#### Stratospheric Age-of-Air: Sensitivity to Finite Volume 1 **Remapping Algorithm** 2

# Clara Orbe <sup>1,2</sup>, Lawrence L. Takacs <sup>3</sup>, Amal El Akkraoui <sup>3</sup>, Krzysztof Wargan <sup>3</sup>, Andrea Molod <sup>3</sup>

 $^{1}\rm NASA$ Goddard Institute for Space Studies, New York, NY $^{2}\rm Department$  of Applied Physics and Applied Mathematics, Columbia University, New York, NY $^{3}\rm Global$  Modeling and Assimilation Office, NASA Goddard Space Flight Center, Greenbelt, MD

#### **Key Points:**

3 4

5 6 7

8

16

9	The stratospheric mean age-of-air simulated in GEOS-5 is sensitive to the remap-
10	ping scheme used within the finite-volume dynamical core.
11	This sensitivity in the age-of-air approaches 30% and imprints on the simulated
12	distributions of several long-lived chemical trace gases, including nitrous oxide and
13	methane.
14	The age-of-air sensitivities primarily reflect changes in resolved wave convergence
15	over the Northern Hemisphere midlatitude stratosphere, which impact mean up-
16	welling within the tropical lower stratosphere.

Corresponding author: =name=, =email address=

#### 17 Abstract

Accurately modeling the large-scale transport of trace gases and aerosols is crit-18 ical for interpreting past (and projecting future) changes in atmospheric composition. 19 Simulations of the stratospheric mean age-of-air continue to show persistent biases among 20 chemistry climate models, although the drivers of these biases are not well understood. 21 Here we identify one driver of simulated stratospheric transport differences among var-22 ious NASA Goddard Earth Observing System Version 5 (GEOS-5) candidate model ver-23 sions under consideration for the upcoming GEOS-5 Retrospective analysis for the 21<sup>st</sup> 24 25 Century (GEOS-R21C). In particular, we show that the simulated age-of-air values are sensitive to the so-called "remapping" algorithm used within the finite-volume dynam-26 ical core, which controls how individual material surfaces are vertically interpolated back 27 to standard pressure levels after each horizontal advection time step. Differences in the 28 age-of-air resulting from changes within the remapping algorithm approach  $\sim 1$  year over 29 the high latitude middle stratosphere - or about 30% climatological mean values – and 30 imprint on several trace gases, including methane  $(CH_4)$  and nitrous oxide  $(N_2O)$ . These 31 transport sensitivities reflect, to first order, changes in the strength of tropical upwelling 32 which are driven by changes in resolved wave convergence over northern midlatitudes 33 as (critical lines of) wave propagation shift in latitude. Finally, we show that degrada-34 tions in the simulation of the age-of-air, stratospheric upwelling and zonal wind climate 35 statistics derived from 30-year-long atmosphere-only (AMIP) experiments, translate to 36 degraded skill in the analysis states used within data assimilation experiments. Our re-37 sults strongly support continued examination of the role of numerics in contributing to 38 transport biases in composition modeling. 39

#### 40 Plain Language Summary

Large-scale transport plays a crucial role in distributing climatically important trace 41 constituents in the atmosphere, especially in the stratosphere where transport largely 42 determines the chemical lifetimes of trace gases. One summary of transport in the strato-43 sphere is the "mean age" or the mean transit time since air at a point in the stratosphere 44 was last in the troposphere. Current models used for simulating stratospheric compo-45 sition produce a range of simulated ages, although these differences are poorly under-46 stood. Among other factors, model numerics play a critical role in transport, but few 47 studies have explored the sensitivity of the mean age to the choice of numerical scheme 48 employed within different dynamical cores. Here we use one model to show that the mean 49 age is sensitive to the so-called "remapping" algorithm used within the finite-volume dy-50 namical core that controls how individual material surfaces are vertically interpolated 51 back to standard pressure levels after each horizontal advection time step. This reflects 52 sensitivities in the representation of how waves propagate from the troposphere into the 53 stratosphere. This work suggests that model numerics can be an important factor in con-54 tributing to differences in simulated transport among models. 55

#### <sup>56</sup> 1 Introduction

The chemical and radiative properties of the troposphere and lower stratosphere 57 are strongly influenced by the stratosphere-troposphere exchange of mass and tracers (e.g., 58 Morgenstern and Carver (2001); Hegglin et al. (2006); Pan et al. (2007)). Properly sim-59 ulating the stratospheric circulation and its influence on atmospheric composition in earth 60 system models is important for capturing past decadal trends in surface climate, par-61 ticularly in response to changes in Southern Hemisphere ozone depletion (e.g., Son et 62 al. (2009); Polvani et al. (2011)). In the Northern Hemisphere (NH), the stratospheric 63 circulation's coupling to ozone could represent an important feedback on the climate's 64 response to future increases in greenhouse gases (GHGs), especially over the North At-65 lantic (e.g., Chiodo and Polvani (2019)). On shorter subseasonal timescales, stratospheric 66

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

Key to accurately simulating a consistent representation of coupling between strato-72 spheric dynamics and chemical trace gases is ensuring that a model's underlying trans-73 port circulation is properly represented. To this end, much effort has been paid to de-74 veloping and refining so-called "tracer-independent" metrics of transport (Holzer and Hall 75 (2000)) such as the mean age-of-air (Hall and Plumb (1994)) and to applying these mea-76 sures to rigorously evaluate model transport characteristics in chemistry climate mod-77 els (CCMs) (e.g., Hall et al. (1999); Orbe et al. (2018); Dietmüller et al. (2018); Aba-78 los et al. (2020)). 79

While the assessment of CCMs participating in the SPARC Chemistry Climate Model 80 Validation (SPARC CCMVal) effort showed a marked improvement in simulated trans-81 port characteristics relative to previous intercomparisons (J. Neu et al. (2010)), more re-82 cent analysis of models participating in the SPARC Chemistry Climate Modeling Ini-83 tiative (CCMI) (Eyring et al. (2013)) do not demonstrate any improvement (Dietmüller 84 et al. (2018), see their Figure 3). In particular, although some models produce mean age 85 values that agree well with observational estimates, the CCMI intermodel spread is  $\sim$ 86 50%, with models generally simulating transport that is too vigorous, relative to obser-87 vations. While documenting these transport differences among models is straightforward, 88 understanding the drivers of this spread remains a key challenge and there is still no con-89 sensus on the main drivers of simulated age biases among the current generation of CCMs. 90

A key challenge in identifying the drivers of age-of-air – and other stratospheric trans-91 port – biases is that they reflect the time-integrated effects of advection by the residual 92 mean circulation and eddy diffusive mixing, or the quasi-random transport due to the 93 breaking of Rossby waves (e.g., Holton et al. (1995); Plumb (2002)). Given that the in-94 fluences of mixing and advection are not easily separable, studies have come to differ-95 ent conclusions about the drivers of age biases in models. In particular, the analysis of 96 the CCMVal models showed a strong correlation between the intermodel spread in the 97 age-of-air and lower stratospheric tropical upwelling, whereas Dietmüller et al. (2018) 98 showed 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 us-100 ing either simplified "leaky pipe" models (Plumb (1996); J. L. Neu and Plumb (1999)) 101 or more complete measures of the transport circulation such as the "age spectrum" (e.g., 102 Hall and Plumb (1994); Waugh and Hall (2002))) may prove enlightening, at present there 103 is no consensus on what is driving biases in the simulated age-of-air in models. 104

One potential limitation of using multi-model intercomparisons to understand drivers 105 of age biases is that many aspects of model formulation can influence both stratospheric 106 upwelling and mixing. Thus, while intercomparisons are useful for identifying common 107 model biases, understanding the drivers of these biases is difficult absent single model-108 based process studies. Among these, several aspects of model formulation have been iden-109 tified as influencing simulated mean age distributions. As the mean age is sensitive to 110 vertical motion in the lowermost stratosphere, these include large sensitivities to verti-111 cal resolution (Orbe et al. (2020)) and to spurious vertical mixing either introduced in 112 vertical coordinate transformations in offline chemical transport models (B. Monge-Sanz 113 et al. (2007)) or through use of assimilated winds performed either in offline (e.g., Legras 114 et al. (2004)) or online data assimilation and "nudged" configurations (e.g., Pawson et 115 al. (2007); Orbe et al. (2017); Davis et al. (2022)). These age sensitivities can be still fur-116 ther amplified, depending on whether or not parameterized gravity waves are included 117 (Eichinger et al. (2020)). 118

By comparison, sensitivities of the mean age to underlying tracer numerics have 119 been less well examined, although Eluszkiewicz et al. (2000) documented a large sensi-120 tivity in simulated age-of-air values to the choice of advection scheme. More recently, 121 Gupta et al. (2020) showed differences of  $\sim 25\%$  in the age-of-air across identical exper-122 iments performed using four different dynamical cores, especially between those using 123 spectral versus finite-volume schemes. The experiments employed in that study, how-124 ever, were highly idealized and it is not clear if the strong influence of tracer numerics 125 that they identified is also realized in more comprehensive model simulations with moist 126 physics, especially in the context of model development as carried out in operational mod-127 eling centers. 128

