Changes in Stratospheric Climate and Age-of-Air in Recent GEOS Systems since MERRA-2

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Key Points:

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10	•	The stratospheric mean age-of-air simulated in GEOS is sensitive to the remap-
11		ping scheme used within the finite-volume dynamical core.
12	•	This sensitivity in the age-of-air is large ($\sim 30\%$) and imprints on the simulated
13		distributions of several long-lived trace gases (e.g., N_2O , CH_4).
14	•	The age-of-air sensitivities primarily reflect changes in resolved wave convergence

¹⁵ over the NH extratropical stratosphere.

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16 Abstract

Accurately modeling the large-scale transport of trace gases and aerosols is crit-17 ical for interpreting past (and projecting future) changes in atmospheric composition. 18 Simulations of the stratospheric mean age-of-air continue to show persistent biases in chem-19 istry climate models, although the drivers of these biases are not well understood. Here 20 we identify one driver of simulated stratospheric transport differences among various NASA 21 Global Earth Observing System (GEOS) candidate model versions under consideration 22 for the upcoming GEOS Retrospective analysis for the 21^{st} Century (GEOS-R21C). In 23 24 particular, we show that the simulated age-of-air values are sensitive to the so-called "remapping" algorithm used within the finite-volume dynamical core, which controls how in-25 dividual material surfaces are vertically interpolated back to standard pressure levels af-26 ter each horizontal advection time step. Differences in the age-of-air resulting from changes 27 within the remapping algorithm approach ~ 1 year over the high latitude middle strato-28 sphere – or about 30% climatological mean values – and imprint on several trace gases, 29 including methane (CH_4) and nitrous oxide (N_2O) . These transport sensitivities reflect, 30 to first order, changes in the strength of tropical upwelling in the lower stratosphere (70-31 100 hPa) which are driven by changes in resolved wave convergence over northern mid-32 latitudes as (critical lines of) wave propagation shift in latitude. Our results strongly sup-33 port continued examination of the role of numerics in contributing to transport biases 34 in composition modeling. 35

³⁶ Plain Language Summary

Large-scale transport plays a crucial role in distributing climatically important trace 37 constituents in the atmosphere, especially in the stratosphere where transport largely 38 determines the chemical lifetimes of trace gases. One summary of transport in the strato-39 sphere is the "mean age" or the mean transit time since air at a point in the stratosphere 40 was last in the troposphere. Current models used for simulating stratospheric compo-41 sition produce a range of simulated ages, although these differences are poorly under-42 stood. Among other factors, model numerics play a critical role in transport, but few 43 studies have explored the sensitivity of the mean age to the choice of numerical scheme 44 employed within different dynamical cores. Here we use one model to show that the mean 45 age is sensitive to the so-called "remapping" algorithm used within the finite-volume dy-46 namical core that controls how individual material surfaces are vertically interpolated 47 back to standard pressure levels after each horizontal advection time step. This reflects 48 sensitivities in the representation of how waves propagate from the troposphere into the 49 stratosphere. This work suggests that model numerics can be an important factor in con-50 tributing to differences in simulated transport among models. 51

52 1 Introduction

The chemical and radiative properties of the troposphere and lower stratosphere 53 are strongly influenced by the stratosphere-troposphere exchange of mass and tracers (e.g., 54 Morgenstern and Carver (2001); Hegglin et al. (2006); Pan et al. (2007)). Properly sim-55 ulating the stratospheric circulation and its influence on atmospheric composition in earth 56 system models is important for capturing past decadal trends in surface climate, par-57 ticularly in response to changes in Southern Hemisphere ozone depletion (e.g., Son et 58 al. (2009); Polvani et al. (2011)). In the Northern Hemisphere (NH), the stratospheric 59 circulation's coupling to ozone could represent an important feedback on the climate's 60 response to future increases in greenhouse gases (GHGs), especially over the North At-61 lantic (e.g., Chiodo and Polvani (2019)). On shorter subseasonal timescales, stratospheric 62 ozone changes associated with strong polar vortex states may also modulate Arctic sea 63 level pressure and surface temperatures (e.g., Ivy et al. (2017); Oehrlein et al. (2020)), 64 so much so that seasonal forecast systems employing prognostic ozone show suggestions 65

of increased signal-to-noise ratio in predictions of the North Atlantic Oscillation (B. M. Monge-Sanz et al. (2022)).

Key to accurately simulating a consistent representation of coupling between stratospheric dynamics and chemical trace gases is ensuring that a model's underlying transport circulation is properly represented. To this end, much effort has been paid to developing 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 75 Validation (SPARC CCMVal) effort showed a marked improvement in simulated trans-76 port characteristics relative to previous intercomparisons (J. Neu et al. (2010)), more re-77 cent analysis of models participating in the SPARC Chemistry Climate Modeling Ini-78 tiative (CCMI) (Eyring et al. (2013)) do not demonstrate any improvement (Dietmüller 79 et al. (2018), see their Figure 3). In particular, although some models produce mean age 80 values that agree well with observational estimates, the CCMI intermodel spread is \sim 81 50%, with models generally simulating transport that is too vigorous relative to obser-82 vations. While documenting these transport differences among models is straightforward, 83 understanding the drivers of this spread remains a challenge and there is still no con-84 sensus on what is causing the large spread in simulated ages among the current gener-85 ation of CCMs. 86

A key challenge in identifying the drivers of age-of-air – and other stratospheric trans-87 port – biases is that they reflect the time-integrated effects of advection by the residual 88 mean circulation and eddy diffusive mixing, or the quasi-random transport due to the 89 breaking of Rossby waves (e.g., Holton et al. (1995); Plumb (2002)). Given that the in-90 fluences of mixing and advection are not easily separable, studies have come to differ-91 ent conclusions about sources of age biases in models. In particular, the analysis of the 92 CCMVal models showed a strong correlation between the intermodel spread in the age-93 of-air and lower stratospheric tropical upwelling, whereas Dietmüller et al. (2018) showed 94 that the age spread among the CCMI models was driven by differences in mixing. While 95 future attempts to further distinguish between sources of age biases using either simpli-96 fied "leaky pipe" models (Plumb (1996); J. L. Neu and Plumb (1999)) or more complete 97 measures of the transport circulation such as the "age spectrum" (e.g., Hall and Plumb 98 (1994); Waugh and Hall (2002))) may prove enlightening, at present there is no consen-99 sus on what is causing large simulated age-of-air biases in models. 100

One potential limitation of previous work based on multi-model intercomparisons 101 is that many aspects of model formulation can influence both stratospheric upwelling and 102 mixing. Thus, while intercomparisons are useful for identifying common model biases, 103 understanding the drivers of these biases is difficult absent single model-based process 104 studies. Among these, several aspects of model formulation have been identified as in-105 fluencing simulated mean age distributions. As the mean age is sensitive to vertical mo-106 tion in the lowermost stratosphere, these include large sensitivities to vertical resolution 107 (Orbe et al. (2020)) and to spurious vertical mixing either introduced in vertical coor-108 dinate transformations in offline chemical transport models (B. Monge-Sanz et al. (2007)) 109 or through use of assimilated winds performed either in offline (e.g., Legras et al. (2004)) 110 or online data assimilation and "nudged" configurations (e.g., Pawson et al. (2007); Orbe 111 et al. (2017); Davis et al. (2022)). These age sensitivities can be still further amplified, 112 depending on whether or not parameterized gravity waves are included (Eichinger et al. 113 114 (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 simulated age-of-air values 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 with moist physics, especially in the context of model development as carried out in operational modeling centers.

To better elucidate this influence of tracer numerics on the transport properties simulated in a comprehensive global model context, here we document the sensitivity of the stratospheric mean age in several recent versions of the NASA Global Earth Observing System (GEOS) general circulation model (Molod et al., 2015). The versions examined here represent different stages in model development since the Modern-Era Retrospective Analysis for Research and Applications Version 2 (MERRA-2; Gelaro et al. (2017)).

