds, relative to MERRA-2, especially above 70 hPa. This change in winds occurs at both C180 (Fig. 10, left panel) and C360 (Fig. 10, right panel) resolutions.

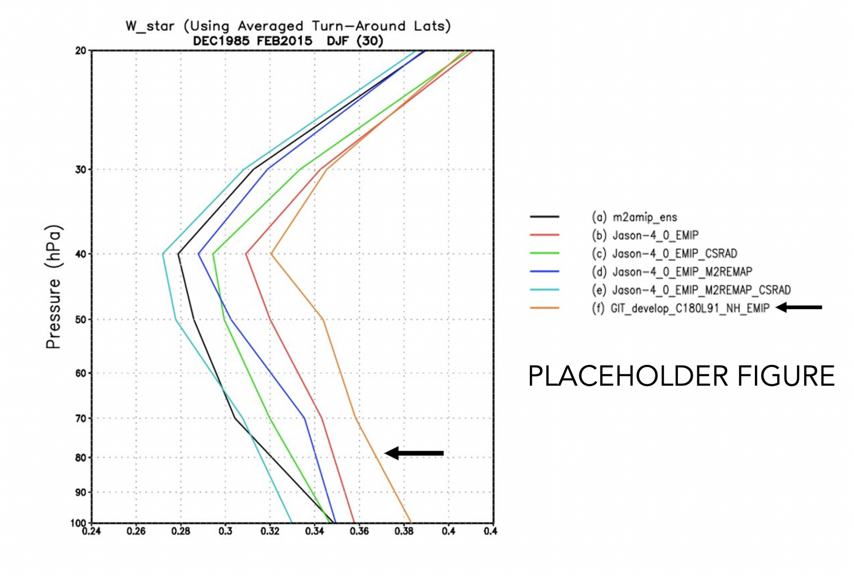

Figure 7. The DJF climatological mean vertical residual mean velocity, w^*, averaged between the turnaround latitudes for the CTRL (red line; Table 2, row 1), CSRAD (green line; Table 2, row 2), M2REMAP (blue line; Table 2, row 3) and combined CSRAD+M2REMAP (cyan line; Table 2, row 4) experiments. MERRA-2 is shown in black. This figure still needs to be refined.

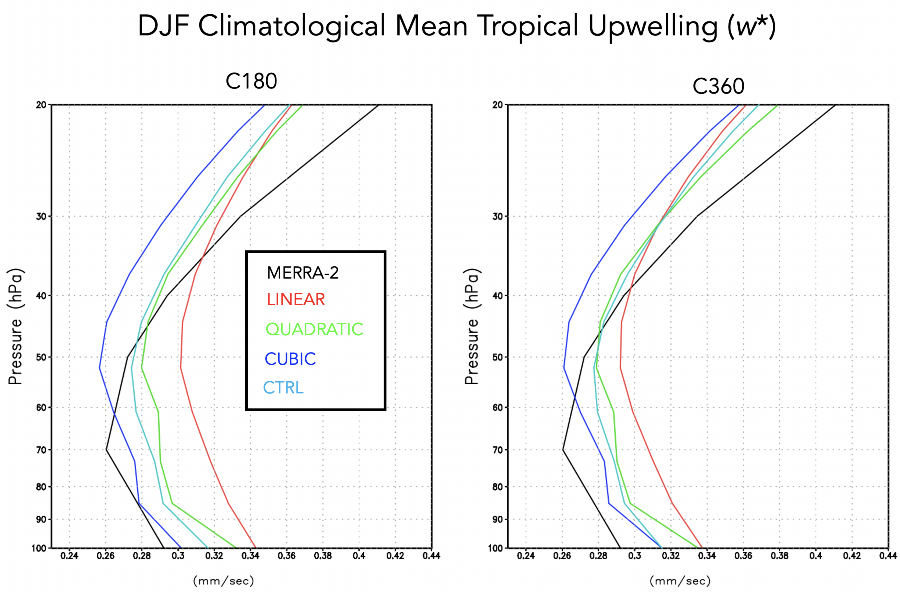

Figure 8. The DJF climatological mean vertical residual mean velocity, w^*, averaged between the turnaround latitudes for the CTRL (cyan line; Table 2, row 1), LINEAR (green line; Table 2, row 5), QUADRATIC (blue line; Table 2, row 6) and CUBIC (cyan line; Table 2, row 7) experiments. MERRA-2 is shown in black.

