Stratospheric transport in a three-dimensional isentropic coordinate model

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Received 20 September 2001; revised 28 December 2001; accepted 8 January 2002; published 8 August 2002.

[1] A new version of the Model of Atmospheric Transport and Chemistry (MATCH) is developed, which uses a coordinate that is terrain-following near the surface and becomes isentropic in the upper troposphere. Starting from a simulation of age of air and water vapor in a standard version of National Center for Atmospheric Research’s Middle Atmospheric Community Climate Model (MACCM), we use the meteorological fields to drive two versions of the off-line MATCH model: the standard hybrid-pressure coordinate (MATCH) and the new hybrid-isentropic coordinate (IMATCH). An analysis of the age of air estimates from MACCM, MATCH, and IMATCH and observations shows that the hybrid-isentropic model, IMATCH, is better able to capture the observed ages than either the original online MACCM or the hybrid-pressure MATCH model. Comparisons of water vapor distributions in the tropical lower stratosphere in the three different model versions and observations suggest that IMATCH produces a better propagation of the seasonal cycle than the other models. Analysis of the model results and vertical velocities suggests that the improvements in the age of air and the water vapor simulations are largely due to the reduced numerical vertical diffusion in IMATCH in the lower tropical stratosphere region. In this region, diabatic vertical motions are much smaller than reversible adiabatic motions, making simulations less susceptible to numerical errors if the transport is calculated on isentropic surfaces. Because the lower tropical stratosphere acts as the source region for transport into the stratosphere, correct simulation of the transport in the lower tropical stratosphere is crucial for improving model simulations of the stratosphere.

INDEX TERMS: 0341 Atmospheric Composition and Structure: Middle atmosphere—constituent transport and chemistry (3334); 3337 Meteorology and Atmospheric Dynamics: Numerical modeling and data assimilation; KEYWORDS: Isentropic, stratosphere-troposphere exchange, age of air, transport

1. Introduction

[2] Studies suggest that modeled distributions of ozone in the stratosphere are very sensitive to model transport, perhaps even more sensitive to model transport than to model ozone chemistry [e.g., Park et al., 1999]. Here, we isolate the transport in order to evaluate and improve the simulations of three-dimensional transport models. The “models and measurement 2” intercomparisons [Park et al., 1999; Hall et al., 1999] described a general framework for evaluating the transport in stratospheric models and demonstrated some common failings of model transport. Generally, models tend to have ages of air in the polar vortex which are too young, propagate the water vapor signal too quickly upward, and attenuate the water vapor signal too quickly. In large part these model transport problems are blamed on model overestimates of vertical diffusion in the lower tropical stratosphere; evidence suggests that problems in the lower tropical stratosphere will affect constituent distributions throughout the stratosphere, since that region acts as the entry point for transport from the troposphere into the stratosphere [e.g., Hall et al., 1999].

[3] The age of a parcel is defined as the statistical mean transit time for air that has traveled from the troposphere to a given location [Hall and Plumb, 1994]. Since concentrations of SF6 and CO2 are increasing roughly linearly with time in the atmosphere, one can use observations of SF6 and CO2 to estimate how long the parcels have been in the stratosphere, and thus deduce the age of air [e.g., Harnisch et al., 1996; Boering et al., 1996]. These data demonstrate that transport is slow as the air moves upwards in the tropical lower stratosphere, with the ages quickly increasing with altitude. The oldest ages in the stratosphere and mesosphere are calculated to be near the mesopause and in the stratospheric polar vortex. Hall and Plumb [1994] and Hall et al [1999] demonstrated the insensitivity of the age of air in the stratosphere to processes in the troposphere.
Observations of water vapor from satellites and in situ observations show a distinct seasonal signal of water vapor, consistent with different tropopause temperature during different seasons [e.g., Mote et al., 1996, 1998]. The water vapor signal propagates upward and is seen for at least a year in the stratospheric observations [Mote et al., 1996, 1998]. In addition to water vapor, this signal is also seen in another seasonally varying tropospheric gas, carbon dioxide [e.g., Boering et al., 1996; Andrews et al., 1999]. Observations of the rate of propagation and decay of this stratospheric “tape recorder” can be used to estimate key parameters of transport in the tropical lower stratosphere [Hall and Waugh, 1997].

In the almost adiabatic conditions characteristic of the stratosphere, diabatic transport is very weak; indeed, the model errors noted above imply that many models are unable to make it weak enough, especially in the tropical lower stratosphere. Simulating transport accurately, in (say) pressure coordinates is problematic because the model grid does not reflect the underlying constraint that the flow is almost isentropic, making the model transport vulnerable to numerical errors. For example, undulations of the isentropes will manifest themselves as nonzero transport across any surface that is not an isentropic surface. While such transport is reversible in principle, numerical errors may preclude exact cancellation; even a weak “leakage” of rapid isentropic transport into the direction across isentropic surfaces may seriously corrupt the simulation of realistically weak diabatic transport. These difficulties are automatically circumvented in models based on isentropic coordinates, for which the almost horizontal model grid surfaces naturally coincide with the plane of rapid horizontal transport. (Figure 3, in section 3.1, demonstrates the extent to which “vertical” velocities are reduced in this framework.)

For a stratospheric model with an elevated lower boundary a purely isentropic coordinate is appropriate, but since isentropes intersect the Earth’s surface extending an isentropic model into the troposphere has been problematic. Stratospheric three-dimensional (3-D) isentropic models can avoid the bottom boundary condition by not extending the model to the surface [e.g., Chipperfield, 1999]. Here we follow the general methodology of Hsu and Arakawa [1990], Zhu et al. [1992], and Konor and Arakawa [1997] and use a coordinate that is isentropic in the stratosphere but terrain-following at the surface. The coordinate switches smoothly in the troposphere. An alternate approach of switching discontinuously from sigma to isentropic is used by Zapolocny et al. [1991] and subsequent papers. We make these modifications to an off-line transport model which is publicly available and widely used, the National Center of Atmospheric Research (NCAR) Model of Atmospheric Transport and Chemistry (MATCH), which is capable of using general circulation model [Rasch et al., 1997] or forecast center winds [Mahowald et al., 1997a] as input. Here we discuss the changes necessary to convert a hybrid-pressure offline transport model to a hybrid-isentropic model and evaluate the performance of this model relative to traditional hybrid-pressure transport models.