Our focus on transport evaluation is partly in wake of the upcoming release of the 131 GEOS Retrospective analysis for the early 21st Century (GEOS-R21C), which is an at-132 mospheric reanalysis that includes many advances over MERRA-2, and serves as a step 133 towards MERRA-3, a planned coupled Earth system reanalysis. Along with having im-134 plications for GEOS-R21C, our analysis also includes the GEOS-IT Version 5.29.4 dat-135 ing from October 19, 2022 (hereafter simply "GEOS-IT"), which will be used to drive 136 an off-line chemistry reanalysis with a full chemistry model (GEOS-Chem) and an ad-137 vanced Constituent Data Assimilation component to update the chemistry fields. Since 138 this chemical reanalysis will be produced in replay-mode (one-way coupling) whereby 139 the meteorology fields are used to define the background atmospheric flow (Orbe et al., 140 2017), it is imperative that recent tags of GEOS produce a credible representation of trans-141 port processes. 142

In particular, here we document how in the process of evaluating candidate sys-143 tems for GEOS-R21C we found that the mean age was ~ 1 year younger (or $\sim 30\%$ smaller) 144 than the values simulated in the model version used to produce MERRA-2 (Figure 1). 145 The model versions shown in Figure 1 reflect more than 10 years' worth of accumulated 146 changes in model development, most notably changes in radiation, parameterized con-147 vection and, as we focus on here, changes in the model's description of vertical advec-148 tion. More precisely, we show that slight modifications to the so-called "remapping" al-149 gorithm, which is used to transform advected fields from Lagrangian levels to the new 150 pressure levels after each horizontal advection time step, are the primary driver of the 151 age-of-air changes exhibited in recent GEOS-R21C candidate model versions. Thus, whereas 152 Gupta et al. (2020) highlighted large differences between dynamical cores employing spec-153 tral versus finite-volume (FV) numerics, our results show that large transport differences 154 can occur even within a given FV dynamical core, a result which may have broader im-155 plications for other general circulation models employing FV numerics. We begin by dis-156 cussing methods in Section 2 and present key results and conclusions in Sections 3 and 157 4, respectively. 158

159 2 Methods

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2.1 Model Configurations

Here we present results from several versions of GEOS 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 a model version that was used in Phase 1 of CCMI and documented in Orbe et al. (2017) (Fig. 1, red line). A more recent model version that was used in the CCMI Phase 2 simulations (correspondence with Michael Manyin) is also shown (Fig. 1, green line).

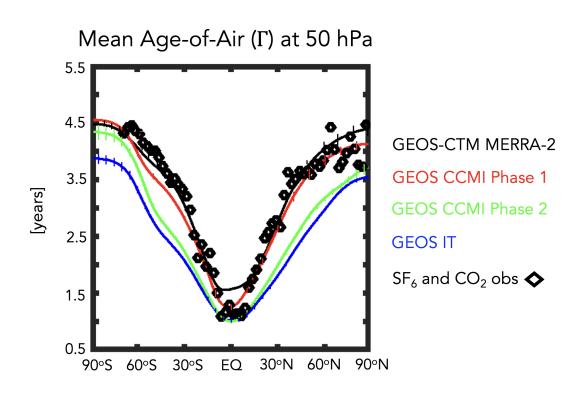


Figure 1. The 2000-2010 climatological annual mean meridional profile of the stratospheric mean age-of-air (Γ), evaluated at 50 hPa. Results from a GEOS-CTM integration constrained with MERRA-2 meteorological fields (black line) as well as free-running GEOS simulations using a model configuration for CCMI Phase 1 (red line), CCMI Phase 2 (green line) and the GEOS-IT Version 5.29.4 dating from October 19, 2022 (hereafter simply "GEOS-IT", blue line) are shown. All simulations are constrained with the same (observed) historical sea surface temperatures. Diamonds correspond to SF₆ and CO₂ in situ based estimates of Γ from Boering et al. (1996) and Engel et al. (2009). Vertical dashed lines denote $\pm \sigma$, the standard deviation of Γ over 2000-2010, for each model simulation.

We begin by comparing 10-year (2000-2010) climatological mean zonally averaged 168 age-of-air profiles at 50 hPa across this subset of model versions, derived from 30-year 169 long atmosphere-only (AMIP) integrations constrained with observed sea surface tem-170 peratures (Figure 1). First, we note that the profiles for the CCMI Phase 1 version of 171 the model are very close to observations (black stars), consistent with the 172 "GEOSCCM" documented age characteristics reported in Dietmüller et al. (2018) (see 173 their Figure 3). In addition, while passive tracers were not integrated within MERRA-174 2, results using the GEOS chemistry transport model (GEOS-CTM, Kouatchou et al. 175 (2015)) constrained with MERRA-2 meteorological fields (black line) also exhibits good 176 agreement with observed values. This good agreement between the CTM-generated age-177 of-air and the observations is consistent with results from a previous GEOS-CTM sim-178 ulation (constrained with MERRA) as documented in Orbe et al. (2017). 179

Moving to more recent development versions of the model (green and blue lines), however, reveals a reduction in the mean age by ~ 1 year over both southern and northern high extratropical latitudes, or a decrease of $\sim 20-30\%$ relative to the MERRA-2 constrained simulation and the observations. As discussed earlier, the green line refers to the CCMI Phase 2 model version, whereas the blue line refers to GEOS-IT. Note that this decrease in the climatological age in both model versions far exceeds the (internal) variations in mean age that occur interannually (vertical bars on solid lines).

Since MERRA-2, numerous updates have been introduced in the GEOS model. This 187 includes replacing the Chou Suarez (Chou & Suarez, 1994) and Chou (Chou, 1990, 1992) 188 radiation codes with the Rapid Radiative Transfer Model for GCMs (RRTMG; Iacono 189 et al. (2008)), which impacts the stratosphere; the introduction of the Grell-Freitas deep-190 convection code (Grell and Freitas (2014); Freitas et al. (2018)), which has a minimal 191 impact on this study; and upgrades to the vertical remapping option from that used in 192 MERRA-2 (hereafter denoted as GMAO FV3 Cubic) to the current updated GDFL remap-193 ping option (hereafter denoted as GFDL FV3 Cubic). Note that both MERRA-2 and 194 current systems use the GFDL FV3 dynamical core (Lin et al., 2017), but differ in terms 195 of this remapping option. 196

As we show in Section 3, the latter transition from the remapping scheme used in 197 MERRA-2 (GMAO FV3) to the scheme used in the current GFDL FV3 core has the largest 198 impact on the simulated age-of-air values. This degradation in simulated transport within 199 the current GFDL FV3 core primarily reflects differences in the implementation of the remapping algorithm, which is used to vertically interpolate individual material surfaces 201 after each horizontal advection step back to the model's reference Eulerian coordinate. 202 In its implementation in MERRA-2 within the GMAO FV3 core (Table 1), this remap-203 ping involves 1) fitting piecewise parabolic (hereafter PPM) functions to input layer-mean 204 values of U, V, Q and tracers; 2) calculating PPM functions to output layer edges; 3) 205 integrating PPM functions between output layer edges to produce new layer-mean val-206 ues of U, V, Q and tracers; 4) calculating total energy (TE) at input mid-layer pressures; 207 5) calculating TE at output mid-layer pressures using cubic interpolation and applying 208 an a-posteriori integral conservation; and, finally, 6) remapping temperatures from to-209 tal energy via T = (TE - K - Φ)/C_p. Here T, U, V, Q, C_p, K and Φ correspond to tem-210 perature, zonal wind, meridional wind, specific humidity, specific heat capacity and ki-211 netic and potential energy, respectively. 212

Differences in the implementation of this remapping algorithm within the current 213 GFDL FV3 core results in degraded simulated stratospheric transport. To demonstrate 214 this in as clean a fashion as possible, we use targeted experiments with the GMAO FV3 215 216 system to show that the degradations in simulated transport when using the remapping option from the GFDL FV3 core resemble changes that occur when using a lower order 217 (quadratic vs. cubic) interpolation scheme in Step 5 of the remapping algorithm (Ta-218 ble 1). This otherwise innocuous change in interpolation order in turn highlights the large 219 sensitivities in transport that can occur even *within* a given finite-volume numerical scheme, 220

Table 1. GMAO FV3 Core Finite-Volume Remapping Algorithm: The remapping algorithm examined in this study controls how individual material surfaces are vertically interpolated back to standard pressure levels. Employing linear – and to a lesser extent – quadratic interpolation in Step 5 produces stratospheric transport characteristics that are more consistent with the most recent GEOS model configurations (green and blue lines, Figure 1), whereas a cubic interpolation is more consistent with older configurations (red and black lines, Figure 1) and with MERRA-2. Here T, U, V, Q, C_p , K and Φ correspond to temperature, zonal wind, meridional wind, specific humidity, specific heat of air at constant pressure and kinetic and potential energy, respectively.

