Transport Diagnostics of GCMs and Implications for 2D Chemistry-Transport Model of Troposphere and Stratosphere

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ABSTRACT

The middle atmosphere version of NCAR Community Climate Model (MACCM2) and the GEOS-STRATAN data assimilation system (DAS) of NASA/GSFC have been used to generate a zonally averaged set of transport parameters (meridional circulation and resolved eddy mixing) for use in two-dimensional (2D) chemistry transport models (CTMs). This was done by performing 3D transport numerical experiments with two orthogonal tracers. Some transport diagnostics from the MACCM2 and DAS are compared with each other, and with other approaches and estimates of horizontal mixing ($K_{yy}$) obtained from satellite data and GCMs. Some differences in the derived $K_{yy}$ values for these passive tracer experiments and using the potential vorticity (PV) methods are discussed, as well as the annual and interannual variations, and the interhemispherical asymmetries in $K_{yy}$ structures. The set of 2D parameters obtained from the MACCM2 transport diagnostics has been used in a 2D CTM to simulate the distribution of CH$_4$, N$_2$O, O$_3$, and the age of air (AOA). These 2D simulations compare well with the zonally averaged results obtained from 3D simulations of these constituents and for AOA in previous studies. The derived 2D transport parameters from the MACCM2 gave an annual cycle of constituent structure and values of mean age that compares well with those of the parent 3D model.

1. Introduction

Three-dimensional (3D) models developed during the last decades have become one of the principal modeling tools for interpretation of the chemical-transport processes in the troposphere and in the lower stratosphere. Some of the major reasons for this are as follows.

1) Three-dimensional chemical-transport models (CTMs) can now interpret the seasonal and interannual variations of total ozone when they are constrained by dynamical fields from general circulation models (GCMs) (Rasch et al. 1995; Shindell et al. 1998) and data assimilation systems (DASs) (Chipperfield et al. 1996).

2) As is commonly accepted, only dynamics from a GCM or DAS is able to credibly reproduce the following features: troposphere–stratosphere exchange (Holton et al. 1995); shift of the center of the polar vortex from the geographical pole; and stratospheric transport barriers and filamentary air intrusion through these barriers (Waugh 1996).

3) Heterogeneous chemical reactions are very temperature sensitive; thus use of the zonally averaged temperatures leads to unrealistic results (Murphy and Ravishankara 1994).

4) Distributions of NO$_x$, HO$_x$, and Br$_y$ concentrations in the upper troposphere and lower stratosphere depend on convective transport (Prather and Jacob 1997; Dvortsov et al. 1998).

Despite recognition of these important features, 2D CTMs, which use quite complete photochemical schemes and relatively simple descriptions of tropospheric–lower stratospheric transport, remain the main conceptual vehicle for our understanding of coupling between stratospheric chemistry and transport and for the analysis of long-term constituent trends. Of course, an advantage of such models is that they are much less computationally demanding compared to 3D CTM simulations. This is especially important for the case of multiyear full chemistry simulations. For example, 2D models have been used to interpret the observed long-term (decadal) and short-term (interannual) ozone changes (1979–95) due to variation of chlorine and bromine emissions, solar cycle effects, solar proton events, and volcanic aerosols specified in the models (Jackman et al. 1996; Solomon et al. 1998; Callis et al. 1997). Although 2D CTMs do offer a convenient format to
analyze the influence of global transport on atmospheric composition, the ways of collapsing a 3D transport effects into a 2D framework are not straightforward (Andrews et al. 1987). The current generation of 2D interactive dynamical, radiative, and photochemical models have their transport formulations based on a quasigeostrophic system of equations utilizing the Garcia-type parameterization for the large-scale mixing ($K_{zz}$) induced by the quasi-stationary planetary waves in the stratosphere (Garcia 1991; Garcia et al. 1992; Summers et al. 1997). The values of vertical mixing ($K_{zz}$) in 2D CTMs are usually adjusted in the troposphere and lower stratosphere (Summers et al. 1997), while at high levels the values of $K_{zz}$ are specified by a Lindzen-type gravity wave parameterization (Garcia and Solomon 1985; Summers et al. 1997) in order to match the observed behavior of long-lived species, and mesospheric temperatures and winds. These 2D models, with parameterized specifications of the planetary and gravity wave forcing, can hardly be expected to adequately reproduce the interhemispherical asymmetries in the position of the surf zones and winter polar vortices, and the seasonal variation in the tropical temperatures, equatorial upwelling, and mixing in the upper troposphere and lower stratosphere. Specification of cumulus transport in 2D CTMs is not usually treated properly. For instance, no 2D models can simulate $^{222}$Rn that matches the zonally averaged $^{222}$Rn distribution simulated by 3D CTMs in the upper troposphere (Jacob et al. 1997).