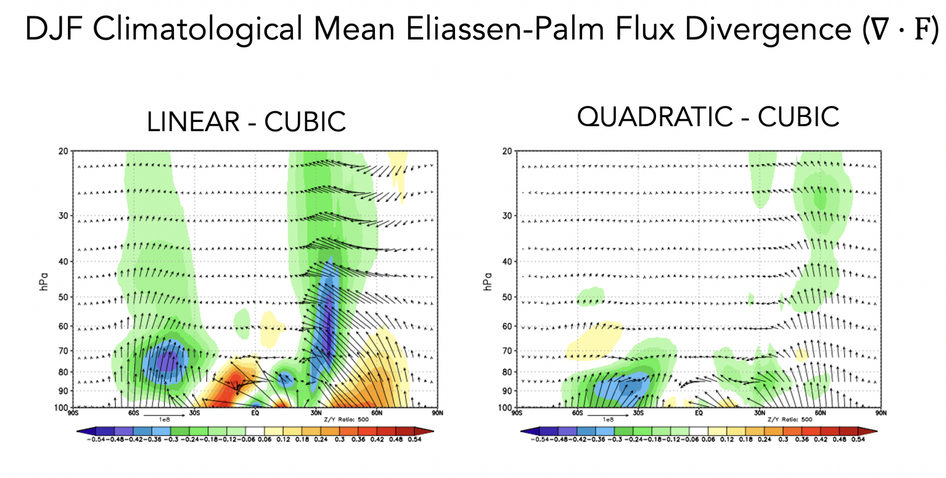

Figure 9. Colors shown anomalies in the DJF climatological mean Eliassen-Palm (EP) flux divergence in the LINEAR (left) and QUADRATIC (right) experiments, relative to the CUBIC model experiment. Arrows denote anomalies in the vertical and meridional EP flux vectors.

Structurally, the increase in zonal wind strength over northern extratropical midlatitudes is reflective of a poleward shift in the zonal winds as the critical latitude, i.e. where the zonal wind is zero, shifts northward in the QUADRATIC and, especially, LINEAR integrations, relative to the CUBIC experiment (Figure 11). Since stationary waves only propagate in westerly zonal flow, the latitude where zonal flow is zero acts a boundary for wave propagation (Hardiman et al. (2014)). As a result, this shift in critical latitude results in enhanced wave propagation in that region.

Figures 10 and 11 highlight how the changes in zonal winds in the LINEAR and QUADRATIC experiments reflect a degradation in model skill, relative to MERRA-2, throughout the entire stratosphere. The changes in upwelling, mean age, chemical trace gases and zonal winds thus provide an coherent and self-consistent picture suggestive of a degradation in the representation of the stratospheric circulation since MERRA-2. That is, an increased bias in the stratospheric northern zonal winds are, via their influence on wave convergence, compromising changes in the strength of the mean meridional overturning circulation and its impact on composition. It is interesting to note that the wind biases also extend into the troposphere and show degraded skill relative to MERRA-2 in the LINEAR and QUADRATIC experiments (Figure 11). Examination of other fields (i.e. tropopause biases, Appendix Figure 3) present somewhat more of a nuanced story that depends more sensitively on latitude and season considered. The improvements in the zonal winds, however, are most relevant for setting the upwelling characteristics within the tropical lower stratosphere via their influence on wave propagation into that region.