Step	REMAP Procedure (MERRA-2, GMAO FV3 Core)
1	Fit PPM functions to
	input layer-mean U, V, Q and tracers
2	Calculate PPM to output layer edges
3	Integrate PPM functions between output
	layer edges to produce new layer-
	mean U, V, Q and tracers
4	Calculate $TE = C_p T + K + \Phi$
	at input mid-layer pressures
5	Calculate TE at output mid-layer pressures
	using cubic interpolation and
	a-posteriori integral conservation
6	Construct "remapped" T via
~	$T = (TE - K - \Phi)/C_p$

in our case resulting in large differences in lower stratospheric upwelling and a $\sim 30\%$ reduction in the simulated mean age of air.

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2.2 Model Experiments

2.2.1 AMIP vs. EMIP

We begin our analysis by interpreting the results shown in Figure 1, which are all based on historical AMIPs that were performed at the same cubed sphere C180 (approximately half-degree) horizontal resolution. As they represent more official model versions they serve as an important motivation for the experiments that follow. However, there are numerous (potentially compensating) development changes between these model versions which renders it nearly impossible to cleanly identify drivers of differences in their simulated transport.

To this end, in order to investigate the drivers of the differences in Figure 1 we perform targeted modeling experiments aimed at disentangling the influence of individual model development changes on stratospheric transport properties (Table 2). In order to evaluate impacts on transport climate statistics, we consider both a set of climatological AMIP (rows 1-4) as well as so-called "EMIP" (rows 5-7) experiments.

In particular, we carry out 30-year-long AMIP simulations at C180 resolution which we use to infer the climate characteristics of the different model configurations. The "EMIP" experiments – ensembles of 3-month-long integrations initialized on approximately November 15 of each year between 1985 and 2015 – are also used to infer impacts on simulated transport climate. As they are more computationally efficient than AMIPs since all 30 **Table 2. GEOS Model Experiments**: Targeted GEOS model experiments based off a control experiment (row 1) were carried out to identify the influence of radiation (row 2) and changes in the remapping algorithm used since MERRA-2 (row 3), as well as their combined influence (row 4). The influence of the remapping algorithm changes is then interpreted using a simpler set of sensitivity experiments, performed using the GMAO FV3 core, in which only the order of the interpolation scheme used to calculate TE at output mid-layer pressure levels is altered (rows 5-7). Experiments in rows 1-4 are 30-year-long AMIPs run at C180 resolution, whereas rows 5-7 refer to 30-member 3-month-long (DJF) EMIP experiments. Both AMIPs and EMIPs are used for climate statistic evaluation (see Appendix B for more on the correspondence between the two). EMIP experiments are run at both C180 and C360 horizontal resolutions.

Experiment Name	Configuration	Experiment Type	Hor. Resolution
CTRL	Control, GFDL FV3 Core	AMIP (30 yrs.)	C180
CSRAD	Chou-Suarez (1994)	AMIP (30 yrs.)	C180
	Radiation (RAD)		
M2REMAP	GMAO FV3 Core (cubic)	AMIP (30 yrs.)	C180
CSRAD+M2REMAP	Chou-Suarez (1994) RAD	AMIP (30 yrs.)	C180
	GMAO FV3 Core (cubic)		
LINEAR	GMAO FV3 Core (linear)	EMIP (30 mem.)	C180, C360
QUADRATIC	GMAO FV3 Core (quadratic)	EMIP (30 mem)	C180, C360
CUBIC	GMAO FV3 Core (cubic)	EMIP (30 mem)	C180, C360

3-month-long integrations may be run in parallel, they are performed at both C180 and
 C360 (approximately quarter-degree) resolutions in order to examine the sensitivity of
 our results to changes in horizontal resolution.

As shown in Appendix B, comparisons of the December-January-February (DJF) 245 vertical profile of tropical upwelling show excellent agreement between EMIP and AMIP 246 integrations carried out using the same model configuration (Appendix Figure B1). This 247 somewhat incidental result represents, to the best of our knowledge, the first time that 248 EMIP-based statistics have been shown to converge well to those from AMIPs for the 249 stratospheric metrics considered in this study. This suggests that EMIPs, relative to AMIPs, 250 may be used to provide a computationally more efficient initial assessment of the impacts 251 of model changes on the stratospheric circulation. 252

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2.2.2 Model Development Changes

Moving next to the precise model development changes examined, 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 AMIP experiments, which aim to distinguish between the age-of-air changes resulting from changes in radiation versus changes in the handling of the REMAP algorithm that occurred in the transition from MERRA-259 2 to the current FV3 cores (Section 3.2.1).

Specifically, these include experiments in which we a) replace RRTMG with the radiation from Chou and Suarez (1994) (CSRAD; Table 2, row 2), b) replace the current
FV3 REMAP approach with the settings used in the GMAO FV3 core when running
MERRA-2 (i.e., M2REMAP; Table 2, row 3) and c) combine these two changes (CSRAD+M2REMAP;
Table 2, row 4)

Table 2, row 4).

As we show in Section 3.2.1, the M2REMAP experiment produces larger changes 265 in age-of-air, compared to the experiment in which only the radiation is altered (CSRAD). 266 Interpreting this result, however, is not straightforward since there are several differences 267 in the implementation of the remapping algorithm between the GMAO and GFDL FV3 cores that are interdependent and, thus, difficult to isolate cleanly. To this end, in or-269 der to simplify the problem we focus the remainder of our investigation (Section 3.2.2) 270 on examining a clean set of EMIP experiments that are all performed using the GMAO 271 FV3 core remapping settings and that differ from each other only in terms of the order 272 of the interpolation that is used to calculate TE at the mid-layer pressure levels (Step 273 5, Table 1). More precisely, we compare configurations using a linear (LINEAR; Table 274 2, row 5), quadratic (QUADRATIC; Table 2, row 6) and cubic interpolation (CUBIC; 275 Table 2, row 7) scheme, with the latter corresponding to the approach that was used in 276 MERRA-2. To assess the robustness of our findings to changes in horizontal resolution, 277 all three sensitivity experiments are run at both C180 and C360 resolutions. 278

These three numerical schemes are derived from the generic Lagrangian interpolation equation:

$$\mathcal{Q}(\mathcal{P}) = \sum_{k'} a_{k+k'} \mathcal{Q}_{k+k'} \qquad k' = 0, \pm 1, \pm 2, \dots$$
(1)

where \mathcal{P} represents the target output location in $\ln(p)$ and $\mathcal{Q}_{k+k'}$ denotes the surrounding grid-point values at input locations. The coefficients $a_{k+k'}$ are derived through Taylor Series expansions using non-uniform grid spacing given by:

$$a_{k+k'} = \frac{\prod_{m} (\mathcal{P}_{k+m} - \mathcal{P})}{\prod_{m} (\mathcal{P}_{k+m} - \mathcal{P}_{k+k'})} \qquad m = 0, \pm 1, \pm 2, \dots \qquad m \neq k'$$
(2)

For the three schemes, the grid points used are: LINEAR (k, k-1), QUADRATIC (k+1, k, k-1), and CUBIC (k+1, k, k-1, k-2). In all cases, the grid points are chosen such that the target location resides between layers k and k-1.

Note that, while the LINEAR and QUADRATIC experiments do not actually correspond to any of the model versions shown in Figure 1, they highlight the large sensitivity of the mean age to changes in the interpolation scheme that may otherwise seem innocuous. They also provide further evidence of the strong influence of changes in tropical lower stratospheric upwelling strength on the stratospheric mean age in GEOS.