To this end, here we document the sensitivity of the stratospheric mean age in sev-129 eral recent versions of the NASA Goddard Earth Observing System Version 5 (GEOS-130 5) general circulation model (Molod et al., 2015) that represent different stages in model 131 development since MERRA-2 (Gelaro et al. (2017)). Our focus on transport evaluation 132 is in wake of the upcoming release of the GEOS-5 Retrospective analysis for the 21<sup>st</sup> Cen-133 tury (GEOS-R21C), which will serve as an intermediate reanalysis between MERRA-134 2 and MERRA-3 ( $\sim 2025$ ). As GEOS-R21C will be used to drive an off-line chemistry 135 reanalysis (GEOS-R21C-Chem) it is imperative that it produces a credible representa-136 tion of transport processes. 137

In particular, here we document how in the process of evaluating candidate sys-138 tems for GEOS-R21C we found that the mean age was  $\sim 1$  younger than the values sim-139 ulated in the model version used to produce MERRA-2 (Figure 1). The model versions 140 shown in Figure 1 reflect more than 10 years' worth of accumulated changes in model 141 development, most notably changes in radiation, parameterized convection and, as we 142 focus on here, changes in the algorithm used to transform advected fields from Lagrangian 143 levels to fixed pressure levels after each horizontal advection time step. We show that 144 slight modifications in this so-called "remapping" algorithm are the primary driver of 145 the age-of-air changes exhibited in recent GEOS-R21C candidate model versions, a re-146 sult which may have broader implications for other general circulation models using fi-147 nite volume (FV) dynamical cores. We begin by discussing methods in Section 2 and present 148 key results and conclusions in Sections 3 and 4, respectively. 149

#### $_{150}$ 2 Methods

151

#### 2.1 Model Configurations

Here we present results from several versions of GEOS-5 spanning MERRA-2 to 152 more recent candidates for GEOS-R21C. Among these model versions, a subset are more 153 "official" as they have been documented and/or employed in recent model intercompar-154 isons and are highlighted in Figure 1. In particular, these include an intermediary model 155 version that was used in Phase 1 of CCMI and documented in Orbe et al. (2017) (Fig. 156 1, red line). A more recent model version that was used in the CCMI Phase 2 simula-157 tions (correspondence with Michael Manyin) is also shown (Fig. 1, green line). These 158 two configurations correspond to the Heracles 5.3 and Icarus 3.2 versions of the GEOS 159 system, respectively (Amal: I need the actual tag names). 160

We begin by comparing 10-year (2000-2010) climatological mean zonally averaged 161 age-of-air profiles at 50 hPa across this subset of model versions, derived from 30-year 162 long atmosphere-only (AMIP) integrations constrained with observed sea surface tem-163 peratures (Figure 1). First, we note that the profiles for the CCMI Phase 1 version of 164 the model are very close to observations (black stars), consistent with the 165 "GEOSCCM" documented age characteristics reported in Dietmüller et al. (2018) (see 166 their Figure 3). In addition, while passive tracers were not integrated within MERRA-167 2, results using the GEOS chemistry transport model (GEOS-CTM, Kouatchou et al. 168

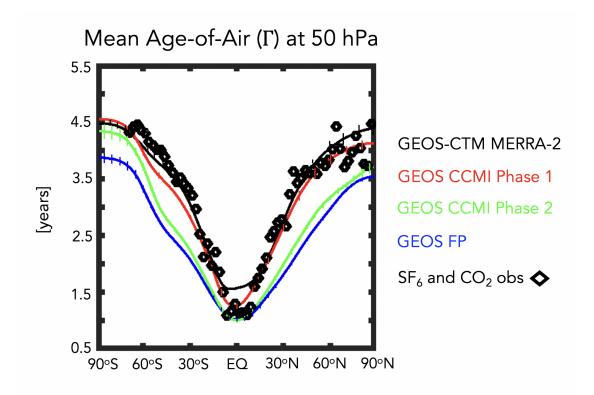


Figure 1. The 2000-2010 climatological annual mean meridional profile of the stratospheric mean age-of-air ( $\Gamma$ ), evaluated at 50 hPa. Results from a GEOS-CTM integration constrained with MERRA-2 meteorological fields (black line) as well as free-running GEOS simulations using a model configuration for CCMI Phase 1 (red line), CCMI Phase 2 (green line) and a more recent GEOS-FP development tag (blue line) are shown. The GEOS model versions to which these configurations correspond are the Heracles 5.3, Icarus 3.2, and Jason 3.6 tags, respectively. All simulations are constrained with the same (observed) historical sea surface temperatures. Diamonds correspond to SF<sub>6</sub> and CO<sub>2</sub> in situ based estimates of  $\Gamma$  from Boering et al. (1996) and Engel et al. (2009). Vertical dashed lines denote  $\pm \sigma$ , the standard deviation of  $\Gamma$  over 2000-2010, for each model simulation.

(2015)) constrained with MERRA-2 meteorological fields (black line) also exhibits good agreement with observed values. This good agreement between the CTM-generated ageof-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), 173 however, reveals a reduction in the mean age by  $\sim 1$  year over both southern and north-174 ern high extratropical latitudes, or a decrease of  $\sim 20{-}30\%$  relative to MERRA-2. As dis-175 cussed earlier, the green line refers to the CCMI Phase 2 model version, whereas the blue 176 177 line refers to an undocumented candidate version (model tag Jason 3.6) that corresponds best to a model configuration similar to what is used in the GEOS forward processing 178 (FP) numerical weather prediction system (Amal: As of which date?). Note that this 179 decrease in the age in both model versions is statistically significant, relative to inter-180 nal variability (vertical bars on solid lines). 181

There are numerous development updates in the model that have occurred since MERRA-2. Therefore, after discussing the model configurations highlighted in Figure 1 in Section 3.1, we then present results from targeted experiments aimed at successively undoing these model updates (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 develop-189 ment was made to the handling of the remapping algorithm within the model's FV dy-190 namical core (Lin, 2004). In particular, vertical motion is realized through the Lagrangian 191 transport of the "floating" vertical coordinate such that after each horizontal advection 192 step the individual material surfaces are vertically interpolated back to standard pres-193 sure levels through FV's so-called "REMAP" algorithm. This is needed because the La-194 grangian surfaces that vertically bound the finite volumes will eventually deform, neg-195 atively impacting the accuracy of the horizontal-to-Lagrangian-surface transport and the 196 computation of the pressure-gradient terms. 197

There are various user-defined parameters and decisions that are made within the 198 remapping algorithm. In its current implementation this involves 1) fitting piecewise parabolic 199 (hereafter PPM) functions to input layer-mean values of T, u, v, q and tracers; 2) cal-200 culating PPM functions to output layer edges; and 3) integrating PPM functions between 201 output layer edges to produce new layer-mean values of T, u, v, q and tracers. Note that 202 T, u, v, q,  $C_p$ , K and  $\Phi$  correspond to temperature, zonal wind, meridional wind, spe-203 cific humidity, specific heat capacity and kinetic and potential energy, respectively. This 204 implementation setup is consistent with what is currently being used in most recent model 205 versions (i.e. blue and green lines, Figure 1) and hereafter is referred to as REMAP Op-206 tion 2 (Table 1, left). 207

The alternative version – which best mimics what was used in MERRA-2 – involves two main changes to this procedure and is hereafter referred to as REMAP Option 1 (Table 1, right; red line in Figure 1). First steps 1) and 3) are performed only for u, v, q and tracers (not T). Second, three additional steps after 3) are added, the first two of which involve calculating total energy (TE) at input mid-layer pressures and then performing cubic interpolation and a posteriori integral conservation at output mid-layer pressures. Finally, temperatures are "remapped" from total energy via T = (TE - K -  $\Phi$ )/C<sub>p</sub>.

When examining Table 1, it is important to note that Options 1 and 2 differ in two main respects. Of these, we find that the simulated ages are most sensitive to the interpolation that occurs within step 5 in REMAP Option 1 (Table 1). The use of TE (as opposed to T), by comparison, is less consequential (Appendix A, Figure A1). To this end, the sensitivity experiments discussed in the next section mainly focus on identifyTable 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  $\Phi$  correspond to temperature, zonal wind, meridional wind, specific heat of air at constant pressure and kinetic and potential energy, respectively.

REMAP Option $2$ (CTRL)	REMAP Option 1 (MERRA-2)
Fit PPM functions to	Fit PPM functions to
input layer-mean T, u, v, q and tracers	input layer-mean u, v, q and tracers
Calculate PPM to output layer edges	Calculate PPM to output layer edges
Integrate PPM functions between output	Integrate PPM functions between output
layer edges to produce new layer-	layer edges to produce new layer-
mean T, u, v, q and tracers	mean u, v, q and tracers
n/a	Calculate $TE = C_pT + K + \Phi$
	at input mid-layer pressures
n/a	Calculate TE at output mid-layer pressures
	using cubic interpolation and
	a-posteriori integral conservation
n/a	Construct "remapped" T via
,	$\mathbf{T} = (\mathbf{TE} - \mathbf{K} - \Phi) / \mathbf{C}_p$
-	Fit PPM functions to input layer-mean T, u, v, q and tracers Calculate PPM to output layer edges Integrate PPM functions between output layer edges to produce new layer- mean T, u, v, q and tracers n/a

ing the age sensitivites in response to changes in the interpolation scheme used in REMAP
 Option 1, not to differences between the use of TE versus T.