Finally, to better understand why these impacts on the winds have such a consequence for the wave convergence properties within the stratosphere, next we examine the zonal structure of these biases in the middle stratosphere (Figure 12). This reveals that the enhanced winds in the LINEAR (and, to a lesser extent, QUADRATIC) integrations are concentrated over the North Pacific (a similar picture emerges within the troposphere, not shown). As this region is the primary region dominating the stationary component of the upward flux of vertical wave activity (Plumb (1985), see their Figure 4) it is perhaps not surprising that this region is having a profound impact on the mean overturning circulation. Again, as with the zonal mean wind changes, the increases in wind strength

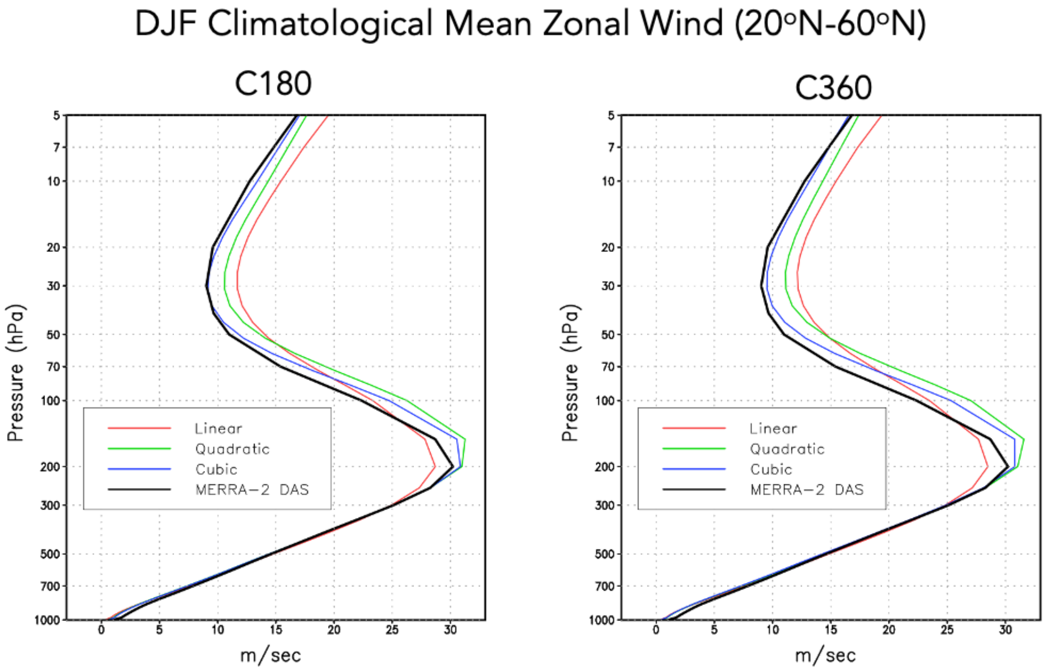

Figure 10. Vertical profiles of the DJF climatological mean zonal mean zonal winds in the LINEAR (red), QUADRATIC (green) and CUBIC (blue) experiments, averaged between 20°N and 40°N. MERRA-2 is shown in the black line. Results for both C180 (left) and C360 (right) experiments are provided.