Self-consistent specification of the large-scale mixing, advection, and convective transport is an important step in the improvement of the 2D formulation in the troposphere and lower stratosphere. Inaccurate representation of the mixing processes is a significant source of error in CTM predictions (Plumb and Mahlman 1987; Hall et al. 1999). In comparison with the coupled CTM strategy, our “2D+” diagnostic approach is to derive the transport formulation from an offline 3D CTM that is driven by the winds, temperature, and convective transports from a parent GCM following the strategy of Plumb and Mahlman (1987, hereafter PM87). These GCM simulations represent the coupling between the troposphere and stratosphere, as well as the wave–mean flow, and wave–wave interactions resolved by the model. This approach relies on the parent 3D dataset, generated by the first principal governing equations. The use of tandem 2D+ and 3D CTM results allows us to address the following tasks:

1) diagnosis of the annual cycle of the zonal mean transport parameters—mixing and convection together with the annual cycle of meridional circulation, temperature, zonal winds, and wave drag, etc;
2) use of the 3D CTM results as a benchmark to validate our 2D transport formulation, as derived from the parent GCM, and to evaluate the practical use of the 2D parameterizations, which are intended to incorporate inherently 3D effects into the 2D formulation; and
3) future application of this methodology to different 3D datasets in helping to diagnose and compare their transport properties more quantitatively in the entire troposphere–stratosphere system.

Following the ideas of PM87, in this paper we derive the zonally averaged transport parameters for the 1992–93 STRATAN-DAS developed by Coy et al. (1994) at the Data Assimilation Office (DAO) of the National Aeronautics and Space Administration (NASA) Goddard Space Flight Center (GSFC), and for the middle atmosphere version of the National Center for Atmospheric Research Community Climate Model (MACCM2), described by Boville (1995). The annual and interannual variations of the meridional large-scale mixing coefficients ($K_{zz}$) derived from STRATAN-DAS and MACCM2 are discussed and compared with previous estimates of $K_{zz}$ from models and data. Validation of the flux–gradient relationship (FGR) for estimates of the resolved vertical mixing in the tropical troposphere is tested using the transport experiments employing MACCM2 and CCM3 history tapes. Finally, using the transport parameters obtained from the MACCM2, we discuss the selected comparison between 3D and 2D CTM simulations for $\text{CH}_4$ and $\text{O}_3$, as a possible test of our adopted 2D transport formulation. To increase confidence that our 2D transport formulation is able to reproduce the global mean age distribution from the parent GCM, we perform the age of air (AOA) experiments with our 2D transport model and compare it with the zonally averaged structures of AOA obtained from the 3D transport simulations driven by the MACCM2 (Hall and Waugh 1997a). In the two previous companion papers by Dvortsov et al. (1998) and Smyshlyaev et al. (1998) we used the derived zonally averaged transport parameters from the MACCM2 in order to incorporate the convective transport and longitudinally temperature asymmetries in our 2D+ CTM. The stress of the present study is the transport diagnostics for the large-scale mixing attributable to the dynamics in the parent 3D datasets.

The structure of this paper is the following. Section 2 presents a brief review of previous studies, which derived the transport parameters for 2D modeling. Section 3 is a brief description of the MACCM2 and STRATAN-DAS simulations, and of the numerical transport schemes, that we use here. Section 4 is a discussion of our results for the 2D transport parameters, derived from the parent GCMs, and of comparisons with other techniques for estimation of the large-scale mixing. Section 5 shows some the comparisons of the 2D CTM results with those from 3D transport modeling results. Section 6 presents the summary and conclusions.
2. Condensed review of the zonally averaged transport deduced from the 3D meteorological fields

Conceptual views of the zonally averaged tracer transport in the troposphere and stratosphere have been discussed in many studies (e.g., Mahlman 1985; Tung 1986; PM87; Plumb 1996; Holton et al. 1995). There is also excellent treatment of the subject in chapters 3 and 9 of Andrews et al. (1987). Two commonly used Eulerian transport formulations for 2D CTMs, the residual mean or transformed Eulerian-mean (TEM) meridional circulation (Andrews et al. 1987) and the meridional circulation in isentropic coordinates (Tung 1986) have the property that when only steady adiabatic small-amplitude waves (eddies) are considered, the mean meridional circulation reduces to the Lagrangian-mean circulation in which no eddy transport terms appear explicitly in the passive tracer continuity equation. These formulations for advective transport have been successfully used in 2D simulations of stratospheric constituents (Garcia and Solomon 1985; Ko et al. 1985; Yang et al. 1990).