Finally, it is worth noting other important model development changes that occurred 222 related to the parameterization of deep convection (Grell and Freitas (2014); Freitas et 223 al. (2018)) which could, potentially, have an indirect impact on the stratospheric circu-224 lation through their influence on wave generation in the troposphere. As we show, how-225 ever, while these have a substantial impacts upon their incorporation in a nonhydrostatic 226 version of the model on characteristics like the diurnal cycle of precipitation (Arnold et 227 al. (2020)) and on convective transport within the troposphere (Freitas et al. (2020)), 228 their indirect influence on the stratosphere is less impactful. 229

230

#### 2.2 Model Experiments

In order to investigate the drivers of the differences illustrated in Figure 1 we perform targeted model experiments aimed at further disentangling the influence of recent model development changes on stratospheric transport properties (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
and c) combine these two changes (CSRAD+M2REMAP; Table 2, row 4). Note that
we have also have performed experiments in which RRTMG is reverted back to Chou
(1990) in the longwave, but these changes are less impactful, compared to the shortwave
radiation changes (not shown).

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 scheme used to calculate TE at output mid-layer pressure levels (rows 5-7). Experiments in rows 1-4 are 30-year-long AMIPs, 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). By comparison, rows 8-9 refer to 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	AMIP $(30 \text{ yrs.})$
	(SW) Radiation	
M2REMAP	MERRA-2 REMAP Option 1 (cubic)	AMIP $(30 \text{ yrs.})$
CSRAD+M2REMAP	Chou-Suarez $(1994)$ SW	AMIP $(30 \text{ yrs.})$
	+ REMAP Option 1 (cubic)	
LINEAR	MERRA-2 REMAP Option 1 (linear)	EMIP $(30 \text{ members})$
QUADRATIC	MERRA-2 REMAP Option 1 (quadratic)	EMIP (30 members)
CUBIC	MERRA-2 REMAP Option 1 (cubic)	EMIP $(30 \text{ members})$
CTRL-DAS	Control, REMAP Option 2	DAS $(1 \text{ yr.})$
CUBIC-DAS	MERRA-2 REMAP Option 1 (cubic)	DAS $(1 \text{ yr.})$

As shown in Section 3.2.1, the M2REMAP experiment produces the largest changes 245 in age-of-air, compared to the altered radiation experiments. To this end, we focus the 246 remainder of our investigation (Section 3.2.2) on examining a clean set of experiments 247 that distinguishes the impact of REMAP Option 1 versus Option 2 on simulated trans-248 port. In particular, we perform three sensitivity experiments that differ from each other 249 only in terms of the calculation of TE at the mid-layer pressure levels, which we perform 250 using a linear (LINEAR; Table 2, row 5), quadratic (QUADRATIC; Table 2, row 6) and 251 cubic interpolation (CUBIC; Table 2, row 7) scheme, with the latter corresponding to 252 the approach that was used in MERRA-2. Note that, while the LINEAR and QUADRATIC 253 experiments do not actually correspond to any of the development tags shown in Fig-254 ure 1, they highlight the large sensitivity of the mean age to changes in the interpola-255 tion scheme that may otherwise seem innocuous. They also provide further evidence of 256 the strong influence of tropical lower stratospheric upwelling strength on stratospheric 257 mean age in GEOS. 258

Finally, in all experiments using REMAP Option 1 (i.e. M2REMAP, CSRAD+ 259 M2REMAP, LINEAR, QUADRATIC, CUBIC) additional modifications to the diver-260 gence damping coefficients were used so as to best ensure consistency with what was used 261 in MERRA-2. Specifically, these include changes to the number of layers for vertical sub-262 grid mixing, the DAS coefficient for barotropic mode damping, the use of 2<sup>nd</sup> vs. 6<sup>th</sup> or-263 der divergence damping and the strength of the divergence damping coefficients. 264

2.3 Analysis Approach 265

266

# 2.3.1 Stratospheric Circulation and Transport Diagnostics

To diagnose the transport circulation we focus primarily on the age-of-air (Hall and 267 Plumb (1994)). This is inferred from an idealized global "clock" or ideal age tracer ( $\Gamma$ ) 268

(Thiele and Sarmiento (1990)) that is defined with respect to all grid points in the first 269 model level. Initially, the ideal age tracer is set to zero throughout the troposphere and 270 thereafter held to zero over the entire Earth's surface, subject to a constant aging of 1 271 year/year throughout the atmosphere. We present here the statistically stationary (equi-272 librated) value of  $\Gamma(\mathbf{r})$ , which is equal to the average time since the air at a location r 273 in the stratosphere last contacted the Earth's surface. In addition to the mean age, we 274 also show results from an idealized e90 tracer that is uniformly emitted over the entire 275 surface layer and decays exponentially at a rate of  $90 \text{ days}^{-1}$  such that concentrations 276 greater than 125 ppb and less than 50 ppb tend to reside in the lower troposphere and 277 stratosphere, respectively (Prather et al. (2011)). As this tracer features strong near-278 tropopause gradients and takes significantly less time to equilibrate, compared to the mean 279 age, it is useful for evaluating stratosphere-troposphere-exchange and transport within 280 the upper troposphere/lower stratosphere (Abalos et al. (2017, 2020); Orbe et al. (2020)). 281

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<sub>2</sub>O) and methane (CH<sub>4</sub>).

As we show in Section 3, the changes in age-of-air across the different model ver-289 sions are strongly tethered to changes in the advective component of the circulation, which 290 we quantify using the Transformed Eulerian Mean (TEM) estimate of the Lagrangian 291 transport of mass by the circulation. Thus, in addition to more standard Eulerian met-292 rics of the circulation (e.g., zonal winds and temperatures), we focus on the vertical com-293 ponent of the TEM residual velocity, defined as  $\overline{w}^* = \overline{w} + \frac{\partial(\psi \cos\phi)}{a\cos\phi\partial\phi}$ , where  $\psi = \overline{v'\theta'}/\frac{\partial\overline{\theta}}{\partial p}$ 294 is the eddy stream function,  $\theta$  refers to potential temperature and overbars and primes 295 denote zonal means and deviations therefrom, respectively (Andrews et al. (1987)). In 296 addition, we interpret the behavior in  $w^*$  using the Eliassen-Palm flux divergence ( $\nabla$ . 297 F), whose horizontal (F( $\phi$ )) and vertical (F(p)) components are respectively defined as  $F(\phi) = acos\phi[\frac{\partial u}{\partial p}\psi - \overline{u'v'}]$  and  $F(p) = acos\phi([f - \frac{\partial ucos\phi}{acos\phi\partial\phi}]\psi - \overline{u'\omega'}).$ 298 299

300

#### 2.3.2 Experimental Setup

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, a clean/meaningful analysis of this set of runs is nonetheless hampered by the structural model differences between them.

Given the limitations of the experiments highlighted in Figure 1, we focus the bulk 307 of our analysis on the model configurations listed in Table 2. For a subset of these model 308 runs (rows 1-4) climatological AMIPS were carried at a C180 resolution and used to in-309 fer the climate characteristics of the different model configurations. For the other exper-310 iments (Table 2, rows 5-7) so-called "EMIPs" – ensembles of 3-month-long integrations 311 initialized on approximately November 15 of each year between 1985 and 2015 - were 312 performed. EMIPs for these experiments were performed at both C180 and C360 res-313 olutions in order to examine the sensitivity of our results to changes in horizontal res-314 olution. All of the experiments listed in Table 2 were integrated using the same ideal-315 ized passive tracer package (including the e90 and  $\Gamma$  tracers) described in Orbe et al. (2017). 316

As shown in Appendix B, comparisons of the the December-January-February (DJF) vertical profile of  $w^*$ , averaged over 1985-2015 and between the tropical turnaround lat-

itudes, show excellent agreement between EMIP and AMIP integrations carried out us-319 ing the same model configuration (Appendix Figure B1). This somewhat incidental re-320 sult, represents, to the best of our knowledge, the first time that EMIP-based statistics 321 have been shown to converge well to those from AMIPs for the stratospheric metrics con-322 sidered in this study. This suggests that EMIPs may provide a computationally more 323 efficient alternative to AMIPs for use in quickly ascertaining the impacts of model changes. 324 We note, however, that this approach is not appropriate for evaluating the time-integrated 325 transport characteristics reflected in the age-of-air. To this end, we show results from 326 both AMIP and EMIP experiments. 327

Finally, in addition to examining the climate statistics of the different model con-328 figurations we also inquire into implications for the analyzed atmospheric states from data 329 assimilation for a subset of the experiments (Table 2, rows 8-9). Specifically, we exam-330 ine the root-mean-square error of various climate fields (Amal, need description of rel-331 evant metrics/analysis). This evaluation is important given that in GEOS-R21C any un-332 derlying model biases will be partly ameliorated through replaying of the model state 333 to the analysis. Assessing the impact of reduced biases from the free-running model for 334 the analysis state is therefore important for informing the development of GEOS-R21C. 335