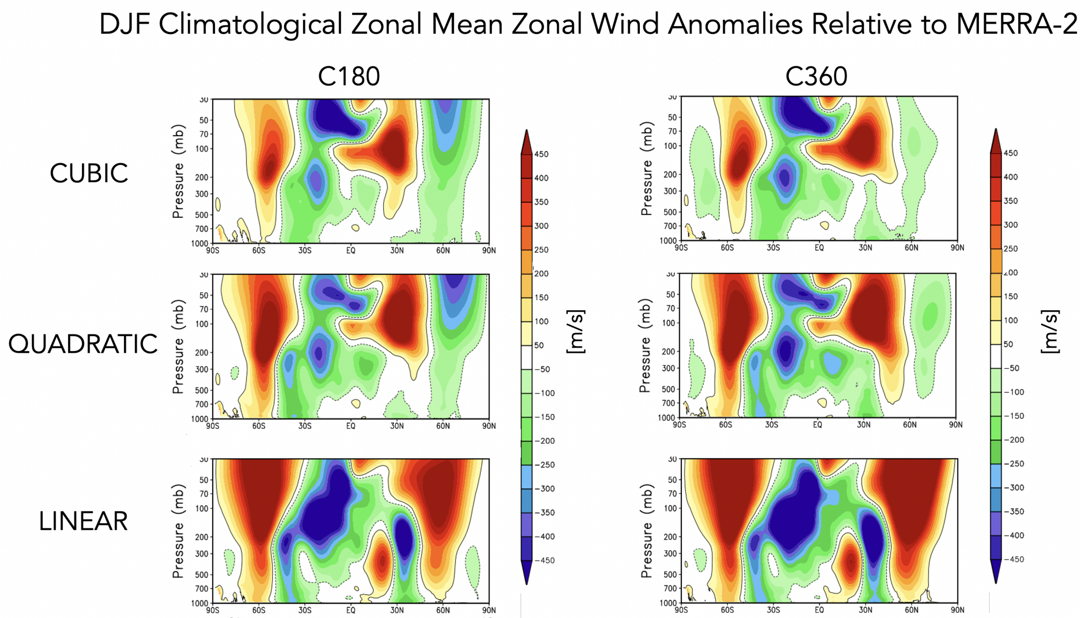

Figure 11. Colors shown anomalies in the DJF climatological mean zonal mean zonal winds in the CUBIC (top), QUADRATIC (middle) and LINEAR (bottom) experiments, relative to MERRA-2. Results for both C180 (left) and C360 (right) experiments are provided.

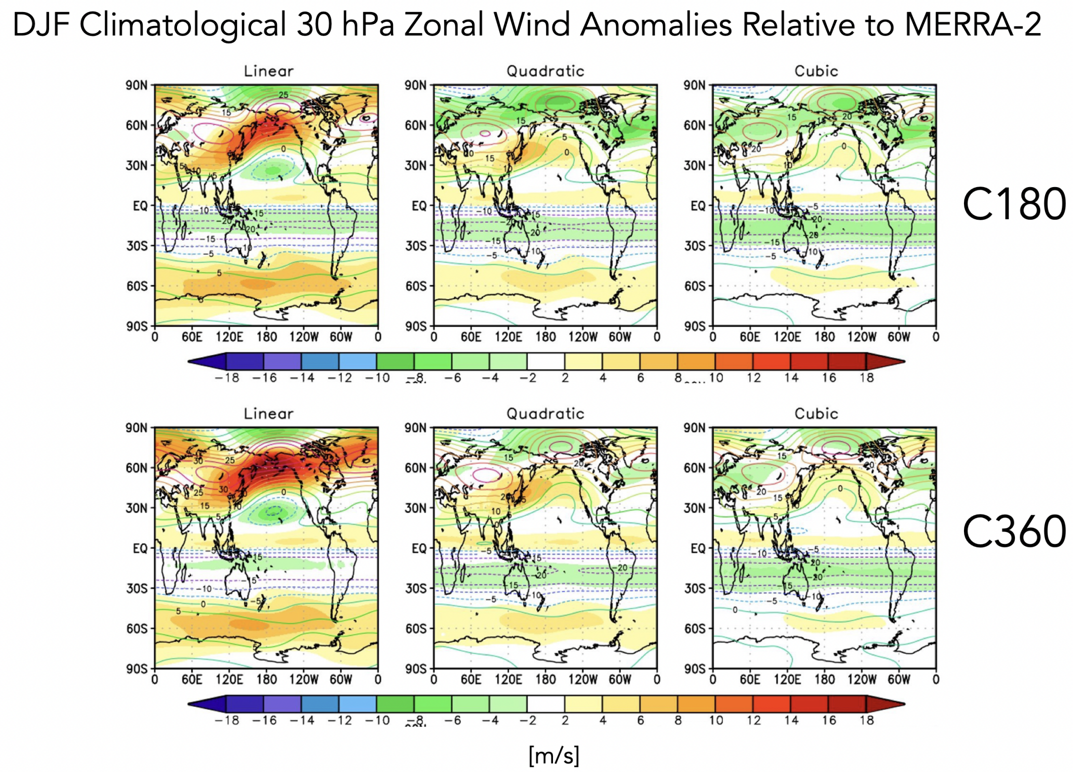

Figure 12. Colors shown anomalies in the DJF climatological mean zonal winds at 30 hPa in the CUBIC (right), QUADRATIC (middle) and LINEAR (left) experiments, relative to MERRA-2. Results for both C180 (top) and C360 (bottom) experiments are provided.