Plumb and Mahlman (1987) introduced the concept of an “effective transport” meridional circulation in the presence of inhomogeneous large-scale resolved diffusion. They discussed differences between this circulation and the Lagrangian-mean and TEM meridional circulations. They showed that the description of tracer transport in terms of the “transport” advective circulation plus diffusion [see Eq. (2.14) in PM87] is a useful fundamental 2D Eulerian framework. Their approach for the evaluation of the transport properties of the Geophysical Fluid Dynamics Laboratory (GFDL) GCM was to take the FGR as the starting point and use a 3D tracer simulation to derive the transport parameters from the zonally averaged tracer gradients and eddy fluxes. To derive the four components of the $K$-tensor, Plumb and Mahlman performed two independent transport simulations with almost-conserved tracers (subject to weak relaxation to some prescribed 2D distributions to preserve the mean tracer gradients in the zone of strong mixing and advection). A pair of artificial horizontally and vertically stratified tracers (sine of the latitude and log pressure vertical coordinate) were used in PM87 to derive the seasonal transport parameters. This approach was not taken to be valid for transport on shorter timescales. We call the PM87 two-tracer technique the orthogonal tracer (OT) approach. The OT approach can be used to calculate the symmetric (irreversible diffusion) and antisymmetric parts of the $K$-tensor. These can then be used to reformulate the 2D Eulerian transport equations in terms of the symmetric part of the eddy fluxes and the “effective transport velocities,” which correspond to a meridional transport streamfunction $\chi_K$. Mathematically $\chi_K$ is expressed by the sum of the Eulerian meridional streamfunction and the antisymmetric part of the $K$-tensor. The validity of such a 2D transport formulation was tested in PM87 by implementing the derived transport parameters in a 2D transport model. Comparison of their 2D and 3D tracer simulations showed that their self-consistent calculations of the eddy and advective transport parameters support, in part, the capability of their 2D transport model to reproduce the zonally averaged tracer distribution obtained from their parent GCM (which extended vertically to 10 mb).

The rest of this section is a brief review of the basic approaches for estimation of the large-scale “resolved” mixing that have been published after PM87. Several of these techniques for estimation of $K_{yy}$ will be compared in section 3 against the OT approach in this study.

Two studies of the horizontal mixing presented by Newman et al. (1988) and Yang et al. (1990) were based on daily National Centers for Environmental Prediction [NCEP, formerly the National Meteorological Center (NMC)] temperatures and geopotential heights. Newman et al. (1988) discussed the derivation of $K_{yy}$ estimates by a use of quasigeostrophic potential vorticity (PV) distribution calculated from winds estimated from 1978–82 NMC data in pressure coordinates between 20° and 85° latitudes (north and south) up to about 50 km. They pointed out that the difference between mixing for PV and for a passive tracer is mainly related to wave dissipation and the nonconservation of PV. They reported that the NMC data indicated that the polar vortex is displaced off the pole during most of the analyzed winter seasons in the stratosphere. For those periods and regions, they argued that their negative $K_{yy}$ estimates, derived from the PV fields, mainly indicated a breakdown of the geostrophic relation. They remarked that the tropospheric $K_{yy}$ values do not suffer from these drawbacks because of the relatively weaker wave amplitudes. They also found that their maximum values of $K_{yy}$ are located in the midlatitudes rather than in the subtropics as predicted by PM87 from their OT experiments in the stratosphere.

Some aspects of the differences between the $K_{yy}$s of the passive tracers and those of PV have been studied by Juckes (1989). He used a shallow water barotropic numerical model to show the differences in the dispersion of a passive tracer and the PV induced by breaking and dissipation of the barotropic waves. His results showed that the difference between the mixing of PV and that of passive tracers (with constant weak loss rates) can be attributed, in part, to chemical eddy effects (see PM87). The major unexplained differences between the $K_{yy}$s calculated from the PV and tracer fields reported by Juckes (1989) were in the vicinity of the winter polar vortex edge. He argued that a possible explanation of such discrepancies is the increase of the PV eddy fluxes due to diabatic changes in PV.