2.4 Observations and Reanalyses

336

While our focus is on interpreting and understanding the different model config-337 urations, we incorporate observations to provide context when possible, although we do 338 not present an exhaustive evaluation of the model's transport characteristics (for that 339 see earlier studies including Orbe et al. (2017, 2018)). However, as the tracers are not 340 directly integrated in MERRA-2 (with the exception of ozone), we compare against in-341 dependent observational estimates. For the mean age we first compare simulated merid-342 ional age profiles at 50 hPa with values derived from in situ aircraft measurements of car-343 bon dioxide  $(CO_2)$ , averaged in 2.5 degree latitude bins over the altitude range 19.5 to 344 21.5 km (Boering et al. (1996), see also Figure 5 in Hall et al. (1999)). 345

We also briefly evaluate impacts of transport biases on the simulated trace gas dis-346 tributions for the CCMI Phase 1 and 2 experiments. The simulated fields of methane 347  $(CH_4)$  are compared with the climatologies derived for 1991–2002 from the Halogen Oc-348 cultation Experiment (HALOE) on board the Upper Atmosphere Research Satellite (UARS) 349 (Grooß and Russell III (2005)). Comparisons of simulated nitrous oxide ( $N_2O$ ) are made 350 against 2005–2015 climatologies derived from the Microwave Limb Sounder (MLS) on 351 the Earth Observing System (EOS) Aura satellite. We use the 190-GHz retrieval from 352 Version 4.2 because the 640-GHz data set ends in summer 2013 due to the failure of the 353  $N_2O$  primary band. 354

For the circulation diagnostics nearly all comparisons are made relative to MERRA-355 2 and comparisons against ERA-5 (not shown) reveal a similar picture. There is one ex-356 ception, however, as special care must be taken when evaluating the (highly derived) TEM 357 circulation. In particular, calculations of the TEM circulation are notoriously sensitive 358 not only to differences in the formulation of the equations (Hardiman et al., 2010), but 359 also to the vertical resolution of the input velocities and associated heat and momentum 360 fluxes that are used to calculate the vertical derivatives in the eddy stream function and 361 EP flux components (Gerber & Manzini, 2016). In this respect, it is essential that com-362 parisons of the simulated TEM circulation must be made using consistent calculations. 363 For the case of the AMIPs shown in Figure 1 and for the targeted experiments listed in Table 2 this is ensured by the use of an identical output vertical grid (consisting of ? lev-365 els, Larry, need number of vertical levels in CSRAD, etc. experiment output). However, 366 comparisons with MERRA-2 are complicated as that data is only available at a lower 367 output vertical resolution (? levels, Larry, how many model output levels are used for 368 calculating  $w^*$  in MERRA2?). This results in spurious differences in the vertical struc-369

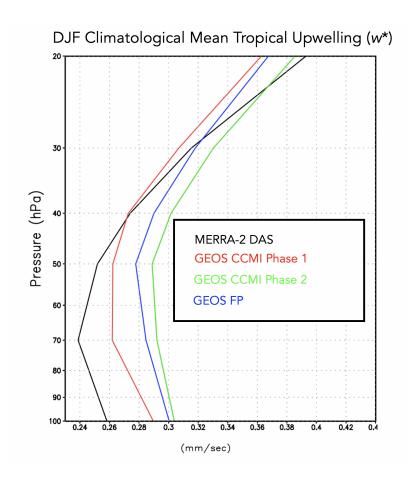


Figure 2. The DJF 1985-1994 climatological mean vertical residual mean velocity,  $w^*$ , averaged between the turnaround latitudes for GEOS model configurations corresponding to the CCMI Phase 1 (red) and Phase 2 (green) submissions and to GEOS-FP (blue). M2AMIP is shown in black. Replace MERRA-2 black line with M2AMIP.

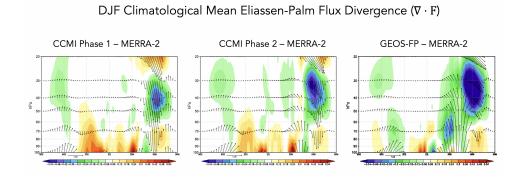


Figure 3. Colors show anomalies in the DJF climatological mean Eliassen-Palm (EP) flux divergence between the CCMI Phase 1 (left), CCMI Phase 2 (middle) and GEOS-FP (right) model versions, relative to MERRA-2. Arrows denote anomalies in the vertical and meridional EP flux vectors (relative to MERRA-2). Replace MERRA-2 with M2AMIP.

ture of the TEM circulation with MERRA-2 that are not physically driven. To this end, 370 when comparing the TEM circulation in the A(E)MIPS, in lieu of MERRA-2 we use re-371 sults from a 30-member AMIP ensemble that was performed using the MERRA-2 sys-372 tem (hereafter M2AMIP) and for which we have output on the higher resolution out-373 put grid. This ensures as apples-to-apples comparison of the TEM in the various GEOS 374 experiments with the MERRA-2 system as possible (note that for non-derived measures 375 (i.e. winds, temperatures) the raw MERRA-2 output is used). Larry/Kris/Amal: Is there 376 a reference for the M2AMIP ensemble?. 377

#### 378 **3 Results**

#### 379

#### 3.1 Reduction in Stratospheric Mean Age Since MERRA-2

We begin by interpreting the reduction in mean age exhibited in more recent model 380 versions in terms of changes in the strength of upwelling in the tropical lower stratosphere. 381 In particular, the reductions in  $\Gamma$  (Figure 1) are consistent with increases in the strength 382 of lower stratospheric tropical upwelling, with  $w^*$  becoming progressively stronger in more 383 recent model tags, relative to MERRA-2 (Figure 2). Though perhaps naive, this rela-384 tionship between lower stratospheric upwelling and the mean age is consistent with the 385 long-term behavior of  $\Gamma$  inferred from both historical and projected future climate sim-386 ulations (Butchart et al. (2010); Abalos et al. (2021)). A strong relationship between the 387 strength of lower stratospheric ascent and the mean age was also shown to hold in the 388 CCMVal models (see Fig. 5.20 in J. Neu et al. (2010)). Nevertheless, it is important to 389 note that a clear relationship between  $w^*$  and  $\Gamma$  is not a priori expected, as the age-of-390 air is also known to be very sensitive to mixing, which may be important in interpret-391 ing differences among the CCMI Phase 1 models (Dietmüller et al. (2018)). 392

The differences in  $w^*$  highlighted in Figure 2 are associated with enhanced Eliassen-393 Palm flux convergence over NH midlatitudes (Figure 3). Increased wave convergence is 394 evident not only within the subtropical lower stratosphere ( $< 30^{\circ}$ N, 50-100 hPa) but also 395 over higher latitudes and altitudes ( $\sim 40^{\circ}$ -70°N, 20-50 hPa). The fact that differences 396 in extratropical wave convergence imprint on tropical upwelling is consistent with our 397 understanding of the so-called "downward control" principal (Haynes et al. (1991)). In 398 particular, the strength of the residual mean streamfunction  $(\Psi^*)$  is, via downward con-399 trol, directly related to the vertically integrated eddy-induced total zonal force above that 400 level and has contributions both from the (resolved wave) Eliassen-Palm flux divergence 401

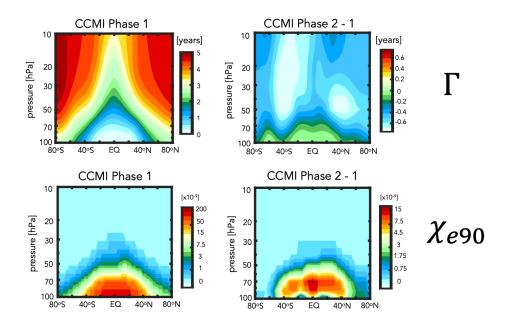


Figure 4. The climatological mean (2000-2010) distribution of the mean age-of-air ( $\Gamma$ ) (left, top) and e90 idealized tracers (left, bottom) for the CCMI Phase 1 model configuration. Climato-logical differences between the CCMI Phase 2 and Phase 1 model configurations are shown in the left panels.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

(Figure 3) as well as parameterized waves (not shown). The tropical upward mass flux - defined as  $\Psi^*_{\text{max}}$ - $\Psi^*_{\text{min}}$  evaluated at the turnaround latitudes (e.g. Rosenlof (1995)) – is therefore directly dependent on the wave forcing aloft.