2. Description of Models

In this study we use three related models: the general circulation model (GCM) from NCAR called the Middle Atmosphere Community Climate Model version 3 (MACCM), MATCH, and the isentropic version of the MATCH model (IMATCH). We calculate the age of air in the MACCM simulation (which calculates the dynamics online), as well as archiving sufficient information to drive the MATCH and IMATCH offline models, where “offline” indicates that the dynamics (temperature, humidity, surface pressure, surface fluxes and winds) are input to the model and not derived within the model. MACCM averaged fields are input to the offline models every 6 hours.

2.1. MACCM

The MACCM is the middle atmosphere version of the Climate System Model’s atmospheric model [Boville and Gent, 1998; Kiehl et al., 1998]. The dry convective mixing parameterization and boundary layer scheme is an updated version of the nonlocal Hotzlag and Boville [1993] scheme. The moist convective mixing parameterization uses the Zhang-McFarlane scheme [Zhang and McFarlane, 1995]. Adective transport of trace species use the semi-Lagrangian transport scheme [Rasch and Williamson, 1990]. The horizontal resolution is T63, with 128 × 64 points in a quasi-linear grid [Williamson, 1997]. The dynamical equations are solved using a semi-Lagrangian technique [Williamson and Olson, 1994] with a time step of 3600 s. The version of the MACCM we use is based on the studies by Sassi et al. [2002] [see also Boville, 1995]. We use two simulations of the MACCM. The first simulation is the 15-year simulation conducted by Sassi et al. [2002] which is used to derive our online age of air estimates. A second simulation of one year was conducted for this study because we failed to archive sufficient heating rates for IMATCH in the first 15-year simulation. These simulations have similar statistics in terms of their vertical velocities and the ages inferred from MATCH.

2.2. MATCH

We use an offline transport model, MATCH, which is capable of using meteorological fields derived either from a GCM [Rasch et al., 1997] or from forecast analyses [Mahowald et al., 1997a]. We use versions of the model with either the semi-Lagrangian [Rasch and Williamson, 1990] or the flux-corrected advection scheme (“SPITFIRE”) [Rasch and Lawrence, 1998]. Subgrid mixing processes can be derived within the model, and use the same algorithms as in the online MACCM algorithms described above, including dry convective mixing, moist convective mixing and large-scale precipitation processes. In MATCH, the vertical velocity is calculated using the divergence of the winds in a manner consistent with the procedures in MACCM (later versions of MATCH use a slightly different approach, which conserves mass better). The MATCH model has been used for transport studies in the stratosphere [Rasch et al., 1994; Waugh et al., 1997] and troposphere [Rasch et al., 1997; Mahowald et al., 1997a], stratospheric chemistry [Rasch et al., 1995], source inversion studies [Mahowald et al., 1997b]; R. Dargaville, et al., Evaluation of terrestrial carbon cycle model through simulations of the seasonal cycle of CO2: Results from transient simulations consisting of increasing CO2, climate, and land-use effects, submitted to Global Biogeochemical Cycles, 2001], and tropospheric chemistry [e.g., Lawrence et al.,
1999] (transport portion of Brasseur et al. [1998]). Thus modifications to this 3-D transport model should be easily incorporated into future modeling studies.

2.3. IMATCH
[10] The isentropic model is a variation on the hybrid-pressure model MATCH. The only modifications we make are to the input algorithms (we interpolate onto our new coordinate system) and the vertical velocity calculation. Other minor changes are made to the code to allow for a more general coordinate system. We only present results using the semi-Lagrangian advection scheme. The same subgrid scale mixing and moist processes are used as in MATCH.

2.3.1. Isentropic vertical coordinate
[11] Using a generalized vertical coordinate, we move MATCH from a \( \eta \) hybrid-pressure coordinate to a \( z \) hybrid-isentropic vertical coordinate. The hybrid-pressure coordinate system \( (\eta) \) is one at the surface and 0 at the top of the atmosphere and lies on pressure surfaces in the stratosphere (above 78 hPa) and sigma surfaces close to the surface (i.e., terrain-following) (for more details see the CCM3 description [Kiehl et al., 1996]).

[12] We define a new vertical coordinate for the isentropic model, \( \zeta \). We follow the work of Hsu and Arakawa [1990], Zhu et al. [1992], and Konor and Arakawa [1997] in allowing \( \zeta \) to vary smoothly from hybrid to isentropic, but we differ in forcing \( \zeta \) to be completely isentropic above some level \( \eta_0 \) (in the previous work \( \zeta \) is almost isentropic, but never completely isentropic) similar to Thuburn [1993] and Webster et al. [1999]. The constraints on the vertical coordinate due to the construction of the IMATCH model are the following: (1) \( \zeta \) must be monotonically decreasing with height, (2) \( \zeta \) must switch smoothly from hybrid-pressure to isentropic, and (3) \( \zeta \) must be dimensionless (this allows our coordinate to be more general). To meet these criteria, we have chosen the following methodology out of many possibilities. We define

\[
\zeta = [\theta_{\text{max}} - f(\eta)(\theta - \theta_0) - \theta_0]C
\]

\[
f(\eta) = \sin \left( \frac{\pi(1 - \eta)}{2(1 - \eta_0)} \right) \quad \eta > \eta_0
\]

\[
f(\eta) = 1 \quad \eta < \eta_0
\]

\[\eta_0 = 0.3; \theta_0 = 200K; \theta_{\text{max}} = 7000K; C = 1/K\]

We subtract the potential temperature \( (\theta) \) value from \( \theta_{\text{max}} \) (7000 K) so that \( \zeta \) decreases with height and multiply by \( C \) (1/K) to make \( \zeta \) dimensionless. The parameter \( \eta_0 \) controls where the model becomes completely isentropic \( (\eta_0 = 0.3) \) implies around 300 hPa), while \( \theta_0 \) must be chosen to be less than the lowest surface potential temperature (which is \( \sim 240 \) K in our case). The \( \zeta \) model surfaces are chosen such that the average pressure at which they are located is similar to the pressure of that level in the hybrid-pressure model. Because of the variability in temperatures in the troposphere, the resolution of the isentropic and hybrid-pressure models differs in some regions of the atmosphere, especially in the middle troposphere. Below about 100 hPa in the tropics there are roughly 16 levels in IMATCH, but there are 20 at the winter poles (18 in MATCH or MACCM).