Finally, in all experiments using the MERRA-2 remapping approach (i.e., M2REMAP, 292 CSRAD+M2REMAP, LINEAR, QUADRATIC, CUBIC) additional modifications to the 293 divergence damping coefficients were used so as to best ensure consistency with what was 294 used in MERRA-2. Specifically, these include changes to the number of layers for ver-295 tical subgrid mixing, the coefficient for barotropic mode damping, the use of 2nd vs. 6th 296 order divergence damping and the strength of the divergence damping coefficients. Com-297 pared to the impact of moving from the CTRL to M2REMAP experiments, these ad-298 ditional changes have a much smaller impact on lower stratospheric upwelling in the model 299 (not shown) and hereafter will not be discussed further. 300

301 2.3 Analysis Approach

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2.3.1 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 the bottom model level as follows: 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 $\Gamma(\mathbf{r})$, 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 310 also show results from an idealized e90 tracer that is uniformly emitted over the entire 311 surface layer and decays exponentially at a rate of 90 $days^{-1}$ such that concentrations 312 greater than 125 ppb and less than 50 ppb tend to reside in the lower troposphere and 313 stratosphere, respectively (Prather et al. (2011)). As this tracer features strong near-314 tropopause gradients and takes significantly less time to equilibrate, compared to the mean 315 age, it is useful for evaluating stratosphere-troposphere-exchange and transport within 316 the upper troposphere/lower stratosphere (Abalos et al. (2017, 2020); Orbe et al. (2020)). 317

Both the mean age and e90 tracers were integrated in all of the AMIP experiments shown in Figure 1 and listed in Table 2 (rows 1-4), which were run using the same idealized passive tracer package described in Orbe et al. (2017). Note that the mean age tracer was not integrated in the EMIP experiments given its much longer characteristic timescale in the stratosphere (\sim 3-5 years). As such, the EMIP simulations, which do not exceed one year, are not appropriate for evaluating the time-integrated transport characteristics reflected in the age-of-air.

In addition to carrying the idealized tracers, two of the experiments shown in Figure 1 were also run with full interactive chemistry and correspond to the two CCMI (Phase 1 and Phase 2) integrations (red and green lines, Figure 1). Both simulations employ the same Global Modeling Initiative (GMI) chemical mechanism (Strahan et al. (2013)) and are therefore useful in evaluating the impact of age differences on real trace gas distributions. In particular, as shown in Section 3.1 results from these experiments show significant imprints of the age-of-air changes on nitrous oxide (N₂O) and methane (CH₄).

2.3.2 Circulation Diagnostics

As we show in Section 3, the changes in age-of-air across the different model ver-333 sions are strongly tethered to changes in the advective component of the circulation, which 334 we quantify using the Transformed Eulerian Mean (TEM) estimate of the Lagrangian 335 transport of mass by the circulation. Thus, in addition to more standard Eulerian met-336 rics of the circulation (e.g., zonal winds and temperatures), we focus on the vertical com-337 ponent of the TEM residual velocity, defined as $\overline{w}^* = \overline{w} + \frac{\partial(\psi \cos\phi)}{a\cos\phi\partial\phi}$, where $\psi = \overline{v'\theta'}/\frac{\partial\overline{\theta}}{\partial p}$ is the eddy stream function, θ refers to potential temperature, a is the Earth's radius 338 339 and overbars and primes denote zonal means and deviations therefrom, respectively (Andrews 340 et al. (1987)). In addition, we interpret the behavior in w^* using the Eliassen-Palm flux 341 divergence $(\nabla \cdot \mathbf{F})$, whose horizontal $(\mathbf{F}(\phi))$ and vertical $(\mathbf{F}(p))$ components are respec-342 tively defined as $F(\phi) = a\cos\phi[\frac{\partial u}{\partial p}\psi - \overline{u'v'}]$ and $F(p) = a\cos\phi([f - \frac{\partial\overline{ucos\phi}}{acos\phi\partial\phi}]\psi - \overline{u'\omega'}).$ 343

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2.4 Observations and Reanalyses

While our focus is on interpreting and understanding the different model config-345 urations, we incorporate observations to provide context when possible, although we do 346 not present an exhaustive evaluation of the model's transport characteristics (for that 347 see earlier studies including Orbe et al. (2017, 2018)). However, as the tracers are not 348 directly integrated in MERRA-2 (with the exception of ozone), we compare against in-349 dependent observational estimates. For the mean age we first compare simulated merid-350 ional age profiles at 50 hPa with values derived from in situ aircraft measurements of car-351 bon dioxide (CO_2) , averaged in 2.5 degree latitude bins over the altitude range 19.5 to 352 21.5 km (Boering et al. (1996), see also Figure 5 in Hall et al. (1999)). 353

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 (CH₄) 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 (N₂O) are made

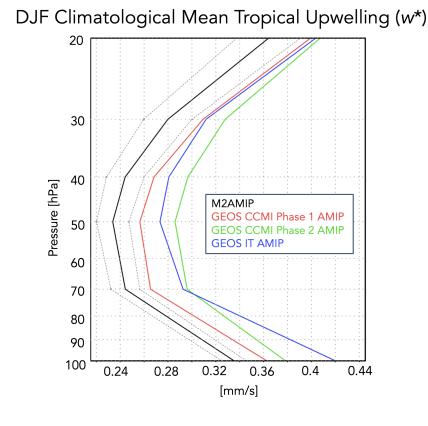


Figure 2. The DJF 1985-1994 climatological mean vertical residual mean velocity, w^* , averaged at each level between the turnaround latitudes for GEOS free-running AMIP simulations using the model configurations corresponding to the CCMI Phase 1 (red) and Phase 2 (green) submissions and to GEOS-IT (blue). M2AMIP is shown in black, with black dashed lines denoting ± 1 standard deviation.

against climatologies derived from the Microwave Limb Sounder (MLS) on the Earth Observing System (EOS) Aura satellite. Climatologies over the same period (2005–2015) are used to evaluate both the model and the observations. 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 N₂O primary band.

For the circulation diagnostics nearly all comparisons are made relative to the MERRA-364 2 data assimilation (DAS) reanalysis product, noting that comparisons against ERA-5 365 (not shown) reveal a similar picture. One exception, however, is the vertical component 366 of the TEM circulation (w^*) , which shows some differences in vertical structure between the MERRA-2 DAS and a 30-member ensemble of (free-running) AMIP integrations pro-368 duced using the MERRA-2 model, hereafter referred to as M2AMIP (Collow et al., 2017)(Ap-369 pendix Figure A1, right). As the free-running model results shown in Figure 1 show more 370 consistency with the vertical profile of M2AMIP, not MERRA-2, we compare w^* in all 371 free-running GEOS experiments with M2AMIP, noting that for non-derived measures 372 (i.e., winds, temperatures), the raw MERRA-2 output is used. 373

The differences in w^* between M2AMIP and the MERRA-2 DAS may reflect the 374 influence of temperature increments in the DAS (MERRA-2) which can drive spurious 375 vertical transport in assimilated products (Weaver et al., 1993; Orbe et al., 2017). In par-376 ticular, Weaver et al. (1993) showed that the imbalance between the thermal and veloc-377 ity fields at the time an observation is ingested during the assimilation cycle can excite 378 unwanted inertial-gravity wave modes that manifest strongly in the residual vertical winds. 379 While this impact of the increments may explain the differences in w^* , we reserve a more-380 in depth examination for future work as our focus in on the transport characteristics of 381 the free-running GEOS system. 382

383 3 Results

384

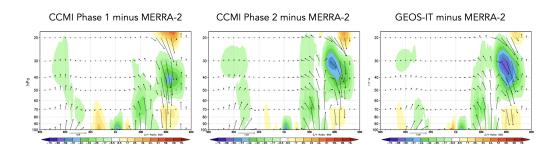
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3.1 Reduction of Stratospheric Mean Age in GEOS Models Since MERRA-2

We begin by interpreting the reduction in mean age exhibited in more recent model 386 versions in terms of changes in the strength of upwelling in the tropical lower stratosphere. 387 In particular, the reductions in Γ (Figure 1) are consistent with increases in the strength 388 of lower stratospheric tropical upwelling, with w^* becoming progressively stronger in more 389 recent model versions, relative to MERRA-2 (Figure 2). Note that these increases in w^* 390 across model versions exceed those due to internal variability alone (black dotted lines, 391 Fig. 2). Furthermore, while the increases in w^* occur throughout the stratosphere, we 392 focus on the changes occurring between 70 and 100 hPa as these are most relevant to 393 determining the tropical upward mass flux and associated strength of the mean overturn-394 ing circulation. 395

Though perhaps naive, the relationship between lower stratospheric upwelling and 396 the mean age suggested by comparing Figure 1 and Figure 2 is consistent with the long-397 term behavior of Γ inferred from both historical and projected future climate simulations 398 (Butchart et al. (2010); Abalos et al. (2021)). A strong relationship between the strength 300 of lower stratospheric ascent and the mean age was also shown to hold in the CCMVal 400 models (see Fig. 5.20 in J. Neu et al. (2010)). Nevertheless, it is important to note that 401 a clear relationship between w^* and Γ is not a priori expected, as the age-of-air is also 402 known to be very sensitive to mixing, which may be important in interpreting differences 403 among the CCMI Phase 1 models (Dietmüller et al. (2018)). 404

The differences in w^* highlighted in Figure 2 are associated with enhanced Eliassen-Palm flux convergence over NH midlatitudes (Figure 3). Increased wave convergence is evident not only within the subtropical lower stratosphere (< 30°N, 50-100 hPa) but also over higher latitudes and altitudes (~ 40°-70°N, 20-50 hPa). The fact that differences



DJF Climatological Mean Eliassen-Palm Flux Divergence ($\nabla \cdot F$)

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

in extratropical wave convergence imprint on tropical upwelling is consistent with our understanding of the so-called "downward control" principle (Haynes 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 the gravity wave drag scheme's 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.