While the reduction in  $\Gamma$  (Figure 1) of ~ 30% at 50 hPa is significant, it is neither 405 clear if this change is representative of other altitudes within the stratosphere nor how 406 this age bias imprints on real chemical species. To this end, we begin by comparing the 407 full latitude-pressure distribution of changes in  $\Gamma$  and another passive tracer (e90) (Fig-408 ure 4) between the CCMI Phase 1 and Phase 2 model configurations (red and green lines, 409 Figure 1). In particular, we find that the changes in both passive tracers – large reduc-410 tions in  $\Gamma$  within both hemispheres (Fig. 4, top right) and increased values of e90 within 411 the lower stratosphere (Fig. 4, bottom right) – are reflective of an overall increase in the 412 strength of the transport circulation. This is highlighted in the CCMI Phase 2 - 1 model 413 differences for the passive tracer distributions (Fig. 4, right panels) which are shown in 414 the absence of robust observational constraints of  $\Gamma$  at higher altitudes (or any obser-415 vational constraints for e90, for that matter). The reduced/increased stratospheric bur-416 dens of the age and e90 tracers are consistent with stronger upwelling in the CCMI Phase 417 2 model configuration (Figure 2). 418

<sup>419</sup> While the observational constraints on  $\Gamma$  presented in Figure 1 and the departure <sup>420</sup> of  $w^*$  away from MERRA-2 suggest that transport properties of the newer model con-<sup>421</sup>figurations are moving in the wrong direction, it is relevant to ask whether or not the <sup>422</sup> trace gas satellite measurements also support this conclusion. Indeed, comparisons with <sup>423</sup> observations show larger biases in N<sub>2</sub>O (Fig. 5, top panels) and CH<sub>4</sub> (Fig. 5, bottom pan-<sup>424</sup> els), increasing from 10% to 30% in the CCMI Phase 2 model configuration, depending <sup>425</sup> on the species. The patterns of these biases are generally consistent with the biases in

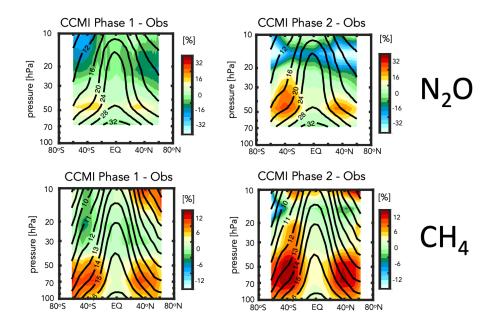


Figure 5. Colors shown anomalies in the simulated distributions of nitrous oxide  $(N_2O)$  (top) and methane (CH<sub>4</sub>) (bottom), relative to the MLS and HALOE observed values, respectively, for the CCMI Phase 1 (left) and Phase 2 (right) GEOS model configurations. Climatological mean observed values are shown in the black contours.

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

437

#### 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  $\Gamma$  shown in Figure 1.

Figure 6 shows the distribution of  $\Gamma$  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  $\Gamma$  is smaller than the change that results from reverting back to REMAP Option 1 (M2REMAP; Table 1; row 3), in which the mean age increases by ~ 1 year. The combined impacts of both

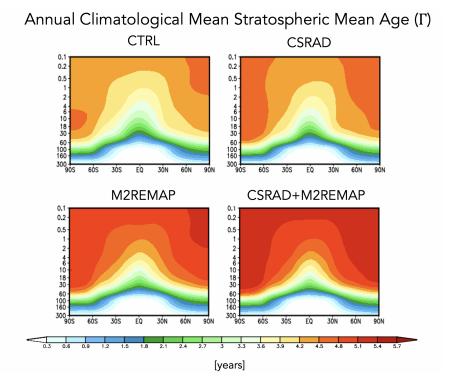


Figure 6. Colors show the simulated 2000-2010 climatological annual mean distributions of the mean age-of-air ( $\Gamma$ ) for the CTRL (top left; Table 1, row 1), CSRAD (top right; Table 1, row 2), M2REMAP (bottom left; Table 1, row 3) and combined CSRAD+M2REMAP (bottom right; Table 1, row 4) experiments.

changes (CSRAD+M2REMAP; Table 1 row 4) is roughly linear, with age values of ~
5.5 years over high latitudes at 50 hPa, consistent with the values simulated by the GEOSCTM MERRA-2 integration (black line, Figure 1) and with the CCMI Phase-1 version
of the model (red line, Figure 1).

Next we ask if the behavior of  $\Gamma$  exhibited in Figure 6 can be interpreted in terms 453 of changes in the strength of lower stratospheric tropical upwelling and extratropical wave 454 convergence, as our previous analysis of the CCMI experiments suggested. Indeed, Fig-455 ure 7 shows that values of upwelling decrease in the CSRAD and M2REMAP experiments, 456 relative to the CTRL integration. The increase in upwelling resulting from both changes 457 (CSRAD+M2REMAP) is still larger, consistent with the larger age decreases in that ex-458 periment. This change in the behavior of  $w^*$  within the tropical stratosphere can be in-459 terpreted in terms of changes in the Eliassen Palm flux convergence over NH midlati-460 tudes (not shown), which features smaller values in the CSRAD, M2REMAP (and CSRAD+ 461 noindentMSREMAP) experiments. Note that our examination of the changes in 462

 $w^*$  are derived from EMIP integrations, which we showed previously converge (for DJF) to the statistics derived from corresponding AMIP experiments.

465

#### 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
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-

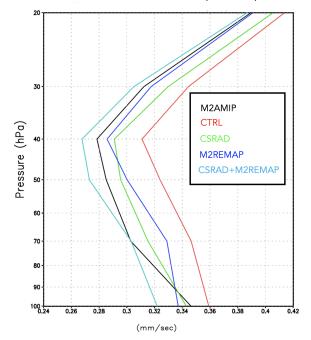


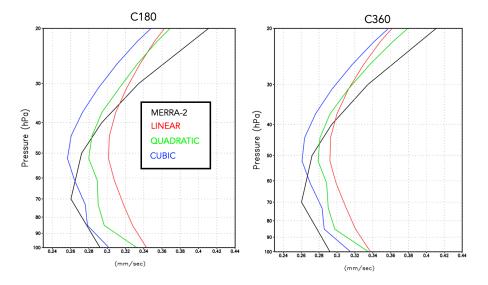
Figure 7. The DJF climatological mean vertical residual mean velocity,  $w^*$ , averaged between the turnaround latitudes for the CTRL (red line; Table 2, row 1), CSRAD (green line; Table 2, row 2), M2REMAP (blue line; Table 2, row 3) and combined CSRAD+M2REMAP (cyan line; Table 2, row 4) experiments.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

layer pressures using cubic, quadratic and linear interpolation 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 474 of interpolation scheme, with  $w^*$  progressively increasing in strength moving from the 475 CUBIC to QUADRATIC to LINEAR schemes. This sensitivity is robust across horizon-476 tal resolutions as the same suite of experiments performed at C360 exhibit the same sen-477 sitivity (Fig. 8, right panels). While no current model tag actually employs a linear scheme, 478 this suite of experiments highlights the strong sensitivity to choice of interpolation scheme 479 within the remapping algorithm; to the best of our knowledge, this result has not been 480 reported in the literature. Furthermore, as we show next, this clean set of experiments 481 allow us to inquire mechanistically into the processes that are driving the changes in wave 482 convergence over midlatitudes, unencumbered by differences in horizontal resolution, physics, 483 etc. 484

Consistent with our expectations based on the analysis of the previous experiments, 485 the drivers of the changes in  $w^*$  are related to increased wave convergence moving from 486 the CUBIC to QUADRATIC to LINEAR schemes (Figure 9). Over extratropical lat-487 itudes, the zonal force associated with this enhanced wave convergence is associated with 488 enhanced downwelling at high latitudes that, through mass balance, is accompanied by 489 enhanced upwelling in the tropics. This indirect impact of higher latitude wave drag is 490 evident in Appendix Figure C1, which show stronger upwelling/downwelling in LINEAR 491 and QUADRATIC experiments over the tropics/polar region. 492

# DJF Climatological Mean Tropical Upwelling (w\*)



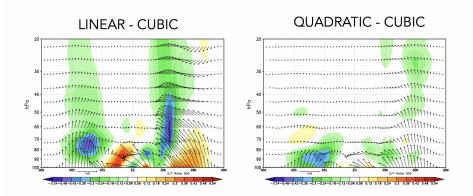
### DJF Climatological Mean Upwelling (w\*)

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), and QUADRATIC (blue line; Table 2, row 6) experiments. MERRA-2 is shown in black. Replace MERRA-2 with M2AMIP.

Next we exploit the fact that these experiments only differ with respect to the interpolation scheme in order inquire further 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 MERRA2, especially above 70 hPa. This change in winds occurs at both C180 (Fig. 10, left panel)
and C360 (Fig. 10, right panel) resolutions.