Because of the hybrid-isentropic nature of the coordinate close to the ground, the boundary layer remains approximately similarly resolved (four or five levels below 800 hPa). However, at \( \sim 230 \) hPa in the tropics, the difference between levels is 100 hPa in IMATCH, while MACCM and MATCH have 30 hPa differences between levels. Figure 1 shows the vertical resolution of the hybrid pressure and isentropic models in pressure (Figure 1a) and potential temperature (Figure 1b).

2.3.2. Isentropic vertical velocity
[13] By calculating the derivative of equation (1) we can analytically derive the vertical velocity:

\[
\frac{dz}{dt} = -\frac{df}{d\eta} \frac{d\theta}{dt} \quad \frac{d\theta}{dt} = -\frac{df}{d\eta} \quad f(\eta) = \sin \left( \frac{\pi(1 - \eta)}{2(1 - \eta_0)} \right) \quad \eta > \eta_0
\]

\[
\frac{df}{d\eta} = -\cos \left( \frac{\pi(1 - \eta)}{2(1 - \eta_0)} \right) \quad \frac{\pi}{2} \frac{d\eta}{d\theta} \quad \eta < \eta_0
\]

\[
\frac{d\eta}{d\theta} = 0 \quad \eta < \eta_0
\]

The vertical velocity on the \( \eta \) surfaces \( (d\eta/dt) \) is taken from the MACCM simulations. The term \( d\theta/dt \) is the heating rate in potential temperature units per unit time and is taken from the MACCM. Note that \( d\eta/dt = -(1/K) d\theta/dt \) above \( \eta_0 = 0.3 \) or 300 hPa. Because the MACCM actually calculates the hybrid-pressure vertical velocity \( (d\eta/dt) \) from tendencies in the horizontal mass flux and because the heating rates only directly affect the temperature tendency in the MACCM, it is quite possible that the heating rates used as vertical velocities in IMATCH and the horizontal winds will not be consistent. These inconsistencies derive from several sources. First of all, while the mean heating rates on an isentropic surface should sum to close to 0.03 K/d on a monthly basis in the stratosphere [Olageur et al., 1992], the mean heating rates on the isentropic surfaces using our methodology can be as large as 0.3 K/d in the stratosphere for the January monthly mean. This large of a discrepancy can affect our tracer distributions [Olageur et al., 1992], and we plan to remove these mean errors in future versions of the model, similar to Chipperfield [1999]. A second source of inconsistency is more local: the mass convergence into or out of a grid cell may not be consistent with the mass change in the cell derived from interpolating the pressures onto the isentropic surfaces at two adjacent time steps. We not explicitly account for these inconsistencies, but rather use equation (3) for vertical velocities and the MACCM horizontal winds interpolated onto the isentropic-hybrid coordinate for our advection. Our advection scheme, the semi-Lagrangian scheme, does not conserve mass, so that the masses are “fixed” to be conserved after advection occurs [Rasch and Williamson, 1990]. We test the sensitivity of our results to the fixer to ensure robust results.

2.4. Model Simulations
[14] Two constituent experiments were conducted with the MACCM, MATCH, and IMATCH models. The first experiment used a constituent with a constant surface tracer
flux, with no sinks, which can be used to calculate the age of the air. The second constituent, which was included only in some simulations, was water vapor. Only the MACCM has the water vapor source in the stratosphere due to methane oxidation, but we do not expect that source of water to be large enough to impact our analysis of stratospheric transport.

Table 1 shows the various model simulations. We conducted two sets of simulations. In the first set, we examined the sensitivity of the hybrid-pressure coordinate to the configuration of the existing standard-hybrid models. First, we ran the 15-year on-line simulation of MACCM and a parallel offline simulation of MATCH (MATCH-SPFC) using the same 15 years of meteorological fields as input. We also examined the impact of the interannual variability by comparing MATCH-SPFC to a run repeating the first year of meteorology (MATCH-SPF). In addition, we considered the impact of the advection scheme: in MATCH-SPF we use the “SPITFIRE” scheme, while in MATCH-SLT we use the semi-Lagrangian scheme using the same input meteorology. In the second set of simulations, we looked specifically at the effects of moving to a hybrid-isentropic coordinate in the offline model. Because we accidentally did not archive all the heating terms in the troposphere in the 15-year MACCM simulation, we were forced to rerun that model for one year, which resulted in slightly different meteorology. We repeated a similar experiment to MATCH-SPF with the new winds (MATCH-SPFA) to be sure that they had similar transport as MATCH-SPF. Thus the IMATCH and MATCH-SPFA simulations can be directly compared, with the only differences being the vertical coordinate and the advection scheme; the meteorology is exactly the same. Since studies in the first set indicated very little sensitivity in the advection scheme (MATCH-SLT vs. MATCH-SPF), the main differences between these two simulations (IMATCH and MATCH-SPFA) will be the vertical coordinate. We also wanted to be