One subtlety to note is that the wave convergence changes shown in Figure 3 occur at high latitudes and are directly associated with downwelling over the polar region. It is then via mass balance that anomalously strong downwelling associated with enhanced flux convergences must be accompanied by enhanced upwelling in the tropics. This indirect impact of higher latitude wave drag reflects an "extratropical pumping" mechanism (Holton et al., 1995), which is illustrated more clearly in Section 3.2.2 in the context of the LINEAR, QUADRATIC and CUBIC experiments.

While the reduction in Γ (Figure 1) of ~ 30% at 50 hPa is significant, it is neither 424 clear if this change is representative of other altitudes within the stratosphere nor how 425 this age bias imprints on real chemical species. To this end, we begin by comparing the 426 full latitude-pressure distribution of changes in Γ and another passive tracer (e90) (Fig-427 ure 4) between the CCMI Phase 1 and Phase 2 model configurations (red and green lines, 428 Figure 1). In particular, we find that the changes in both passive tracers – large reduc-429 tions in Γ within both hemispheres (Fig. 4, top right) and increased values of e90 within 430 the lower stratosphere (Fig. 4, bottom right) – are reflective of an overall increase in the 431 strength of the transport circulation. This is highlighted in the CCMI Phase 2-1 model 432 differences for the passive tracer distributions (Fig. 4, right panels) which are shown in 433 the absence of robust observational constraints of Γ at higher altitudes (or any obser-434 vational constraints for e90, for that matter). The reduced/increased stratospheric bur-435 dens of the age and e90 tracers are consistent with stronger upwelling in the CCMI Phase 436 2 model configuration (Figure 2). 437

⁴³⁸ While the observational constraints on Γ presented in Figure 1 and the departure ⁴³⁹ of w^* away from MERRA-2 suggest that transport properties of the newer model con-⁴⁴⁰figurations are moving in the wrong direction, it is relevant to ask whether or not the

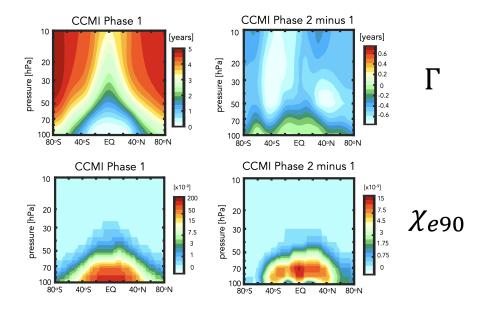


Figure 4. The climatological mean (2000-2010) distribution of the mean age-of-air (Γ) (left, top) and e90 idealized tracers (left, bottom) for the CCMI Phase 1 model configuration. Climatological differences between the CCMI Phase 2 and Phase 1 model configurations are shown in the right panels. Note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

trace gas satellite measurements also support this conclusion. Indeed, comparisons with observations show larger biases in N₂O (Fig. 5, top panels) and CH₄ (Fig. 5, bottom panels), increasing from 10% to 30% in the CCMI Phase 2 model configuration, depending on the species. Recall that the same chemistry mechanism is used in both CCMI Phase 1 and 2 simulations.

The patterns of the trace gases biases are generally consistent with the biases in the mean age (Fig. 4). This comports with well-known correlations between the mean age and stratospheric trace gases, reinforcing the fact that model transport inaccuracies can significantly affect simulations of important long-lived chemical species in the stratosphere (Hall et al. (1999)).

The fact that the mean age changes have a significant imprint on the simulated trace gases is consequential for the GEOS-R21C 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

460

3.2.1 Radiation versus REMAP Algorithm

⁴⁶¹ As discussed in Section 2, among the model changes that were made since MERRA-⁴⁶² 2, the changes in radiation and the FV remapping algorithm are most likely to directly ⁴⁶³ have impacted the stratospheric circulation. We therefore begin by assessing which of ⁴⁶⁴ these changes dominates the decreases in Γ shown in Figure 1.

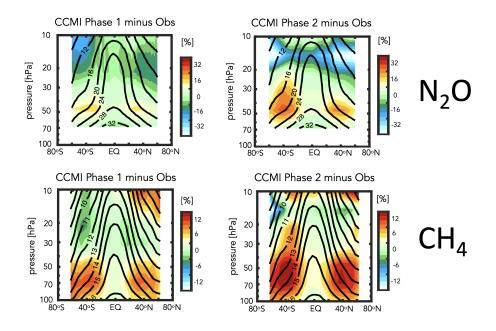


Figure 5. Colors shown anomalies in the simulated distributions of nitrous oxide (N_2O) (top) and methane (CH₄) (bottom), relative to the MLS and HALOE observed values, respectively, for the CCMI Phase 1 (left) and Phase 2 (right) GEOS model configurations. Climatological mean observed values are shown in the black contours.

Figure 6 shows the distribution of Γ for experiments in which the longwave, short-465 wave, and REMAP updates since MERRA-2 have successively been undone. Relative 466 to the control experiment (CTRL; Table 2, row 1), the transition back to Chou and Suarez 467 (1994) in the shortwave and Chou (1990, 1992) in the longwave results in an increase in 468 the mean age of ~ 0.5 years throughout the stratosphere (CSRAD; Table 2, row 2). Though 469 significant, this change in Γ is smaller than the change that results from applying the 470 remapping approach used in MERRA-2 (M2REMAP; Table 2; row 3), in which the mean 471 age increases by ~ 1 year. The combined impacts of both changes (CSRAD+M2REMAP; 472 Table 2 row 4) is roughly linear, with age values of ~ 5.5 years over high latitudes at 50 473 hPa, consistent with the values simulated by the GEOS-CTM MERRA-2 integration (black 474 line, Figure 1) and with the CCMI Phase-1 version of the model (red line, Figure 1). 475

Next we ask if the behavior of Γ exhibited in Figure 6 can be interpreted in terms 476 of changes in the strength of lower stratospheric tropical upwelling and extratropical wave 477 convergence, as our previous analysis of the CCMI experiments suggested. Indeed, Fig-478 ure 7 shows that values of upwelling decrease in the CSRAD and M2REMAP experiments, 479 relative to the CTRL integration. The increase in upwelling resulting from both changes 480 (CSRAD+M2REMAP) is still larger, consistent with the larger age decreases in that ex-481 periment. This change in the behavior of w^* within the tropical stratosphere can be in-482 terpreted in terms of changes in the Eliassen Palm flux convergence over NH midlati-483 tudes (not shown), which features smaller values in the CSRAD, M2REMAP (and CSRAD+ 484 MSREMAP) experiments. Note that our examination of the changes in w^* are derived 485 from EMIP integrations, which we showed previously converge (for DJF) to the statis-486 tics derived from corresponding AMIP experiments. 487

It is important to note that, while the reduced values of w^* in the M2REMAP experiment (Fig. 7), represent an improvement, relative to the CTRL integration, these

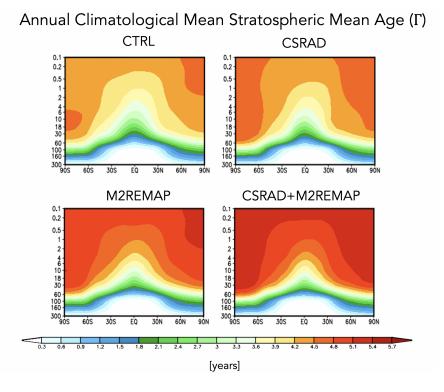


Figure 6. Colors show the simulated 2000-2010 climatological annual mean distributions of the mean age-of-air (Γ) for the CTRL (top left; Table 2, row 1), CSRAD (top right; Table 2, row 2), M2REMAP (bottom left; Table 2, row 3) and combined CSRAD+M2REMAP (bottom right; Table 2, row 4) experiments.