over the North Pacific represent degraded model skill relative to MERRA-2. Note that comparisons with ERA-5 reveal a similar bias (not shown).

3.2.3 FV REMAP Algorithm: Sensitivity of DAS Analysis State

Up to this point our focus has been on evaluating the various model configurations via use of 30-year long AMIPs, which are required for deriving the integrated transport statistics (i.e. age-of-air) that reflect the long timescales relevant to setting the stratospheric transport circulation. However, this not only poses practical challenges for model development purposes (which may be ameliorated, for some variables, through use of EMIPs), but it is also not obvious how the time-integrated model biases inferred from AMIPS manifest in a data assimilation (DAS) context. To this end, here we briefly comment on implications for the DAS analysis state.

In particular, we compare two DAS experiments one mimicking MERRA2 (d46aremp2) and one mimicking the control configuration (d46actrl) (Table 2, rows 8-9). As in the previous section, we also consider the robustness of results to changes in horizontal resolution.

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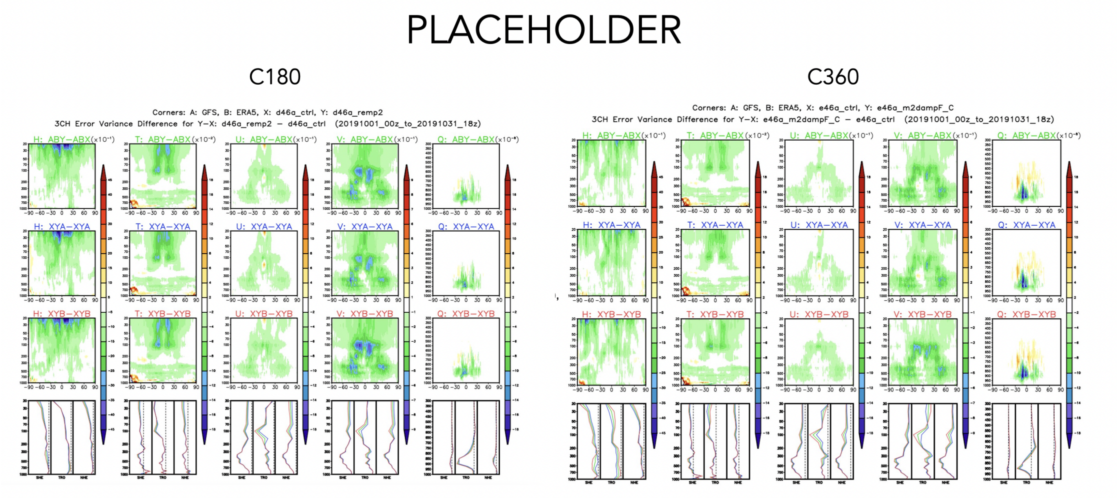

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4 Conclusions

Here we have presented an analysis aimed at understanding changes in the representation of the stratospheric circulation occurring in several model configurations of GEOS-5 moving from MERRA-2 to more recent candidate systems for GEOS-R21C. Through the use of targeted model experiments oriented at disentangling various model development updates, we have identified a key role played by changes in the handling of the remapping algorithm within the model's finite-volume dynamical core. Our key results are as follows:

#1. The stratospheric mean age-of-air in GEOS-5 is sensitive to the degree of the interpolation scheme that is used to calculate layer-mean values of total energy, u, v and tracers. Different handling of details in the vertical remapping algorithm (REMAP Option 1 vs. 2) result in mid-stratospheric (50 hPa) age-of-air differences of ∼1 year over high latitudes, or about 30% climatological mean values.