<table>
<thead>
<tr>
<th>Name</th>
<th>Model Description</th>
<th>Description</th>
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<tbody>
<tr>
<td>MACCM</td>
<td>MACCM3</td>
<td>base for all other simulations</td>
</tr>
<tr>
<td>MATCH-SLT</td>
<td>MATCH</td>
<td>use SLT advection</td>
</tr>
<tr>
<td>MATCH-SPF</td>
<td>MATCH3.3.19</td>
<td>use SPITFIRE advection</td>
</tr>
<tr>
<td>MATCH-SPFC</td>
<td>MATCH3.3.19</td>
<td>use SPITFIRE advection with interannual variability</td>
</tr>
<tr>
<td>MATCH-SPFA</td>
<td>MATCH3.3.19</td>
<td>use different year from MACCM (same year as for the isentropic model)</td>
</tr>
<tr>
<td>IMATCH</td>
<td>IMATCH</td>
<td>default isentropic version</td>
</tr>
<tr>
<td>IMATCH-NOFIX</td>
<td>IMATCH</td>
<td>do not use the SLT fixer</td>
</tr>
</tbody>
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sure that the mass fixer used with the SLT scheme was not important in our IMATCH results, and so conducted a run where the masses were not fixed (IMATCH-NOFIX). The first year of the IMATCH simulation (when the interpolations to the new coordinate system are conducted) is about 3 times slower than the default MATCH model. For subsequent years, we read the interpolated values into the model, and then the IMATCH and MATCH versions run approximately equally quickly.

3. Results

[16] We compare the models to available observations and to each other in the following section. Our goal is to demonstrate the viability of an offline isentropic transport model, as well as evaluate the transport in our new model compared with observations and existing models.

3.1. Vertical Velocity

[17] The January monthly and zonal-mean vertical velocities calculated in the isentropic model are shown in Figure 2. Note that the $\frac{dc}{dt} = (-1/K) \frac{db}{dt}$ from the MACCM runs for $\eta < \eta_0 = 0.3$ or approximately 300 hPa. The annual average lower tropical stratospheric heating rates (or vertical velocities) in the lower tropical stratosphere are 0.62 K/d (averaged close to 70 hPa from 15°N to 15°S) for the MACCM fields used in the IMATCH simulation, roughly consistent with (although slightly larger than) observational estimates of heating rates [e.g., Rosenlof, 1995], and averages for the longer periods of the MACCM simulation are similar. Overall, the heating rates predicted in the MACCM and thus the stratospheric vertical velocities in the IMATCH model seem consistent with observations.

[18] As described above, both the MATCH and IMATCH model calculate the vertical velocities from the 6-hourly averaged output from the MACCM model, either from the divergence of the winds (MATCH) or from the MACCM vertical velocities and heating rates (IMATCH). The mean vertical velocities on the hybrid-pressure coordinate from the MACCM and the MATCH model are very similar to each other (not shown). The standard deviation of the vertical velocities, however, vary substantially by model. Figure 3 shows the ratio of the standard deviation to the mean vertical velocity for January for the MACCM (Figure 3a), MATCH (Figure 3b), and IMATCH (Figure 3c) models. These values were calculated by considering the averaged 6-hourly output for all models, and are standard deviations over longitude and time. Note that the standard deviation in the online model is often close to twice as large as in the offline model (Figure 3d); there is some filtering of the winds when we use averaged 6-hourly fields (horizontal winds and surface pressure tendency) to derive our vertical velocities in the MATCH offline model.

[19] A comparison of Figure 3a, 3b and 3c, show that in the lower tropical stratosphere (17–22 km, 20°N to 20°S), the MACCM or MATCH have ratios of standard deviation to mean for the vertical velocity of 10-100+; while the ratio of the standard deviation to the mean for the IMATCH model is 0.1 to 10, usually 1 or 2 orders of magnitude smaller in IMATCH than in MACCM (see Figure 3e) or even MATCH (not shown). This is consistent with our expectation that much of the higher frequency variability is adiabatic. In addition, the IMATCH model has much smaller variability (by over 1 order of magnitude) in the vertical velocities in the polar vortex region.

3.2. Age of Air Simulations

[20] The age of air is estimated using the zonal and monthly mean concentrations for a tracer that is linearly increasing with time in the troposphere. By calculating the lag time since a given concentration was seen at the tropical tropopause (~190 hPa), an age is calculated for each latitude and level. The MACCM, MATCH, and IMATCH simulations were conducted for 15, 10, and 18 years, respectively, at which time none of the ages were changing more than 0.05 yr/yr in the polar regions. The IMATCH-NOFIX case was simulated for only 10 years, and compared against the IMATCH simulation at the same time. There is no significant difference between the IMATCH and IMATCH-NOFIX simulations (not shown), indicating that the age of air model results we obtain for the IMATCH simulations are not sensitive to the “mass fixer.”

[21] Figure 4 shows the age of air calculations for the MACCM, MATCH-SLT, MATCH-SPF, MATCH-SPFC,
Figure 3. Variability of vertical velocity as measured by the ratio of the standard deviation divided by the mean vertical velocity during January for (a) online MACCM model ($\frac{d\bar{y}}{dt}$), (b) MATCH ($\frac{d\bar{y}}{dt}$), and (c) IMATCH ($\frac{d\bar{z}}{dt}$). Figure 3d shows the ratio of the standard deviations for the MATCH/MACCM 6-hourly average vertical velocities for January. The ratios have been interpolated onto the hybrid-pressure vertical coordinate for comparison. Notice that Figure 3d is shown using a different scale than the rest of the figures and thus uses contours instead of a gray scale. Figure 3e shows the ratio of the variability in IMATCH divided by the variability in MACCM, or the ratio of the field in Figure 3c divided by the field in Figure 3a.
Figure 4. Calculated age of air relative to the tropopause for the (a) MACCM, (b) MATCH-SLT, (c) MATCH-SPFC, (d) MATCH-SPF, (e) MATCH-SPFA, and (f) IMATCH simulations. The IMATCH simulation has been interpolated onto the hybrid grid for this figure. The 4.0 age is denoted by a thicker black line, while the ages over 5.0 years are in the crosshatched region.
MATCH-SPFA, and IMATCH for January. The vertical coordinate used for some of the figures and analysis in this paper is the log pressure coordinate: $Z/(km) = -16\log_{10}(p/p_0)$. For the IMATCH model, we interpolate onto the same vertical grid as the hybrid pressure models. These ages are shown for January, but similar ages are seen in July as well.