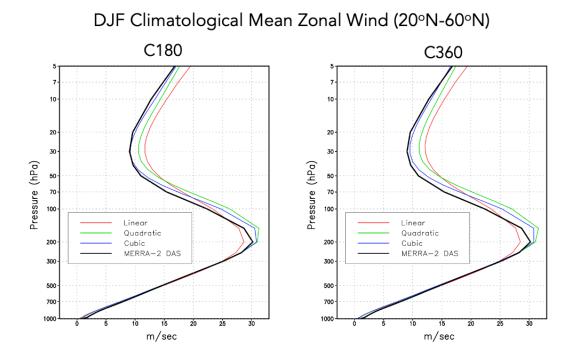
Structurally, the increase in zonal wind strength over northern extratropical midlatitudes is reflective of a poleward shift in the zonal winds as the critical latitude, i.e. where the zonal wind is zero, shifts northward in the QUADRATIC and, especially, LIN-EAR integrations, relative to the CUBIC experiment (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 508 QUADRATIC experiments reflect a degradation in model skill, relative to MERRA-2, 509 throughout the entire stratosphere. The changes in upwelling, mean age, chemical trace 510 gases and zonal winds thus provide a coherent and self-consistent picture suggestive of 511 a degradation in the representation of the stratospheric circulation since MERRA-2. That 512 is, an increased bias in the stratospheric northern zonal winds are, via their influence on 513 wave convergence, compromising changes in the strength of the mean meridional over-514 turning circulation and its impact on composition. It is interesting to note that the wind 515 biases also extend into the troposphere and show degraded skill relative to MERRA-2 516 in the LINEAR and QUADRATIC experiments (Figure 11). Examination of other fields 517 (i.e. tropopause biases, Appendix Figure D1) present somewhat more of a nuanced story 518



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

**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.



**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.

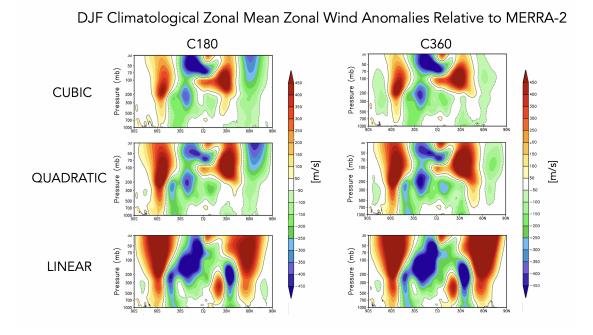


Figure 11. Colors shown anomalies in the DJF climatological mean zonal mean zonal winds in the CUBIC (top), QUADRATIC (middle) and LINEAR (bottom) experiments, relative to MERRA-2. Results for both C180 (left) and C360 (right) experiments are provided.

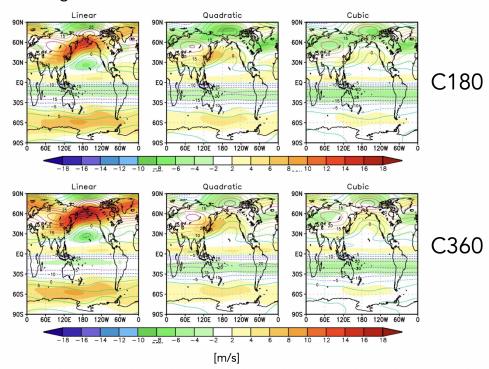
that depends more sensitively on latitude and season considered. The improvements in the zonal winds, however, are most relevant for setting the upwelling characteristics within the tropical lower stratosphere via their influence on wave propagation into that region.

Finally, to better understand why these impacts on the winds have such a conse-522 quence for the wave convergence properties within the stratosphere, next we examine the 523 zonal structure of these biases in the middle stratosphere (Figure 12). This reveals that 524 the enhanced winds in the LINEAR (and, to a lesser extent, QUADRATIC) integrations 525 are concentrated over the North Pacific at both C180 (Fig. 12, left) and C360 (Fig. 12, 526 right) resolutions (a similar picture emerges within the troposphere, not shown). As this 527 region is the primary region dominating the stationary component of the upward flux 528 of vertical wave activity (Plumb (1985), see their Figure 4) it is perhaps not surprising 529 that this region is having a profound impact on the mean overturning circulation. Again, 530 as with the zonal mean wind changes, the increases in wind strength over the North Pa-531 cific represent degraded model skill relative to MERRA-2. Note that comparisons with 532 ERA-5 reveal a similar bias (not shown). 533

534

#### 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 535 via use of 30-year long AMIPs, which are required for deriving the integrated transport 536 statistics (i.e. age-of-air) that reflect the long timescales relevant to setting the strato-537 spheric transport circulation. However, this not only poses practical challenges for model 538 development purposes (which may be ameliorated, for some variables, through use of EMIPs), 539 but it is also not obvious how the time-integrated model biases inferred from AMIPS man-540 ifest in a data assimilation (DAS) context. To this end, here we briefly comment on im-541 plications for the DAS analysis state. 542



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

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.

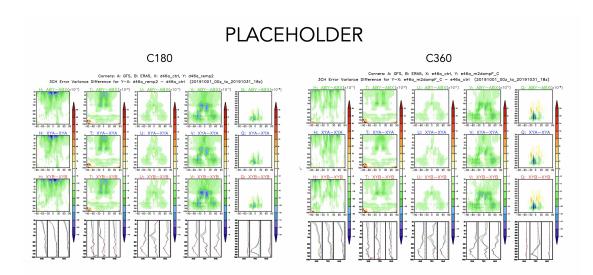


Figure 13. Need to fill in when figure has been decided.

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 res olution.

Need to write when receive Amal's new figure (current Figure 13 is only a place-holder).

#### 549 4 Conclusions

Here we have presented 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-5 similar to that which was used to produce MERRA-2. Using targeted model experiments oriented at disentangling various model development updates, we have identified a key role played by changes in 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 treatment of 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 sensitivities reflect, to first order, changes in the strength of trop ical 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 conver gence 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 man ifest in AMIPs, also translate to degradations in the DAS analysis states of a broad range
 of variables. These results are not sensitive to horizontal resolution.

Although our focus here has been on the stratospheric transport circulation, motivating our use of tracer-independent metrics like the age-of-air, our results have clear <sup>571</sup> implications for constituent transport in GEOS-R21C. In particular, we showed that the <sup>572</sup> increased age-of-air biases correspond to increased biases in the representations of  $CH_4$ <sup>573</sup> and N<sub>2</sub>O moving from the CCMI Phase 1 to Phase 2 model configuration. This com-<sup>574</sup> ports with well-known correlations between the mean age and stratospheric trace gases, <sup>575</sup> reinforcing the fact that model transport inaccuracies continue to significantly affect sim-<sup>576</sup> ulations 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 577 (1987)). The sensitivities in the age-of-air documented herein are also consistent in spirit 578 579 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 580 remain large sensitivities even within a given (FV) dynamical core. Furthermore, we also 581 show that that statistics derived from long AMIPS also manifest within a data assim-582 ilation context, which raises important questions as to the degree to which model biases 583 can be ameliorated through assimilation of observations. 584

Looking forward, our findings support and build on the recommendation proposed 585 in Gupta et al. (2020) for the construction of dynamical core benchmark tests aimed at 586 determining how underlying AGCM numerics impact climatological transport proper-587 ties. In particular, in addition to the age-of-air, the authors propose a range of strato-588 spheric circulation diagnostics that should be evaluated including the zonal mean zonal 589 winds, eddy temperature variance and zonal spectra of eddy kinetic energy. Our anal-590 ysis reveals an important role to be played by the climatological zonal mean wind struc-591 ture as it impacts wave convergence over midlatitudes; we therefore also recommend ex-592 plicit consideration of the Eliassen Palm flux convergence and tropical upwelling  $(w^*)$ 593 fields as they may be crucial for interpreting age-of-air changes. 594

<sup>595</sup> One somewhat incidental – but practical - result from our analysis is that the statis-<sup>596</sup> tics of  $\nabla$ ·F and  $w^*$  are well approximated by ensembles of so-called EMIP integrations. <sup>597</sup> As these are substantially easier to run that AMIPs these could provide a "first pass" <sup>598</sup> when evaluating new proposed model development changes, without the immediate need <sup>599</sup> to integrate AMIP-style experiments. We emphasize, however, that this statement should <sup>600</sup> only apply to a first stage in model development as the age-of-air will reflect the time <sup>601</sup> 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. Future work will focus on examining these impacts.

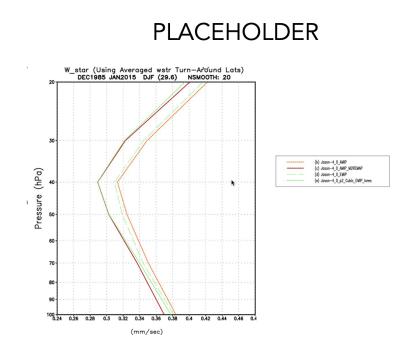


Figure A1. The DJF climatological mean vertical residual mean velocity,  $w^*$ , averaged between the turnaround latitudes for the CUBIC experiment (Table 2, row 7) (? colored line) and a CUBIC experiment performed using T, not TE, denoted CUBIC–T (? colored line). Results are based on 30-member ensemble EMIP experiments.

## Appendix A Sensitivity of REMAP to Temperature (T) vs. Total Energy (TE)

Whereas the modeling experiments listed in Table 2 (rows 5-7) focus on the sen-611 sitivity of Step 5 in REMAP Option 1 to the choice of interpolation scheme, another dif-612 ference between REMAP Options 1 and 2 is the use of TE versus T, respectively. To test 613 the impact of this difference, we ran a new experiment (CUBIC-T) which is identical 614 to the CUBIC experiment (Table 2, row 7), except that T is remapped from input layer 615 mean pressure locations to standard output layer mean locations directly using cubic in-616 terpolation (i.e., no computation of TE or a-posteriori energy conservation applied). Ap-617 pendix Figure A1 shows that this has little impact on the strength of tropical upwelling, 618 suggesting that the  $w^*$  differences between REMAP Options 1 and 2 are dominated by 619 sensitivities to the choice of interpolation scheme, not the use of TE versus T. 620

# Appendix B Correspondence between EMIP and AMIP $w^*$

<sup>622</sup> Appendix Figure B1 shows the close correspondence in DJF climatological mean <sup>623</sup>  $w^*$ , averaged between the turnaround latitudes, from AMIP and EMIP experiments us-<sup>624</sup> ing the CUBIC configuration.