Salby et al. (1990) continued to use the barotropic framework to study the discrepancies between the $K_{yy}$s estimated from the eddy PV fluxes, assuming the FGR, and those calculated from the Lagrangian dispersion of particles. They showed that the differences in $K_{yy}$ es-
timated by their techniques at middle and high latitudes follow from the nonconservative behavior of the zonally averaged PV, which is controlled by the competition between horizontal eddy transports and the thermal drive in their model. A brief summary of their findings is as follows. Under adiabatic conditions, eddy stirring alone would tend to destroy the polar vortex in a couple of weeks, while thermal dissipation modifies that behavior by confining irreversible mixing to low latitudes, where diabatic effects give small damping of the wind fields. Salby et al. (1990) concluded that outside the Tropics, even if the eddy dispersion is small, a sizable flux of PV results from the diabatic effects acting on large scales. They pointed out that this nondispersive diabatic source of eddy PV flux at middle and high latitudes may represent an important source of error in the estimation of passive tracer mixing when $K_{yy}$ values are calculated from the eddy PV fluxes.

Garcia (1991) proposed a parameterization of planetary wave (PW) breaking for use in 2D CTMs in the stratosphere, using the barotropic instability criterion. Briefly, the PW breaking and associated horizontal mixing are assumed to occur in those regions where the eddy PV gradient exceeds the zonally averaged value. Furthermore, Randel and Garcia (1994) have tested the $K_{yy}$ estimates based on this PW breaking parameterization using 1979–90 climatological averages of the stratospheric geopotential heights produced by the NCEP analyses between 100 and 1 mb. They confirmed the results of PM87, Juckes (1989), and Salby et al. (1990) that the PW breaking and associated horizontal mixing mainly occur in the subtropics. Garcia et al. (1992) applied the PW breaking parameterization for the transport of surface source gases in the middle atmosphere. Comparison of their model results with observations for CH$_4$ and N$_2$O revealed reasonable agreement in tropical and polar regions. It is necessary to mention that Garcia’s (1991) parameterization of PW breaking can be applied to 2D models that fully couple dynamics, radiation, and chemistry. That provides an opportunity to study the possible feedbacks between dynamical, photochemical, and radiative processes in the middle atmosphere.

Diagnostic formulation of 2D transport in isentropic coordinates was initially proposed by Tung (1986) and further developed by Yang et al. (1990). In their diagnostic approach, the meridional circulation is derived from the net heating rates computed from the observations of temperature and radiatively active species. Eddy fluxes are then parameterized using horizontal mixing coefficient along isentropes, calculated by balancing the zonally averaged terms in the momentum equation with the divergence of the Eliassen–Palm flux. This approach has been successfully used to simulate stratospheric tracer transport in Yang et al. (1990). Sassi et al. (1990) have applied Tung’s diagnostic approach for calculations of stratospheric $K_{yy}$ values using the Limb Infrared Monitor of Stratosphere (LIMS) data for December 1978 and January–February 1979 in the Northern Hemisphere. They have found that, for the relatively quiet December and January months, Tung’s diagnostic method for $K_{yy}$ estimation gives reasonable results. Some problems in their $K_{yy}$ estimates arose from negative values for $K_{yy}$ and steep PV gradients in the Tropics during February, which was very disturbed dynamically.

To conclude this brief review, we emphasize that the major problem of deriving a proper 2D transport formulation is to derive a self-consistent set of transport velocities and large-scale mixing coefficients, both of which are inherently unmeasurable. The estimates of these magnitudes from satellite temperature and tracer observations for different months, years, and latitudinal zones in the stratosphere (Lyjak 1987; Sassi et al. 1990; Stanford et al. 1993; Schoeberl et al. 1997) give interesting and useful information for further validation of 2D transport formulations and conceptual models for transport in the real world (Holton et al. 1995; Plumb 1996; Hall et al. 1998).

The reported estimates of $K_{yy}$ in the stratosphere, based on different models, datasets, and approaches vary by a factor of more than 2 (even sometimes by an order of magnitude). This means that further analyses of observations and model diagnostics are needed to separate the impact of interannual variability of atmospheric dynamics from differences in the methods of estimating the unmeasurable transport characteristics.