changes are, in isolation, accompanied by a cold bias (~4-6 K) in the tropical lower strato-490 sphere (Fig. 8a). Unlike the upwelling changes, this represents a degradation in model 491 skill, increasing the temperature bias in that region, relative to MERRA-2 (Fig. 8 b,c). 492 While this temperature bias is concerning in isolation, it is decoupled from the changes in residual mean upwelling which, rather, are more sensitive to the changes in *extratrop*-494 *ical* wave convergences (described further in the next section). Furthermore, the increased 495 temperature bias in the M2REMAP experiment appears to be tethered to other updates 496 that were made in the CTRL model (specifically the radiation progression from Chou-497 Suarez to RRTMG). In particular, the M2AMIP ensemble, which also employs the GMAO 498 cubic remapping option, features a much smaller temperature bias in the tropical lower 499 stratosphere, relative to MERRA-2 (~ 0.2 K) (Fig. 8d). This suggests that the ampli-500 fied temperature bias moving from the CTRL to M2REMAP experiments needs to be 501 interpreted in the context of other model development changes that were introduced, par-502 ticularly in the radiation scheme and its coupling to convection. 503

504

3.2.2 FV REMAP Algorithm: Sensitivity of Climate Statistics

Having shown in the previous section that the largest changes in the mean age were 505 realized through the differences in implementation of the remapping algorithm between 506 the GMAO FV3 core used in MERRA-2 and in current FV3 core configurations, we now 507 investigate further the sensitivity of the transport circulation to the choice of remapping 508 interpolation scheme. In particular, we compare simulations run with the GMAO FV3 509 remapping settings in which total energy is calculated at new mid-layer pressures using 510 cubic, quadratic and linear interpolation prior to the aposterior integral conservation (Ta-511 ble 2, rows 5-7). In addition, in this section we seek to understand how the changes in 512 the Eliassen-Palm flux convergence over NH midlatitudes arise via analysis of the large-513 scale wind structure. 514

Figure 9 (left panel) shows a clear sensitivity in tropical upwelling to the choice of 515 interpolation scheme, with w^* progressively increasing in strength moving from the CU-516 BIC to QUADRATIC to LINEAR schemes. This sensitivity is robust across horizontal 517 resolutions as the same suite of experiments performed at C360 exhibit the same sen-518 sitivity (Fig. 9, right panel). While no current model version actually employs a linear 519 scheme, this suite of experiments highlights the strong sensitivity to choice of interpo-520 lation scheme within the remapping algorithm; to the best of our knowledge, this result 521 has not been reported in the literature. 522

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.

Interestingly, the increases in w^* moving from the CUBIC to QUADRATIC schemes 526 not only manifests in free-running AMIP simulations, but also in AMIP simulations in 527 which GEOS is constrained (or replayed, following Orbe et al. (2017)) to MERRA-2 me-528 teorological fields, using the MERRA-2 GMAO cubic interpolation (Fig. 10, blue line) 529 and the GFDL FV3 core remapping approach (Fig. 10, red line). While there is a gen-530 eral increase in w^* in the former, however, both simulations, lie within the range of MERRA2-531 DAS, suggesting that replay does act to ameliorate some of the upwelling biases man-532 ifest in the underlying unconstrained models. While not the focus of this study, this im-533 pact of the remapping approach on simulations run in replay mode will be examined fur-534 ther in future work. 535

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 11). Over extratropical latitudes, the zonal force associated with this enhanced wave convergence is associated with enhanced downwelling at high latitudes that, through mass balance, is accompanied by

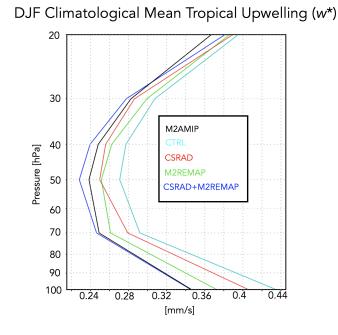


Figure 7. The DJF 1985-2015 climatological mean vertical residual mean velocity, w^* , averaged at each level between the turnaround latitudes for the CTRL (cyan line; Table 2, row 1), CSRAD (red line; Table 2, row 2), M2REMAP (green line; Table 2, row 3) and combined CSRAD+M2REMAP (blue line; Table 2, row 4) experiments. M2AMIP is shown in black.

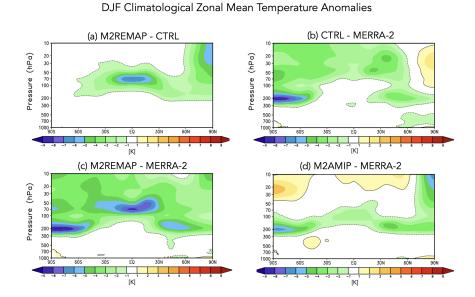
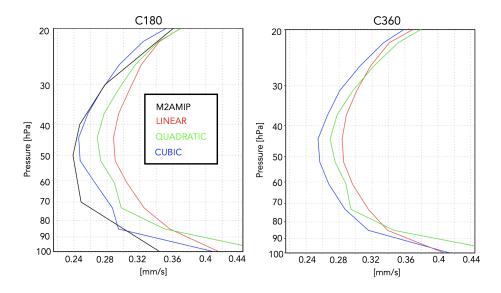


Figure 8. Anomalies in DJF 1985-2015 climatological mean zonal mean temperatures: M2REMAP - CTRL (a), CTRL - MERRA-2 (b), M2REMAP - MERRA-2 (c) and M2AMIP - MERRA-2 (d).



DJF Climatological Mean Upwelling (w*)

Figure 9. The DJF 1985-2015 climatological mean vertical residual mean velocity, w^* , averaged at each level between the turnaround latitudes for the LINEAR (red line; Table 2, row 5), QUADRATIC (green line; Table 2, row 6) and CUBIC (blue line; Table 2, row 7) experiments. M2AMIP is shown in black. Results from C180 and C360 EMIP experiments are shown in the left and right panels, respectively.

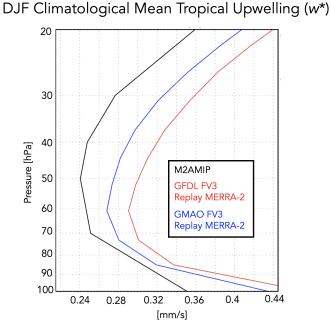


Figure 10. The DJF 2005-2015 climatological mean vertical residual mean velocity, w^* , averaged at each level between the turnaround latitudes for two GEOS replay AMIP simulations constrained with MERRA-2 meteorological fields using remapping approaches from the MERRA-2 GMAO FV3 cubic core (blue line) and the GFDL FV3 core (red line). MERRA-2 DAS is shown in black.

DJF Climatological Mean Eliassen-Palm Flux Divergence ($\nabla \cdot F$)

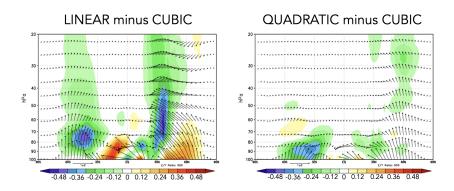


Figure 11. Colors shown anomalies in the DJF 1985-2015 climatological mean Eliassen-Palm (EP) flux divergence in the LINEAR (left) and QUADRATIC (right) experiments, relative to the CUBIC model experiment. Arrows denote anomalies in the vertical and meridional EP flux vectors.

enhanced upwelling in the tropics. This indirect impact of higher latitude wave drag is
 evident in Appendix Figure C1, which shows stronger upwelling/downwelling in the LIN EAR and QUADRATIC experiments over the tropics/polar region.