#### <sup>625</sup> 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).

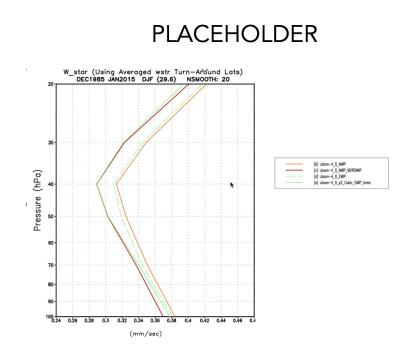


Figure B1. PLACEHOLDER FIGURE: The DJF climatological mean vertical residual mean velocity,  $w^*$ , averaged between the turnaround latitudes for the CTRL experiment (Table 2, row 1). Results based on a 30-year-long AMIP experiment (dotted orange line) and a 30-member ensemble of three-month-long EMIP experiments (dashed green line) are shown.

#### 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.

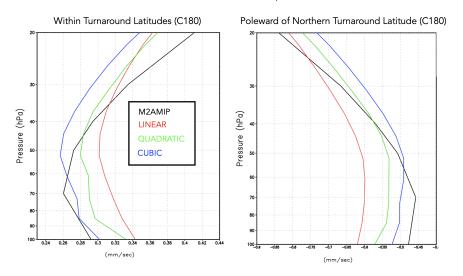
632 Appendix D Tropopause Pressures

Appendix Figure D1 compares boreal winter tropopause pressures among the LIN EAR, QUADRATIC and CUBIC experiments, relative to MERRA-2.

- 635 Open Research Section
- 636 TBD
- 637 Acknowledgments
- 638 TBD

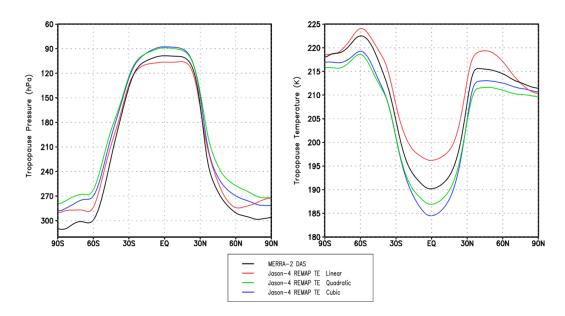
# 639 References

- Abalos, M., Calvo, N., Benito-Barca, S., Garny, H., Hardiman, S. C., Lin, P., ...
- others (2021). The brewer-dobson circulation in cmip6. Atmospheric Chemistry and Physics, 21(17), 13571–13591.
- Abalos, M., Orbe, C., Kinnison, D. E., Plummer, D., Oman, L. D., Jöckel, P., ...
- others (2020). Future trends in stratosphere-to-troposphere transport in ccmi



# DJF Climatological Mean Upwelling (w\*)

Figure C1. Left: 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), and QUADRATIC (blue line; Table 2, row 6) experiments. M2AMIP is shown in black. Right: As in left panel, except averaged over latitudes poleward of the northern turnaround latitude. Results are shown for C180 experiments. Replace MERRA-2 black line with M2AMIP



C180 EMIP 30-yr DJF Climatology (Dec 1985 - Feb 2015)

Figure D1. 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.

645	models. Atmospheric Chemistry and Physics, 20(11), 6883–6901.
646	Abalos, M., Randel, W. J., Kinnison, D. E., & Garcia, R. R. (2017). Using the arti-
647	ficial tracer e90 to examine present and future utls tracer transport in waccm.
648	Journal of the Atmospheric Sciences, $74(10)$ , $3383-3403$ .
649	Andrews, D., Holton, J., & Leovy, C. (1987). Middle Atmosphere Dynam-
650	ics. Academic Press, $60$ , $489$ . doi: $10.1175/1520-0469(2003)060(0103)$ :
651	$CEOOAL\rangle 2.0.CO;2$
652	Arnold, N. P., Putman, W. M., & Freitas, S. R. (2020). Impact of resolution and
653	parameterized convection on the diurnal cycle of precipitation in a global
654	nonhydrostatic model. Journal of the Meteorological Society of Japan. Ser. II.
655	Boering, K. A., Wofsy, S., Daube, B., Schneider, H., Loewenstein, M., Podolske, J.,
656	& Conway, T. (1996). Stratospheric mean ages and transport rates from obser-
657	vations of carbon dioxide and nitrous oxide. Science, 274(5291), 1340–1343.
658	Butchart, N., Cionni, I., Eyring, V., Shepherd, T., Waugh, D., Akiyoshi, H.,
659	others (2010). Chemistry–climate model simulations of twenty-first century
660	stratospheric climate and circulation changes. Journal of Climate, $23(20)$ ,
661	5349 - 5374.
662	Chiodo, G., & Polvani, L. M. (2019). The response of the ozone layer to quadru-
663	pled co 2 concentrations: Implications for climate. Journal of climate, $32(22)$ ,
664	7629–7642.
665	Chou, MD. (1990). Parameterizations for the absorption of solar radiation by o
666	2 and co 2 with application to climate studies. Journal of Climate, $3(2)$ , 209–
667	217.
668	Chou, MD. (1992). A solar radiation model for use in climate studies. Journal of
669	Atmospheric Sciences, $49(9)$ , 762–772.
670	Chou, MD., & Suarez, M. J. (1994). An efficient thermal infrared radiation param-
671	eterization for use in general circulation models.
672	Davis, N. A., Callaghan, P., Simpson, I. R., & Tilmes, S. (2022). Specified dynamics
673	scheme impacts on wave-mean flow dynamics, convection, and tracer transport in $convection = 0.0(1)$ 107 214
674	in cesm2 (waccm6). Atmospheric Chemistry and Physics, 22(1), 197–214.
675	Dietmüller, S., Eichinger, R., Garny, H., Birner, T., Boenisch, H., Pitari, G., oth-
676	ers (2018). Quantifying the effect of mixing on the mean age of air in ccmval-2 and ccmi-1 models. <i>Atmospheric Chemistry and Physics</i> , 18(9), 6699–6720.
677	Eichinger, R., Garny, H., Šácha, P., Danker, J., Dietmüller, S., & Oberländer-Hayn,
678	S. (2020). Effects of missing gravity waves on stratospheric dynamics; part 1:
679	climatology. Climate Dynamics, 54 (5), 3165–3183.
680	Eluszkiewicz, J., Hemler, R. S., Mahlman, J. D., Bruhwiler, L., & Takacs, L. L.
681	(2000). Sensitivity of age-of-air calculations to the choice of advection scheme.
682	Journal of the atmospheric sciences, 57(19), 3185–3201.
683	Eyring, V., Lamarque, JF., Hess, P., Arfeuille, F., Bowman, K., Chipperfield,
684 685	M. P., others (2013). Overview of igac/sparc chemistry-climate model
686	initiative (ccmi) community simulations in support of upcoming ozone and
687	climate assessments. SPARC newsletter, $40$ (Januar), 48–66.
688	Freitas, S. R., Grell, G. A., Molod, A., Thompson, M. A., Putman, W. M., Santos e
689	Silva, C. M., & Souza, E. P. (2018). Assessing the grell-freitas convection
690	parameterization in the nasa geos modeling system. Journal of Advances in
691	Modeling Earth Systems, $10(6)$ , $1266-1289$ .
692	Freitas, S. R., Putman, W. M., Arnold, N. P., Adams, D. K., & Grell, G. A. (2020).
693	Cascading toward a kilometer-scale gcm: Impacts of a scale-aware convection
694	parameterization in the goddard earth observing system gcm. <i>Geophysical</i>
695	Research Letters, 47(17), e2020GL087682.
696	Gelaro, R., McCarty, W., Suárez, M. J., Todling, R., Molod, A., Takacs, L.,
697	others (2017). The modern-era retrospective analysis for research and applica-
698	tions, version 2 (merra-2). Journal of climate, $30(14)$ , $5419-5454$ .
699	Gerber, E. P., & Manzini, E. (2016). The dynamics and variability model intercom-