[22] The estimates of age of air from observations of CO$_2$, or from SF$_6$ (which should be corrected for the mesosphere sink) suggest ages of air in the polar vortex of 5 to 6 years [e.g., Harnisch et al., 1996; Hall et al., 1999; Andrews et al., 1999; Moore et al., 2002]. The MACCM simulation is typical of many GCMs in that it calculates an age of 4.5 years in the polar vortex. The MATCH-SLT, MATCH-SPF, MATCH-SPFC, and MATCH-SPFA simulations have similar ages to the MACCM simulation in the polar stratospheric vortex, although slightly younger (4.0 years) than the online model. The MATCH-SLT simulation is slightly older than the MATCH-SPF simulation in the mesosphere; the only difference between these two simulations is the advection scheme. There is only a small effect of interannual variability, which can be seen by comparing the continuous meteorology simulation (MATCH-SPFC) with two 1 year repeating meteorology simulations (MATCH-SPF and MATCH-SPFA). The IMATCH simulations show the oldest ages in the polar vortex, ages above 5.5 years, more consistent with the observations. The general shape of the age profiles is consistent with observations for all models (class B of Hall et al. [1999]). Notice the horizontal gradient at the top of the IMATCH age of air simulation. This is due to the tilting of the isentropic levels with respect to pressure and the top boundary condition of the model (fixed at 0.1 Pa). It is clear from Figure 4 that IMATCH has the largest vertical gradient in the lower stratosphere of the model simulations, and for much of the stratosphere has ages approximately a year older than the other models.

[23] There is a strong horizontal gradient of age in the lower stratosphere, as seen in Figure 5a in both the observations [Harnisch et al., 1996; Boering et al., 1996; Andrews et al., 1999; Elkins et al., 1996; Moore et al., 2002] (summarized by Hall et al. [1999]) and the models, although the models, with the exception of the IMATCH simulation, underestimate the observed gradient. Notice that the estimates of age from SF$_6$ may be biased by up to several years due to a mesospheric sink of SF$_6$ [e.g., Hall and Waugh, 1998]. We compare our simulations to the available observations of age of air in the lower tropical stratosphere in Figure 5b. IMATCH captures the rate of age increase with height better than the hybrid-pressure models, but that there is still a discrepancy between the predictions from the isentropic model and the observations. Figures 5c and 5d show comparisons of the model results with age of air estimates from the observations in midlatitudes and high latitudes. Overall, the comparison of model-based versus observational estimates of age of air suggest that the IMATCH model simulation is substantially more realistic than the other models presented here.

[24] Note that our study implies a much smaller sensitivity to advection schemes than shown by Eluszkiwicz et al. [2000], more consistent with a previous comparison [Hall et al., 1999]. Here, we see very little difference between ages inferred from different advection schemes (SPITFIRE versus semi-Lagrangian). These are similar schemes to what were used by Eluszkiwicz et al. [2000]. This suggests that the sensitivity to the advection schemes may depend on the time step as well as on the “noisiness” of the vertical velocity.

[25] The mean heating rates from the MACCM simulation indicate a 0.62 K/d upward motion in the tropical lower stratosphere. This implies it would take ~1 year to ascend from the tropopause (~390 K) to 600 K, which is ~24 km in this model. Notice that the age of air is much older than 1 year at 24 km in the tropics, which demonstrates the importance of horizontal mixing [e.g., Neu and Plumb, 1999]. We explore the role of horizontal mixing in more detail later in the paper.

3.3 Water Vapor and the Tape Recorder

[26] Water vapor and carbon dioxide concentrations are observed to enter the stratosphere with a distinct seasonal cycle, which propagates upwards into the lower stratosphere [e.g., Mote et al., 1996; Boering et al., 1996]. The carbon dioxide seasonal cycle is associated with the seasonal cycle in the terrestrial biosphere, while the water vapor signal is indicative of changes in the mean tropopause temperature since colder temperatures precipitate out more water vapor. The models considered here have moist convective and large-scale precipitation parameterizations, although it is unclear whether moist parameterizations play a role in the stratospheric water vapor signal. Previous comparisons of the transport into the stratosphere show that many 3-D models tend to propagate and attenuate this signal too quickly [e.g., Park et al., 1999; Hall et al., 1999].

[27] Figure 6 demonstrates the propagation of the water vapor signal upward into the stratosphere in IMATCH. The mean water vapor in the stratosphere is 2.6 ppmv in the MACCM and MATCH simulations, while it is 3 ppmv in IMATCH. The observational estimates for water vapor in the tropical lower stratosphere suggest values close to 2.7 ppmv (4.4 ppmv [Weinstock et al., 1995]). Notice that the isentropic model has 10% higher water vapor in the stratosphere than observed. The higher mean water vapor in the stratosphere is probably due to the slightly warmer tropopause temperatures in IMATCH (due to the interpolation).