Next we exploit the fact that these experiments only differ with respect to the in-544 terpolation scheme in order to inquire further into the drivers of the wave convergence 545 changes. To this end, Figure 12 compares profiles of the zonal mean zonal wind between 546 the CUBIC, QUADRATIC and LINEAR experiments, averaged over the region of en-547 hanced wave convergence (i.e. 20°N-60°N). The experiments featuring stronger wave con-548 vergence (LINEAR and QUADRATIC) are also simulations with stronger zonal winds, 549 relative to MERRA-2, especially above 70 hPa. This change in winds occurs at both C180 550 (Fig. 12, left panel) and C360 (Fig. 12, right panel) resolutions. 551

Structurally, the increase in zonal wind strength over northern extratropical mid-552 latitudes is reflective of a poleward shift in the zonal winds as the critical latitude, i.e. 553 where the zonal wind is zero, shifts northward in the QUADRATIC and, especially, LIN-554 EAR integrations, relative to the CUBIC experiment (Figure 13). Since stationary waves 555 only propagate in westerly zonal flow, the latitude where zonal flow is zero acts a bound-556 ary for wave propagation (Hardiman et al. (2014)). As a result, this shift in critical lat-557 itude results in enhanced wave propagation and convergence over middle and high lat-558 itudes. 559

Figures 12 and 13 highlight how the changes in zonal winds in the LINEAR and 560 QUADRATIC experiments reflect a degradation in model skill, relative to MERRA-2, 561 throughout the entire stratosphere. The changes in upwelling, mean age, chemical trace 562 gases and zonal winds thus provide a coherent and self-consistent picture suggestive of 563 a degradation in the representation of the stratospheric circulation since MERRA-2. That 564 is, an increased bias in the stratospheric northern zonal winds are, via their influence on 565 wave convergence, compromising changes in the strength of the mean meridional over-566 turning circulation and its impact on composition. It is interesting to note that the wind 567 biases also extend into the troposphere and show degraded skill relative to MERRA-2 568 in the LINEAR and QUADRATIC experiments (Figure 13). Examination of other fields 569

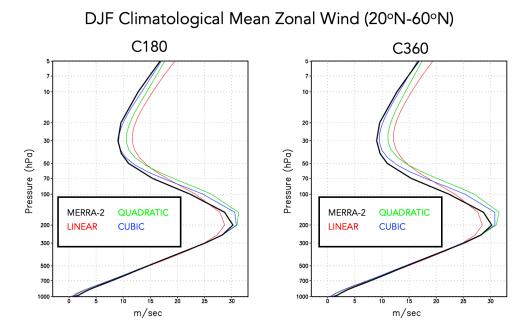


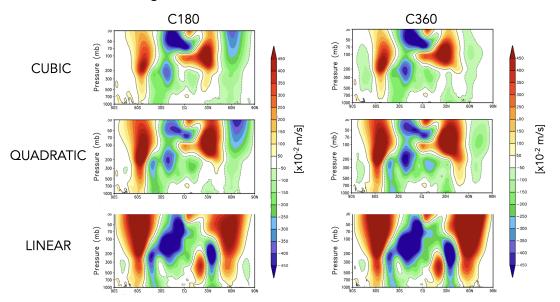
Figure 12. Vertical profiles of the DJF 1985-2015 climatological mean zonal mean zonal winds in the LINEAR (red), QUADRATIC (green) and CUBIC (blue) experiments, averaged between 20°N and 60°N. MERRA-2 is shown in the black line. Results for both C180 (left) and C360 (right) experiments are shown.

(i.e. tropopause biases, Appendix Figure D1) present somewhat more of a nuanced story
that depends on other changes that made to the model since MERRA-2, as shown in Figure 8 and discussed in Section 3.2.1. 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 conse-575 quence for the wave convergence properties within the stratosphere, next we examine the 576 zonal structure of these biases in the middle stratosphere (Figure 14. This reveals that 577 the enhanced winds in the LINEAR (and, to a lesser extent, QUADRATIC) integrations 578 are concentrated over the North Pacific at both C180 (Fig. 14, top) and C360 (Fig. 14, 579 bottom) resolutions (a similar picture emerges within the troposphere, not shown). As 580 this region is the primary region dominating the stationary component of the upward 581 flux of vertical wave activity (Plumb (1985), see their Figure 4) it is perhaps not surpris-582 ing that this region is having a profound impact on the mean overturning circulation. 583 Again, as with the zonal mean wind changes, the increases in wind strength over the North 584 Pacific represent degraded model skill relative to MERRA-2. Note that comparisons with 585 ERA-5 reveal a similar bias (not shown). 586

587 4 Conclusions

Here we have performed an analysis aimed at understanding differences in the representation of the stratospheric circulation in recent candidate systems for GEOS-R21C, relative to older versions of GEOS similar to the model used to produce MERRA-2. Using targeted experiments oriented at disentangling various model development updates, we have identified a key role played by changes in the implementation of the remapping



DJF Climatological Zonal Mean Zonal Wind Anomalies Relative to MERRA-2

Figure 13. Colors shown anomalies in the DJF 1985-2015 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 shown.

algorithm within the model's finite-volume dynamical core. Our key results are as follows:

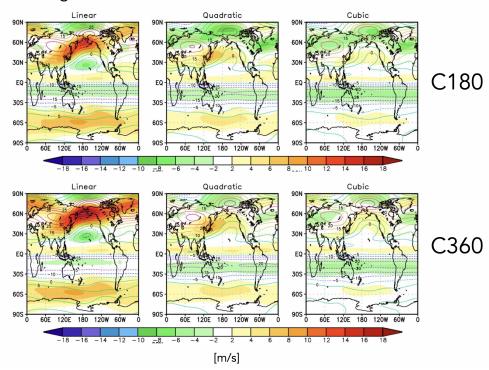
⁵⁹⁵ #1. The stratospheric mean age-of-air in GEOS is sensitive to the degree of the ⁵⁹⁶ interpolation scheme that is used to calculate layer-mean values of total energy, U, V and ⁵⁹⁷ tracers. Different treatment of the vertical remapping algorithm result in mid-stratospheric ⁵⁹⁸ (50 hPa) age-of-air differences of ~ 1 year over high latitudes, or about 30% climatolog-⁵⁹⁹ ical mean values.

#2. The increased age-of-air biases in more recent GEOS configurations are reflected in the increased biases in simulated trace gases, including CH₄ and N₂O.

#3. The age-of-air sensitivities 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.

#4. The degradation of upwelling statistics manifest in AMIPs, also translate to
 degradations in configurations of GEOS in which the meteorological fields are constrained
 or "replayed" to MERRA-2.

An important caveat should be mentioned in relation to Conclusion 3 listed above, which highlights the leading role played by *extratropical* wave convergences in the behavior of tropical upwelling in the model. While this is consistent with our understanding that the Brewer-Dobson Circulation is, to first order, determined by extratropical wave flux convergences, in practice this means that other undesirable biases may emerge in the tropics (i.e., tropical temperatures, Figure 8). Our analysis of the M2AMIP ensemble, however, suggests that this tropical temperature bias is not a necessary conse-



DJF Climatological 30 hPa Zonal Wind Anomalies Relative to MERRA-2

Figure 14. Colors shown anomalies in the DJF 1985-2015 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 shown.

quence of the GMAO FV3 remapping scheme but, rather, emerges in tandem with other changes that were made in the model. Nonetheless, Figure 8 suggests that improvements in transport associated with the GMAO remapping scheme must be carefully weighed in the broader context of other model development choices.

Interestingly, preliminary analysis suggests that our findings may also translate to 621 replay configurations of GEOS (Figure 10), although the effect is muted, relative to free-622 running configurations. As a rigorous evaluation of the stratospheric circulation in re-623 play and DAS configurations is beyond the scope of the current study, future work will 624 625 therefore focus on assessing the extent to which the free-running model biases reported here are expressed when the model is run in data assimilation mode. It also bears em-626 phasizing that our findings do have immediate implications for the (free-running) sub-627 seasonal forecast and coupled chemistry climate applications of the GEOS model cur-628 rently in operation. 629

In addition to its implications for GEOS, our results more generally 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.

Looking forward, our findings support and build on the recommendation proposed 636 in Gupta et al. (2020) for the construction of dynamical core benchmark tests aimed at 637 determining how underlying AGCM numerics impact climatological transport proper-638 ties. In particular, in addition to the age-of-air, the authors propose a range of strato-639 spheric circulation diagnostics that should be evaluated including the zonal mean zonal 640 winds, eddy temperature variance and zonal spectra of eddy kinetic energy. Our anal-641 ysis reveals an important role to be played by the climatological zonal mean wind struc-642 ture as it impacts wave convergence over midlatitudes; we therefore also recommend ex-643 plicit consideration of the Eliassen Palm flux convergence and tropical upwelling (w^*) 644 fields as they may be crucial for interpreting age-of-air changes. 645

⁶⁴⁶ One somewhat incidental – but practical - result from our analysis is that the statis-⁶⁴⁷ tics of ∇ ·F and w^* are well approximated by ensembles of so-called EMIP integrations. ⁶⁴⁸ As these are substantially easier to run than AMIPs these could provide a "first pass" ⁶⁴⁹ when evaluating new proposed model development changes, without the immediate need ⁶⁵⁰ to integrate AMIP-style experiments. We emphasize, however, that this statement should ⁶⁵¹ only apply to a first stage in model development as the age-of-air will reflect the time ⁶⁵² 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 identified here, the former could potentially influence the age both directly through changes in thermal structure and indirectly by modifying wave propagation and/or generation in the troposphere.