#2. The age-of-air sensitivies reflect, to first order, changes in the strength of tropical upwelling associated with the Brewer-Dobson circulation which are in turn are driven by changes in EP flux convergence over northern midlatitudes. Changes in wave convergence reflect shifts in (critical lines of) wave propagation that originate in the troposphere over the Pacific Ocean, a region of strong upward wave activity.

#3. The degradation of age-of-air, upwelling and zonal wind climate statistics manifest in AMIPs, also translate to degradations in the DAS analysis states of a broad range of variables. Both DAS- and AMIP-based findings are not sensitive to horizontal resolution.

Although our focus here has been on the transport circulation, motivating our use of tracer-independent metrics like the age-of-air, our results have clear implications for constituent transport in GEOS-R21C. In particular, we showed that the increased age-of-air biases correspond to increased biases in the representations of CH_4 and N_2O moving from the CCMI Phase 1 to Phase 2 model configuration. This comports with well-known correlations between the mean age and stratospheric trace gases, reinforcing the fact that model transport inaccuracies continue to significantly affect simulations of important long-lived chemical species in the stratosphere (Hall et al. (1999)).

Our results highlight the key role played by model numerics in transport (e.g., Rood (1987)). The sensitivities in the age-of-air documented herein are also consistent in spirit with the findings in Gupta et al. (2020) who showed significant age differences occurring between spectral versus finite-volume numerics. Our results, however, suggest that there remain large sensitivities even within a given (FV) dynamical core. Furthermore, we also show that that statistics derived from long AMIPS also manifest within a data assimilation context, which raises important questions as to the degree to which model biases can be ameliorated through assimilation of observations.

Looking forward, our findings support and build on the recommendation proposed in Gupta et al. (2020) for the construction of dynamical core benchmark tests aimed at determining how underlying AGCM numerics and resolution impact climatological transport properties. In particular, in addition to the age-of-air, the authors propose a range of stratospheric circulation diagnostics that should be evaluated including the zonal mean zonal winds, eddy temperature variance and zonal spectra of eddy kinetic energy. Our analysis reveals an important role to be played by the climatological zonal mean wind structure as it impacts wave convergence over midlatitudes; we therefore also recommend explicit consideration of the Eliassen Palm flux convergence and tropical upwelling (w^*) fields as they may be crucial for interpreting age-of-air changes.

One somewhat incidental – but practical - result from our analysis is that the statistics of $\nabla \cdot$F and w^* are well approximated by ensembles of so-called EMIP integrations. As these are substantially easier to run that AMIPs these could provide a "first pass" when evaluating new proposed model development changes, without the immediate need to integrate AMIP-style experiments. We emphasize, however, that this statement should only apply to a first stage in model development as the age-of-air will reflect the time integrated impacts of both advection and mixing.

Finally, we conclude by noting that, while we have focused on sensitivities within the FV remapping algorithm, our results have highlighted important sensitivities to changes in radiation and, to a lesser extent, changes in parameterized convection. Though not the dominant drivers of the age-of-air changes exhibited here, the former could potentially both directly influence the age through changes in thermal structure and indirectly influence the age by modified wave propagation and/or generation in the troposphere. Future work will focus on examining these influences.