In this paper, we show some results of deriving the zonally averaged transport parameters from the MACCM2 GCM (Boville 1995) and STRATAN-DAS (Coy et al. 1994). The selection of these two 3D temperature and wind datasets for our transport studies is not arbitrary. Use of the MACCM2 as a middle atmosphere GCM in earlier stratosphere–troposphere chemistry–transport studies of Randel et al. (1994) and Rasch et al. (1995) showed that the MACCM2 winds and temperatures let them reproduce reasonably well the observed zonally averaged structures of ozone, CH$_4$, and N$_2$O. The wind and temperature fields generated by STRATAN-DAS (Coy et al. 1994) have been used successfully in various 3D transport studies (Douglass et al. 1996; Yudin et al. 1997) for the interpretation of constituents measured by Upper Atmosphere Research Satellite (UARS) as well as for NO$_x$ simulations using different scenarios for aircraft exhausts (Weaver et al. 1995).

3. Tracer transport numerical experiments driven by MACCM2 and STRATAN-DAS

Descriptions of the MACCM2 and STRATAN-DAS can be found in Boville (1995) and Coy et al. (1994), respectively. Here, we briefly summarize the basic aspects of these datasets and list the numerical transport schemes that we used in our 3D- and 2D-transport tracer experiments.
The 1992–93 STRATAN-DAS temperature and winds are archived every 6 h on a uniform horizontal grid with 4° latitudinal and 5° longitudinal resolution on 46 sigma-pressure hybrid vertical levels extending to 54 km (0.04 mb). Our 3D tracer experiments, with assimilative winds, were performed using the transport scheme developed by Lin and Rood (1996), on the same grid. This numerical transport scheme has advantages in its economic use of computer resources and in providing one of the best representations of vertical advection on nonuniform vertical grids. Numerical tests of this scheme in comparison with the semi-Lagrangian transport (SLT) scheme used in the MACCM2 transport calculations have been discussed in detail by Lin and Rood (1996). Our additional tests of this scheme against Prather’s (1986) second-order moments advective scheme in 2D-transport experiments showed that both schemes have comparable numerical accuracy.

The MACCM2 temperature winds were also stored every 6 h, after GCM simulation with T42 × 21 truncation, with equivalent horizontal grid spacing of about 5.6° in longitude and 2.8° in latitude on 44 sigma-pressure vertical levels from the surface to about 76 km. We performed our transport experiments on NCAR computers using the CTM of Rasch et al. (1997), which employs a SLT scheme and implicit diffusion transport in the vertical direction.

4. Zonally averaged diagnostics of transport from MACCM2 and STRATAN-DAS

For diagnostics of the large-scale mixing and transport velocities from the above-mentioned 3D datasets, we performed the analogous set of OT experiments as PM87 for estimates of the effective transport velocities and determination of the K-tensor. Some details of these experiments with a discussion of the selected relaxation rates that are needed to preserve spatial gradients of the orthogonal tracers are found in the appendix. Our different tracer experiments indicated that the specification of relaxation rates appeared to be a weakness of the OT strategy, especially in polar regions and in the middle and upper stratosphere where vertical and meridional velocities are large and have a strong annual cycle. We found, however, that the difference between estimates of Kyy obtained with “zero” and “nonzero” relaxation rates are significantly less than the difference between eddy mixing derived from the PV eddy fluxes and from the OT approach.

This is illustrated in Fig. 1, where the annual and latitudinal variations of the Kyy values obtained using the OT approach with zero (first column) and nonzero (second column) relaxation rates, and the PV technique (third column), applied to the MACCM2 output, are plotted at selected heights. There are significant differences between the values of Kyy derived by the OT and PV techniques from the MACCM2 in high and middle latitudes of the southern winter hemisphere. It is interesting to note that the major discrepancy between the two approaches for the derivation of Kyy is found at the edge and inside the Southern Hemisphere (SH) polar vortex, where the impact of PWs with the first three zonal wavenumbers is important. Such features support the conceptual picture drawn by Salby et al. (1990) that the nondispersive diabatic source of eddy PV flux at stratospheric middle and high latitudes is similar in nature to the thermal dissipation of PWs and may represent an important source of error in Kyy values estimated from the eddy PV fluxes. Less discrepancies in the magnitudes of Kyy, obtained by the PV and OT techniques are seen in the northern stratosphere above 30 km.