700	parison project (dynvarmip) for cmip6: assessing the stratosphere–troposphere
701	system. Geoscientific Model Development, $9(9)$ , $3413-3425$ .
702	Grell, G. A., & Freitas, S. R. (2014). A scale and aerosol aware stochastic convective
703	parameterization for weather and air quality modeling. Atmospheric Chemistry
704	and Physics, 14(10), 5233–5250.
705	Grooß, JU., & Russell III, J. M. (2005). A stratospheric climatology for o 3, h 2
706	o, ch 4, no x, hcl and hf derived from haloe measurements. Atmospheric chem-
707	istry and physics, 5(10), 2797–2807.
708	Gupta, A., Gerber, E. P., & Lauritzen, P. H. (2020). Numerical impacts on tracer
709	transport: A proposed intercomparison test of atmospheric general circula-
710	tion models. Quarterly Journal of the Royal Meteorological Society, 146(733),
711	3937–3964.
712	Hall, T. M., & Plumb, R. A. (1994). Age as a diagnostic of stratospheric transport.
713	Journal of Geophysical Research: Atmospheres, 99(D1), 1059–1070.
714	Hall, T. M., Waugh, D. W., Boering, K. A., & Plumb, R. A. (1999). Evaluation
715	of transport in stratospheric models. Journal of Geophysical Research: Atmo-
716	spheres, 104 (D15), 18815–18839.
717	Hardiman, S. C., Andrews, D. G., White, A. A., Butchart, N., & Edmond, I. (2010).
718	Using different formulations of the transformed eulerian mean equations and
719	eliassen-palm diagnostics in general circulation models. Journal of the atmo-
720	spheric sciences, 67(6), 1983–1995.
721	Hardiman, S. C., Butchart, N., & Calvo, N. (2014). The morphology of the brewer-
722	dobson circulation and its response to climate change in cmip5 simulations.
723	Quarterly Journal of the Royal Meteorological Society, 140(683), 1958–1965.
724	Haynes, P., McIntyre, M., Shepherd, T., Marks, C., & Shine, K. P. (1991). On the
725	"downward control" of extratropical diabatic circulations by eddy-induced
726	mean zonal forces. Journal of the Atmospheric Sciences, $48(4)$ , $651-678$ .
727	Hegglin, M. I., Brunner, D., Peter, T., Hoor, P., Fischer, H., Staehelin, J., Weers,
728	U. (2006). Measurements of no, no y, n 2 o, and o 3 during spurt: implica-
729	tions for transport and chemistry in the lowermost stratosphere. Atmospheric
730	chemistry and physics, $6(5)$ , 1331–1350.
731	Holton, J. R., Haynes, P. H., McIntyre, M. E., Douglass, A. R., Rood, R. B., & Pfis-
732	ter, L. (1995). Stratosphere-troposphere exchange. <i>Reviews of geophysics</i> ,
733	33(4), 403-439.
734	Holzer, M., & Hall, T. M. (2000). Transit-time and tracer-age distributions in geo-
735	physical flows. Journal of the atmospheric sciences, 57(21), 3539–3558.
736	Iacono, M. J., Delamere, J. S., Mlawer, E. J., Shephard, M. W., Clough, S. A., &
737	Collins, W. D. (2008). Radiative forcing by long-lived greenhouse gases:
738	Calculations with the aer radiative transfer models. Journal of Geophysical
739	Research: Atmospheres, 113(D13).
	Ivy, D. J., Solomon, S., Calvo, N., & Thompson, D. W. (2017). Observed connec-
740	tions of arctic stratospheric ozone extremes to northern hemisphere surface
741	climate. Environmental Research Letters, $12(2)$ , $024004$ .
742	Kouatchou, J., Molod, A., Nielsen, J., Auer, B., Putman, W., & Clune, T. (2015).
743	Geos-5 chemistry transport model user's guide (Tech. Rep.).
744	Legras, B., Pisso, I., Berthet, G., & Lefèvre, F. (2004). Variability of the lagrangian
745	turbulent diffusivity in the lower stratosphere. <i>Atmospheric Chemistry and</i>
746	Physics Discussions, 4(6), 8285–8325.
747	Lin, SJ. (2004). A "vertically lagrangian" finite-volume dynamical core for global
748	
749	models. Monthly Weather Review, 132(10), 2293–2307. Moled A. Takaga I. Suarga M. & Bagmaister, I. (2015). Development of the
750	Molod, A., Takacs, L., Suarez, M., & Bacmeister, J. (2015). Development of the
751	geos-5 atmospheric general circulation model: Evolution from merra to merra2.
752	Geoscientific Model Development, 8(5), 1339–1356.
753	Monge-Sanz, B., Chipperfield, M., Simmons, A., & Uppala, S. (2007). Mean age of
754	air and transport in a ctm: Comparison of different ecmwf analyses. Geophysi-

355	cal Research Letters, $34(4)$ .
755	Monge-Sanz, B. M., Bozzo, A., Byrne, N., Chipperfield, M. P., Diamantakis, M.,
756	
757	Flemming, J., others (2022). A stratospheric prognostic ozone for seam-
758	less earth system models: performance, impacts and future. Atmospheric
759	Chemistry and Physics, 22(7), 4277–4302.
760	Morgenstern, O., & Carver, G. D. (2001). Comparison of cross-tropopause transport
761	and ozone in the upper troposphere and lower stratosphere region. Journal of
762	Geophysical Research: Atmospheres, 106(D10), 10205–10221.
763	Neu, J., Strahan, S., Braesicke, P., Douglass, A., Huck, P., Oman, L., Tegtmeier,
764	S. (2010). Sparc ccmval (2010), sparc report on the evaluation of chemistry-
765	climate models: Chapter 5: Transport. SPARC.
766	Neu, J. L., & Plumb, R. A. (1999). Age of air in a "leaky pipe" model of strato-
767	spheric transport. Journal of Geophysical Research: Atmospheres, 104(D16),
768	19243–19255.
769	Oehrlein, J., Chiodo, G., & Polvani, L. M. (2020). The effect of interactive ozone
770	chemistry on weak and strong stratospheric polar vortex events. Atmospheric
771	Chemistry and Physics, 20(17), 10531–10544.
772	Orbe, C., Oman, L. D., Strahan, S. E., Waugh, D. W., Pawson, S., Takacs, L. L., &
	Molod, A. M. (2017). Large-scale atmospheric transport in geos replay simula-
773	tions. Journal of Advances in Modeling Earth Systems, $9(7)$ , 2545–2560.
774	Orbe, C., Rind, D., Jonas, J., Nazarenko, L., Faluvegi, G., Murray, L. T., oth-
775	
776	
777	atmosphere—2. validation of large-scale transport and evaluation of cli-
778	mate response. Journal of Geophysical Research: Atmospheres, 125(24),
779	e2020JD033151.
780	Orbe, C., Yang, H., Waugh, D. W., Zeng, G., Morgenstern, O., Kinnison, D. E.,
781	others (2018). Large-scale tropospheric transport in the chemistry-climate
782	model initiative (ccmi) simulations. Atmospheric Chemistry and Physics,
783	<i>18</i> (10), 7217–7235.
784	Pan, L. L., Wei, J., Kinnison, D., Garcia, R., Wuebbles, D., & Brasseur, G. P.
785	(2007). A set of diagnostics for evaluating chemistry-climate models in the ex-
786	tratropical tropopause region. Journal of Geophysical Research: Atmospheres,
787	<i>112</i> (D9).
788	Pawson, S., Stajner, I., Kawa, S. R., Hayashi, H., Tan, WW., Nielsen, J. E.,
789	Livesey, N. J. (2007). Stratospheric transport using 6-h-averaged winds from
790	a data assimilation system. Journal of Geophysical Research: Atmospheres,
791	112(D23).
792	Plumb, R. A. (1985). On the three-dimensional propagation of stationary waves.
793	Journal of Atmospheric Sciences, $42(3)$ , 217–229.
794	Plumb, R. A. (1996). A "tropical pipe" model of stratospheric transport. Journal of
795	Geophysical Research: Atmospheres, 101(D2), 3957–3972.
796	Plumb, R. A. (2002). Stratospheric transport. Journal of the Meteorological Society
797	of Japan. Ser. II, 80(4B), 793–809.
798	Polvani, L. M., Waugh, D. W., Correa, G. J., & Son, SW. (2011). Stratospheric
799	ozone depletion: The main driver of twentieth-century atmospheric circulation
800	changes in the southern hemisphere. Journal of Climate, 24(3), 795–812.
801	Prather, M. J., Zhu, X., Tang, Q., Hsu, J., & Neu, J. L. (2011). An atmospheric
802	chemist in search of the tropopause. Journal of Geophysical Research: Atmo-
803	<i>spheres</i> , 116(D4).
804	Rood, R. B. (1987). Numerical advection algorithms and their role in atmospheric
805	transport and chemistry models. Reviews of geophysics, 25(1), 71–100.
806	Rosenlof, K. H. (1995). Seasonal cycle of the residual mean meridional circulation
807	in the stratosphere. Journal of Geophysical Research: Atmospheres, 100(D3),
808	5173-5191.

Son, S.-W., Tandon, N. F., Polvani, L. M., & Waugh, D. W. (2009). Ozone hole and

southern hemisphere climate change. Geophysical Research Letters, 36(15). 810

- Strahan, S., Douglass, A., & Newman, P. (2013). The contributions of chemistry 811 and transport to low arctic ozone in march 2011 derived from aura mls obser-812
- vations. Journal of Geophysical Research: Atmospheres, 118(3), 1563–1576. 813 Thiele, G., & Sarmiento, J. (1990). Tracer dating and ocean ventilation. Journal of 814 815
  - Geophysical Research: Oceans, 95(C6), 9377–9391.
- Waugh, D., & Hall, T. (2002). Age of stratospheric air: Theory, observations, and 816 models. Reviews of Geophysics, 40(4), 1–1. 817