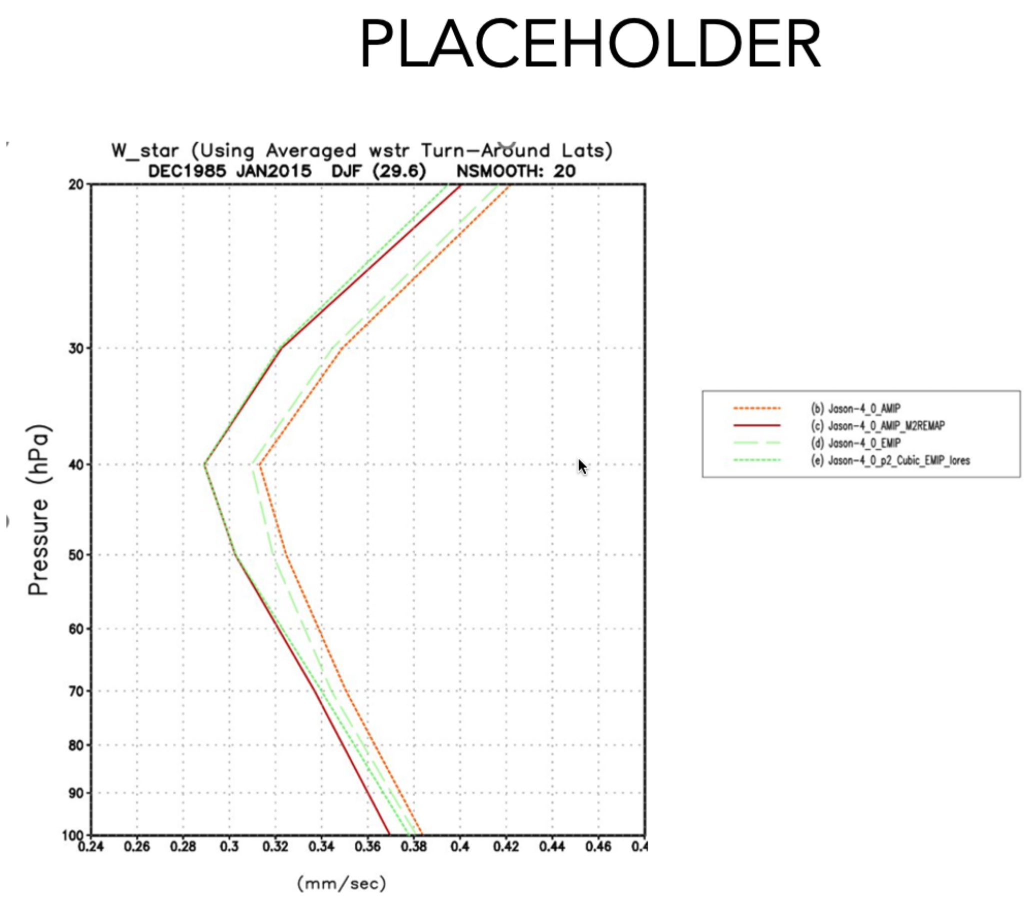

Figure A1. The DJF climatological mean vertical residual mean velocity, w^*, averaged between the turnaround latitudes for the CTRL experiment (Table 2, row 1). Results based on a 30-year-long AMIP experiment (dotted orange line) and a 30-member ensemble of three-month-long EMIP experiments (dashed green line) are shown.