[28] Model simulations and observations are more easily compared if the phase and amplitude of the water vapor are calculated relative to the tropopause [see Hall et al., 1999]. Figure 7 shows the phase and amplitude propagation of water vapor in the models, compared against observations of water vapor plus methane and carbon dioxide [Mote et al., 1998; Boering et al., 1996; Andrews et al., 1999; Hall et al., 1999]. The phase and amplitude of the water vapor signal in the models are calculated relative to the tropopause, which is defined here as the maximum amplitude of the water vapor signal (17 km in the models not 16 km as in the observations). The IMATCH model much better captures the phase. If one considers the attenuation of the water vapor signal in height, MATCH does better than IMATCH, but due to the slower propagation speed in IMATCH, the attenuation in time is slightly better in IMATCH (compared with MATCH-SPFA), as discussed below. Notice that there is a discrepancy between the in situ and satellite observed attenuation, which Hall et al. [1999] discuss in more detail.
Figure 5. Comparison of the model and observation derived age of air (a) horizontal cross section at 20 km (pressure height), (b) tropical age of air (15°N to 15°S), (c) midlatitude age of air (40°N) and high latitude age of air (65°N) as a function of height. From Hall et al., [1999], the triangles and diamonds represent ages inferred from the SF₆ and CO₂ observations, respectively. Observations are, in Figure 5a, latitudinal profile of in situ aircraft measurements from the Stratospheric Photochemistry Aerosol and Dynamics Experiment (SPADE), Airborne Southern Hemisphere Ocean Experiment/Measurements for Assessing the Effects of Stratospheric Aircraft (ASHOE/MAESA), Stratospheric Tracers of Atmospheric Transport (STRAT), and photochemistry of Ozone Loss in the Arctic Regions in Summer (POLARIS) for CO₂ and from ASHOE/MAESA (one deployment only), STRAT, and POLARIS for SF₆. Data points are averaged in 2.5 degree latitude bins for both tracers, and between 19.5–21.5 km for CO₂ and 19–21 km for SF₆. In Figure 5b, Vertical Observations in the Middle Stratosphere (OMS) balloon profiles at 7°N are averaged in 1 km altitude bins over three flights for in situ CO₂ (one February, two November 1997) and over two flights for in situ SF₆ (February, November 1997). In Figure 5c, in situ SF₆ and CO₂ mean ages from a single OMS balloon flight of September 1996, at 35°N, are binned in altitude as in Figure 5b, and mean age from SF₆ whole-air samples, September 1993, from 44°N (asterisks) [Harnisch et al., 1996]. In Figure 5d, in situ CO₂ and SF₆ mean ages are from the OMS balloon flights of June 1997, 65°N, and whole-air SF₆ samples at 68°N inside (crosses; average of four flights) and outside (asterisks; single flight) the polar vortex (from Harnisch et al. [1996], OMS SF₆ data provided courtesy J. W. Elkins and F. L. Moore). The dotted line is MACCM, the dashed line is MATCH-SLT, the dash-dotted line is MATCH-SPFC, the dash-dot-dotted line is MATCH-SPFA, and the heavy gray solid line is for IMATCH.
Owing to satellite problems in detecting the maximum amplitude at lower altitudes, the magnitude of the satellite attenuation may be uncertain. Unfortunately, there are few in situ data points at high altitudes.

Hall et al. [1999] used the phase and amplitude relationships with height to deduce a phase speed $c$ of the vertical propagation of the signal. They also derive a scale height for the water vapor attenuation ($H_a$), by fitting the decrease of amplitude with height in Figure 7b with an exponential function from 16 to 26 km (100 to 16 hPa). Dividing $H_a$ by the distance traveled in 1 year (based on the phase speed, $c$) gives information on how much the amplitude is reduced in one year and is referred to as $R$. We calculate these same parameters for our models and compare to the observational results reported by Hall et al. [1999] in Table 2. Generally speaking, the isentropic model tends to match the observations more closely than either the online or the hybrid pressure offline model. Differences between the phase speed and attenuation between the different hybrid MATCH-SPF simulations show the effect of interannual variability. We will discuss the interpretation of these concentration characteristics in section 4.

4. Role of Vertical Versus Horizontal Diffusion in the Lower Tropical Stratosphere

In section 3.1 we show that the variability of the vertical velocities is quite different in the various model versions. This alone may explain the differences in the tropical lower stratospheric transport properties (Table 2). However, it is also possible that differences in mixing between the extra-tropics and the tropics contribute to the differences in the concentration characteristics of the lower stratosphere. Hall et al. [1999] and Neu and Plumb [1999] show how a “leaky tropical pipe” (one which has mixing between the tropics and extratropics) influences...
the age of air characteristics of the tropical lower stratosphere. Because the vertical propagation of the water vapor signal and the gradient in the mean age of air have different sensitivities to vertical advection and horizontal and vertical mixing, we can use these tracer signals in combination to estimate the velocity and mixing rates [e.g., Hall and Waugh, 1997; Hall et al., 1999]. In this section, we follow Hall and Waugh [1997] and try to distinguish between the effects of 3-D model vertical diffusion and horizontal diffusion using a 1-D model of the tropical leaky pipe:

$$\frac{\partial \varphi}{\partial t} + Q \frac{\partial \varphi}{\partial \theta} - \frac{1}{\rho} K_0 \frac{\partial}{\partial \theta} \sigma \frac{\partial \varphi}{\partial \theta} = - \frac{1}{\tau} (\varphi - \varphi_s)$$

Where $\varphi(\theta)$ is the tropical concentration as a function of height, $\varphi_s$ is the extratropical concentration, $\theta$ is potential temperature and is used as the vertical coordinate, $Q$ is the mean heating rate, $K_0$ is the vertical diffusion rate (assumed independent of $\theta$), $\tau$ is the mixing time with the extratropics, and $\sigma$ is the isentropic density.

[11] Hall and Waugh [1997] solve this model analytically for a seasonal varying tracer (water vapor or CO$_2$) and for a linearly increasing tracer (age of air). They use the following concentration characteristics from the observations (or models in our case) to constrain the $Q$, $K_0$, and $\tau$ (see Table 3): the upward phase speed of the water vapor signal ($1/K_v$), the height scale of the amplitude of the water vapor signal ($1/K_h$), the age of air in the tropics $80$ K above the tropopause ($\Gamma(\Delta \theta \approx 80^\circ K)$), the vertical gradient of the age of the air in the extratropics ($d \Gamma_{e}/d \theta = m$), and the mean difference in age between the tropics and extratropics on the isentropic surface which skims the tropical tropopause at about $400$ K ($\Gamma_{\text{w}}$). See Hall and Waugh [1997] for the explicit solution. Generally, we follow their methodology with minor changes, so we do not repeat the entire description here. In order to make the vertical extent of the calculations consistent we calculate all variables between the model tropopause (90 hPa or 17 km or 390 K) and a height $\Delta \theta \approx 80$ K above the tropopause (the results are sensitive how far above the tropopause we consider our tropical leaky pipe model to extend with $\Delta \theta \approx 80$ K appearing the best fit to the tropical leaky pipe). Following Hall and Waugh [1997] for the tropical mean age, we average between $15^\circ N$ and $15^\circ S$, and for the extratropical analysis we use averages between 20 and $40^\circ$ north or south. We did a simple sensitivity study where we assumed the tropical pipe extended five more degrees toward the extratropics in the model analysis, and it did not change our results qualitatively.