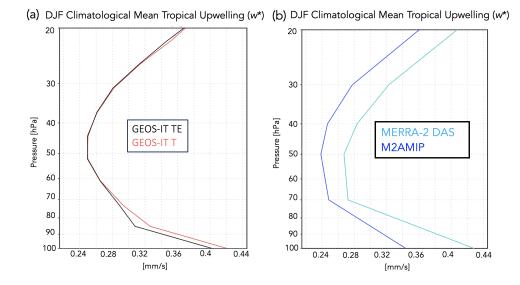


Figure A1. The DJF 1985-2015 climatological mean vertical residual mean velocity, w^* , averaged at each level between the turnaround latitudes compared between two experiments remapping to temperature (T) (red) versus total energy (TE) (black) (a) and between MERRA-2 DAS (cyan) and the M2AMIP ensemble (blue) (b). The underlying model code is consistent with the Version 5.29.4 GEOS-IT model.

⁶⁵⁹ Appendix A Sensitivities in Calculation of TEM Upwelling

There are various aspects of the calculation of the TEM circulation that warrant 660 further comment. First, whereas the modeling experiments listed in Table 2 (rows 5-7) 661 focus on the sensitivity of Step 5 within the GMAO FV3 core remapping algorithm to 662 the choice of interpolation scheme, another difference between the GMAO and GFDL 663 FV3 core remapping approaches is the use of TE versus T, respectively. To test the im-664 pact of this difference, we ran a new experiment which is identical to the CUBIC exper-665 iment (Table 2, row 7), except that T is remapped from input layer mean pressure lo-666 cations to standard output layer mean locations directly using cubic interpolation (i.e., 667 no computation of TE or a-posteriori energy conservation applied). Appendix Figure A1a 668 shows that this has little impact on the strength of tropical upwelling, suggesting that 669 the w^* differences associated with changes in the remapping algorithm are dominated 670 by sensitivities to the choice of interpolation scheme, not the use of TE versus T. 671

Second, the vertical component of the TEM circulation (w^*) shows some differences in vertical structure between MERRA-2 and the 30-member M2AMIP ensemble (Appendix Figure A1b). This difference in vertical structure appears to reflect a difference between DAS and free-running configurations of the model, since other DAS configurations share a similar vertical structure (not shown). Given this difference, we ensure as apples-to-apples a comparison of simulated TEM velocities by comparing all AMIP results to other AMIP experiments.

⁶⁷⁹ Appendix B Correspondence between EMIP and AMIP Upwelling

Appendix Figure B1 shows the close correspondence in DJF climatological mean w^* , averaged at each level between the turnaround latitudes, from AMIP and EMIP ex-

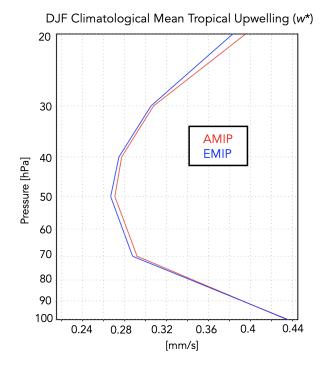
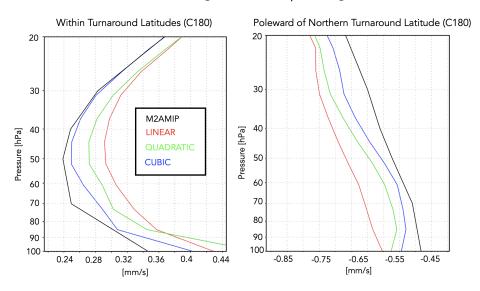


Figure B1. The DJF 1985-2015 climatological mean vertical residual mean velocity, w^* , averaged at each level between the turnaround latitudes for the CTRL experiment (Table 2, row 1). Results based on a 30-year-long AMIP experiment (red line) and a 30-member ensemble of three-month-long EMIP experiments (blue line) are shown.

periments using the same model configuration. This good agreement in upwelling is used to justify the analysis of the EMIP experiments listed in Table 2 (rows 5-7).

⁶⁸⁴ Appendix C Changes in Tropical and High Latitude Upwelling

Appendix Figure C1 compares the behavior in residual mean upwelling among the LINEAR, QUADRATIC and CUBIC experiments over the latitudes between the (tropical) turnaround latitudes (left) and poleward of the northern turnaround latitude (right). The ordering among experiments in both regions reflects how increases in downwelling at high latitudes are, through mass balance, accompanied by enhanced upwelling in the tropics.

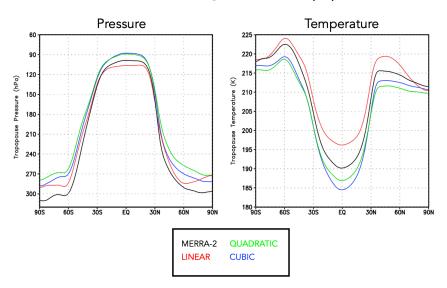


DJF Climatological Mean Upwelling (w*)

Figure C1. Left: The DJF 1985-2015 climatological mean vertical residual mean velocity, w^* , averaged at each level between the turnaround latitudes for the LINEAR (red line; Table 2, row 5), QUADRATIC (green line; Table 2, row 6) and CUBIC (blue line; Table 2, row 7) experiments. M2AMIP is shown in black. Right: As in left panel, except averaged over latitudes poleward of the northern turnaround latitude. Results in both panels are shown for C180 experiments.

⁶⁹¹ Appendix D Tropopause Pressure

Appendix Figure D1 compares boreal winter tropopause pressure and temperature among the LINEAR, QUADRATIC and CUBIC experiments, relative to MERRA-2.



DJF Climatological Mean Tropopause

Figure D1. The DJF 1985-2015 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 shown for the C180 experiments.

694 Acronyms

- 695 **AMIP** Atmospheric Model Intercomparison Project
- $_{696}$ **CH**₄ methane
- 697 CCMs chemistry climate models
- 698 CCMI Chemistry Climate Modeling Initiative
- 699 CCMVal Chemistry Climate Model Validation
- $_{700}$ CO₂ carbon dioxide
- 701 CTRL control
- ⁷⁰² **CTM** chemistry transport model
- 703 **DAS** Data assimilation
- 704 **DJF** December-January-February
- 705 **EMIP** ensemble AMIP
- 706 EOS Earth Observing System
- 707 **EP** Eliassen-Palm
- $_{708}$ FV finite-volume
- 709 **FP** Forward Processing
- 710 **GEOS** Global Earth Observing System
- ⁷¹¹ **GEOS-R21C** GEOS Retrospective analysis for the 21st Century
- 712 **GMI** Global Modeling Initiative
- 713 HALOE Halogen Occultation Experiment
- 714 MERRA-2 Modern-Era Retrospective Analysis for Research and Applications v2
- 715 MLS Microwave Limb Sounder
- $_{^{716}}$ N₂O nitrous oxide
- 717 **NH** northern hemisphere
- 718 **PPM** piecewise parabolic
- 719 **RRTMG** Rapid Radiative Transfer Model for GCMS

- $_{720}$ **SW** shortwave
- 721 **TE** total energy
- 722 **TEM** Transformed Eulerian Mean
- ⁷²³ **UARS** Upper Atmosphere Research Satellite

724 Open Research Section

All output from the GEOS simulations presented has been reprocessed as GrADS control files and binary datasets that are located publicly at https://gmao.gsfc.nasa.gov/

- gmaoftp/corbe/StratAge/Data/. The MERRA-2 data is publicly available at
- https://disc.gsfc.nasa.gov/datasets?project=MERRA-2.

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⁷³⁵ similation Office and core chemistry-climate and chemistry-modeling activities.

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