Appendix A Appendix Figures

Open Research Section

TBD

Acknowledgments

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PLACEHOLDER

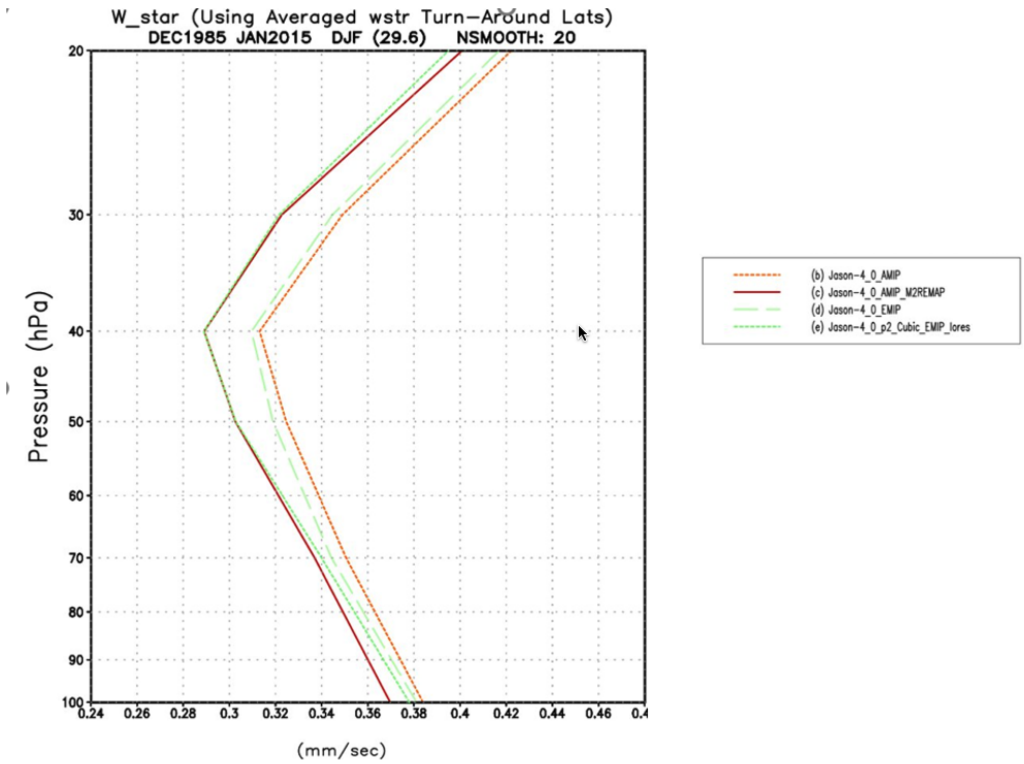

Figure A2. PLACEHOLDER

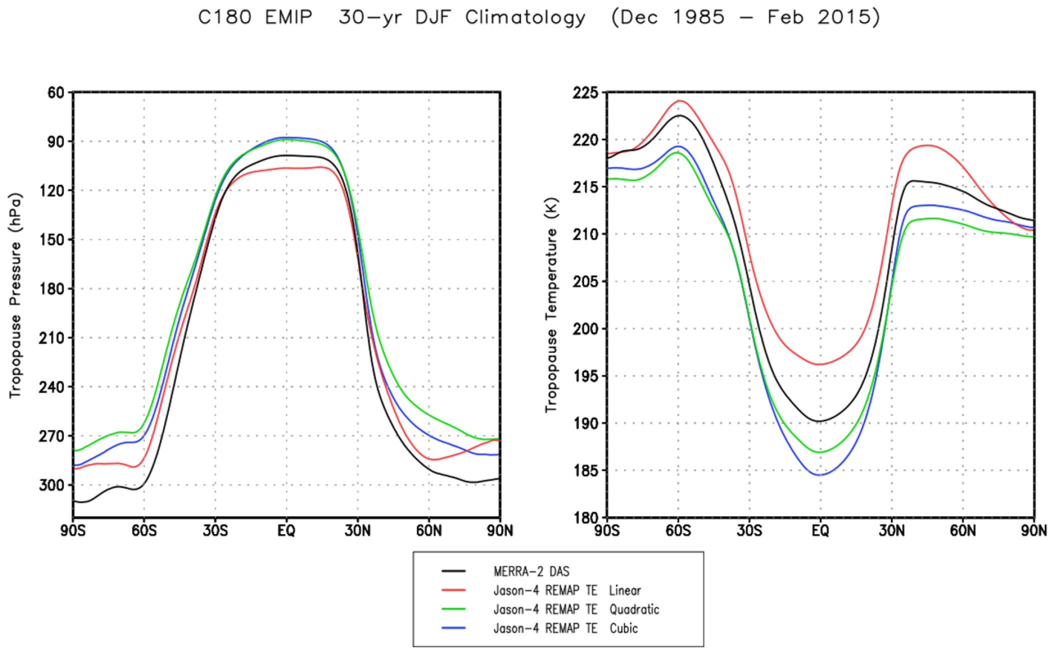

Figure A3. The DJF climatological mean tropopause pressure (left) and temperature (right) in the CUBIC (blue), QUADRATIC (green and LINEAR (red) experiments. MERRA-2 is shown in black. Results are presented for the C180 experiments.

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