Table 2. Summary of Concentration Characteristics in Lower Tropical Stratosphere

<table>
<thead>
<tr>
<th>Measure</th>
<th>Observations</th>
<th>MACCM</th>
<th>MATCH-PFC</th>
<th>MATCH-SPF</th>
<th>MATCH-PFA</th>
<th>IMATCH</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d(\text{age})/d\theta$, yr/km</td>
<td>0.29</td>
<td>0.29</td>
<td>0.22</td>
<td>0.23</td>
<td>0.21</td>
<td>0.21</td>
</tr>
<tr>
<td>$c$, mm/s</td>
<td>0.33</td>
<td>0.23</td>
<td>0.37</td>
<td>0.33</td>
<td>0.39</td>
<td>0.37</td>
</tr>
<tr>
<td>$H_v$, km</td>
<td>7.6</td>
<td>3.8</td>
<td>3.8</td>
<td>4.3</td>
<td>4.2</td>
<td>4.3</td>
</tr>
<tr>
<td>$R$</td>
<td>0.70</td>
<td>0.50</td>
<td>0.33</td>
<td>0.41</td>
<td>0.34</td>
<td>0.37</td>
</tr>
<tr>
<td>Age in polar stratosphere, years</td>
<td>5–6</td>
<td>4.5</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>5.5</td>
</tr>
</tbody>
</table>

$^*$Observational estimates taken from Hall et al. [1999].

[12] Table 3 shows the estimated parameters needed for the 1-D model for the observations [from Hall and Waugh, 1997; Hall et al., 1999] and several versions of the 3-D models. Notice that these are basically the same characteristics as in Table 2, but in different units. We solve for the $Q$, $K_0$, and $\tau$ using an optimization technique instead of solving three simultaneous equations for three unknowns as from Hall and Waugh [1997]. Here our cost function ($\chi^2$) is the sum of the squared differences between the 3-D model and the simple 1-D model derived $K_v$, $K_w$, and $\Gamma(\Delta \theta \approx 80$ K) divided by the uncertainty in the 3d model values for the $K_v$, $K_w$, and $\Gamma(\Delta \theta \approx 80$ K), where we assume a 20% uncertainty:

$$\chi^2 = \left( \frac{K_v(\text{obs}) - K_v(\text{3d})}{0.2 K_v(\text{3d})} \right)^2 + \left( \frac{K_w(\text{obs}) - K_w(\text{3d})}{0.2 K_w(\text{3d})} \right)^2 + \left( \frac{\Gamma(\Delta \theta = 80)(\text{obs}) - \Gamma(\Delta \theta = 80)(\text{3d})}{0.2 \Gamma(\Delta \theta = 80)(\text{3d})} \right)^2$$

The subscript s indicates the estimate from the simple model (1-D) presented in this section, while the 3d subscript indicates the values from 3-D model simulations (Tables 2 and 3). Our results are identical in the case where an exact solution exists (see Table 3), but our method is slightly more flexible, allowing us to solve for only two of the three variables, providing us with the “closest” solution when there is no exact solution and allowing us to evaluate the confidence intervals, as discussed below.

[13] Using the concentration characteristics shown in Table 3 for the observations, Hall and Waugh [1997] showed that the mean motions derived using this methodology (0.55 K/d) are consistent with those derived from independent methods [Rosenlof, 1995], that the observations suggest small vertical diffusion ($K_0 = 0.3$ K$^2$/d) and that the exchange time between the tropics and extra tropics ($\tau$) is about 1.2 years in this region. We also include solutions where some of the observed parameters are updated with values calculated between 16 and 21 km from the HALOE data [from Hall et al., 1999] and where in situ estimated vertical attenuation and propagation of the water vapor signal is used [Andrews et al., 1998; Hall et al., 1999]. These results give a slightly different picture of the observed lower tropical stratospheric circulation than discussed by Hall and Waugh [1997], with more vertical diffusion and less horizontal diffusion. In fact, the horizontal mixing times are quite long (2 years) in this analysis and the mean heating rates are smaller compared to previous studies [e.g., Hall and Waugh, 1997; Hall et al., 1999; Volk et al., 1996; Rosenlof, 1995].
Table 3. Concentration Characteristics for 1-D Model From Observations and Model

<table>
<thead>
<tr>
<th>Description</th>
<th>Base Case</th>
<th>Mean Vertical</th>
<th>Vertical Diffusion $K$</th>
<th>Timescale for Extratropical Motion $Q/K$</th>
<th>Horizontal Mixing $K_w$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observations in situ</td>
<td>0.025</td>
<td>0.92</td>
<td>0.9</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>HALOE</td>
<td>0.0043</td>
<td>0.9</td>
<td>0.9</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>MATCH-SPFC</td>
<td>0.0025</td>
<td>0.9</td>
<td>0.9</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>MATCH-SPFA</td>
<td>0.0026</td>
<td>0.9</td>
<td>0.9</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>MACCM</td>
<td>0.0026</td>
<td>0.9</td>
<td>0.9</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>MATCH</td>
<td>0.0026</td>
<td>0.9</td>
<td>0.9</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>MATCH-SPFA</td>
<td>0.0026</td>
<td>0.9</td>
<td>0.9</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>MATCH</td>
<td>0.0026</td>
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<td>MATCH</td>
<td>0.0026</td>
<td>0.9</td>
<td>0.9</td>
<td>0.004</td>
<td>0.004</td>
</tr>
</tbody>
</table>

Input data for the constrained optimization are bold, the values which are compared in the optimization are italic, and the estimated parameters are in regular type. For the “constrained case,” the mean vertical velocity is input to the optimization.

For several of our model simulations (MACCM, MATCH-SPFC, MATCH-SPFA, IMATCH) we use this simple model to deduce the mean vertical motion and the vertical and horizontal diffusion as shown in Table 3 for the base case. In Table 3, we can see that the solution of the 1-D model tends to put some of the errors from the model transport into the mean vertical velocity, which is probably fairly accurate (section 3.1). In fact, the mean vertical velocities in all four model versions for the base case in Table 3 should be similar (varying slightly due to interannual variability in the MACCM simulation). Especially in the case of the MACCM, the vertical velocities are quite far from the mean calculated in section 3.1. Indeed the mean vertical velocity from section 3.1 is outside the confidence limits (described below) of the $Q$ estimated here in the case of the MACCM, although within the confidence limits for the other models. For unknown reasons, although perhaps related to strong vertical and horizontal mixing, the tropical leaky pipe model does not appear to be a good description of the MACCM simulation when we use three free parameters, although the tropical leaky pipe model does work for the offline models.

Next we repeat the analysis in Table 3 for the base case, but fix the mean vertical velocity to that calculated between 390 and 470 K (shown in Table 3 for the constrained case and equal to 0.61 K/d) and solve only for the values of $K_0$ and $\tau$ (Table 3, constrained case). Similarly, we reanalyze the observational estimates of vertical and horizontal mixing while constraining the mean vertical velocity to be 0.55 K/d (Table 3). This produces estimates of horizontal mixing time (1–1.5 years), which are more consistent with previous studies [e.g., Hall and Waugh, 1997; Volk et al., 1996; Hall et al., 1999]. In this case, results from the analysis of the observations and models appear consistent with our expectations.

Because we are using an optimization approach, we can use the value of the cost function to provide information about the likelihood of different solutions. If we had normally distributed errors and a linear model or many observations (none of which criteria we meet), the values of our cost function ($\chi^2$) (minus the minimum value) of less than 4 would give us the 95% confidence interval of including the correct value of our mixing coefficients [Press et al., 1992]. For studies like ours, which do not meet the strict statistical criteria, we can still set a reasonable value of the cost function to surround our possible solutions, but we cannot be assured that we have a 95% probability of including the real solution. Figure 8 shows the area in $K_0$ and $\tau$ space for which the cost function is less than or equal to 4 for the both models and observations from Table 3 for the constrained case and thus describes the confidence intervals of the variables.

Figure 8 suggests that there is a large range of effective horizontal and vertical diffusion values that may be valid for each model version. Interestingly, this methodology has raised questions about the horizontal mixing rates in this set of models, especially in MACCM and IMATCH, although the overlap in the confidence intervals indicates that the differences between models may not be statistically significant. Importantly, Figure 8 suggests that both the upper and lower bound on the vertical diffusion in IMATCH is smaller than the upper and lower bounds in the other...
models, and that the upper and lower bounds on vertical diffusion in the MACCM are larger than in the other models. Since the confidence intervals partly overlap, it is not clear how statistically significant these differences are, especially for the MACCM and MATCH simulations. With the exception of IMATCH, all the model simulations have a lower bound on vertical diffusion larger than the observations suggest. This analysis supports the argument that the vertical diffusion in IMATCH is smaller than in either MATCH or MACCM, and is more consistent with the observations. This suggests that the strong adiabatic motions seen in Figure 3 are not well represented in the hybrid pressure models, and that numerical vertical diffusion is playing a significant role in the MATCH and MACCM simulations.

5. Summary and Conclusions

This study demonstrates the viability of a new hybrid-isentropic coordinate offline chemical transport model, IMATCH, for use in stratospheric studies using GCM (or forecast center) winds. Simple tests of stratospheric transport as proposed by Hall et al. [1999] suggest that IMATCH does a better job simulating stratospheric transport than either an online model (MACCM) or a standard hybrid-pressure offline model (MATCH). Simulations of age of air suggest that IMATCH obtains ages in the polar vortex of 5.5 years relative to the tropopause, which is similar to observational based estimates, while both MACCM and MATCH tend to simulate young ages of air (4–4.5 years). In addition, IMATCH seems to capture the weak tropical lower stratosphere transport more accurately than the hybrid-pressure models, since it better simulates slow propagation of the tropical water vapor signal.

Our analyses of the vertical velocities (Figure 3) and the transport characteristics (Figure 8) suggest that the IMATCH model better captures the slow vertical transport in the tropical lower stratosphere because of lower numerical vertical diffusion associated with adiabatic motions. The ratio of the standard deviation to the mean vertical velocity is 1–2 order of magnitudes smaller in IMATCH than either hybrid-pressure model in the lower tropical stratosphere and the polar vortex region, showing that in these regions adiabatic vertical motions are much stronger than the diabatic vertical motions. While a perfect numerical algorithm would allow the cancellation of the reversible motions, even a small nonzero transport of mass across the isentropes during adiabatic motions in the lower tropical stratosphere appears to be important. Because the lower tropical stratosphere acts as a very slow entry point for air moving from the troposphere to the stratosphere, correctly simulating the vertical motions in the lower tropical stratosphere is critical for correctly simulating constituent distributions throughout the stratosphere. We present a modified version of the Hall and Waugh [1997] methodology to estimate effective horizontal and vertical diffusion in the lower tropical stratosphere. Results of this analysis are consistent with IMATCH having lower effective vertical diffusion than MACCM or MATCH.

This study suggests that problems with age of air or water vapor simulations in GCMs may not only be related to the physics used in the GCM (e.g., the gravity wave breaking scheme) or the advection schemes, but also to the vertical coordinate used for the transport simulations. Hopefully, this paper provides a methodology and a modeling framework for improving the transport in models used to evaluate the future of stratospheric ozone and other stratospheric chemistry questions. Just as the current MATCH model is publicly available, IMATCH will also be publicly available.

Acknowledgments. N.M. would like to thank Peter Hess, Celal Konor, Akio Arakawa, and Danny Kirk-Davidoff for insightful conversations and to Tim Hall for making data available. We would like to thank...
References