Despite the differences in the PV and OT Kyy estimates at middle and high latitudes, it must be emphasized that in the tropical stratosphere, both methods show weak mixing (Kyy less than 2 × 10^5 m^2 s^-1). The areal extent of this weak mixing is confined by the annual evolution of regions where the mean zonal wind is close to zero, as shown by the dashed–dotted lines in Fig. 1, in the Tropics and sub tropics. These low values of Kyy are consistent with estimates of the tropical–mid-latitude exchange in the 20–28-km region reported by Schoeberl et al. (1997) on the basis of UARS wind and constituent measurements. Their estimated Kyy value of 7 × 10^4 m^2 s^-1 and mixing times longer than 18 months were derived by the examining the phase of the N_2 O/CH_4 ratio with respect to the quasi-biennial oscillation (QBO) winds above 20 km. The magnitudes of horizontal mixing associated with the MACCM2 eddies (Fig. 1) above 20 km are close to observational Kyy estimates. Diagnostics of the STRATAN-DAS horizontal mixing also show the minimum values of tropical Kyy above 20 km, but these Kyy values are larger, in the range of 1–4 × 10^5 m^2 s^-1.

With respect to QBO phases, our diagnostics of the 1992–93 STRATAN-DAS transport properties show some interesting features of interannual variability in the mixing and in the TEM circulation. Figures 2 and 3 present the height–latitude cross section of the mean zonal winds, Kyy-OT, and the TEM meridional streamfunction derived from the STRATAN-DAS for January and July 1992–93. The −5, 0, and 5 m s^-1 mean zonal wind lines (dashed) separate the region of intensive mixing from the region of weak horizontal diffusion (second column of Figs. 2 and 3). Such a correlation between the zero zonal wind line and the magnitudes of Kyy has been also found in PM87 and remarked on by Newman et al. (1988) for quiet winter conditions. From the mean zonal wind structures, we see that 1992 and 1993 are years of different QBO phases in the stratosphere. In 1992 (easterly phase of the QBO), the interhemispheric summer–winter transport in the stratosphere is well developed and high mixing is seen in the SH subtropics (Fig. 3) and in the Northern Hemisphere (NH) midlatitudes (Fig. 2). During 1993 (westerly phase of the QBO), the assimilative system gives a weak summer–winter transport in the middle and low latitudinal re-
regions of the stratosphere, and relatively weak mixing in the winter subtropics and midlatitudes. These transport differences between opposite phases of the QBO support the conceptual picture of Holton and Tan (1980) and of O’Sullivan and Salby (1990) that the displacement of the zero wind line in the Tropics is related to interannual variability of planetary waves at high and middle latitudes in the winter stratosphere. Using barotropic simulations at about 30 mb, O’Sullivan and Salby (1990) showed that during the easterly phase of the QBO, there is amplified exchange of air between the Tropics and middle–high latitudes that is associated with stronger planetary wave transport, which also acts to displace and weaken the polar vortex. The MACCM2 interannual variability in the $K$-tensor and TEM velocities (not shown) is considerably less than that of the
STRATAN-DAS (the MACCM2 does not reproduce the QBO).

Figure 4 shows the Eulerian, TEM, and transport streamfunctions (July and January) calculated from the sixth year of the MACCM2 simulation. Comparing the MACCM2 circulation with the STRATAN-DAS meridional transport (Figs. 2, 3), we find similar structures in the TEM meridional circulation and zonal winds (not shown) in the 1992 STRATAN-DAS and MACCM2. However, in the tropical lower–middle stratosphere the STRATAN-DAS vertical upwelling ($W^* \sim 0.3–0.6$ mm s$^{-1}$) is two times stronger compared with the MACCM2 vertical velocities ($W^* \sim 0.1–0.3$ mm s$^{-1}$) (not shown). These differences in the tropical TEM fields of DAS and GCM likely can explain the differences in the 3D Global Modeling Initiative (GMI) CTM simulations of the N$_2$O and of the mean age driven by the DAO-DAS and MACCM2 [see Figs. 11 and 20 in Hall et al. (1999)].
The MACCM2 transport and TEM meridional streamfunctions (second and third columns Fig. 4) are close to each other in the stratosphere, although there are differences between them in the strong mixing zones: below 20 km in Tropics, and above 20 km in the winter subtropics and midlatitudes. Unfortunately, breakdown of the FGR in the tropical troposphere (see discussion below) and the poorly structured distribution of the antisymmetric part of the $K$-tensor in polar regions prohibited the use of the transport meridional circulation in our 2D transport experiments. In the next section we discuss 2D CTM results obtained using the TEM circulation and symmetric part of $K$-tensor.

Figure 5 presents the $K_{yy}$ distributions estimated by the OT method from the MACCM2 for January, April, July, and November. The July $K_{yy}$ structures in the winter stratosphere derived from the MACCM2 and the 1992 STRATAN-DAS (Fig. 2) have similar patterns in the subtropics and indicate the position of the PW surf zones (Randel and Garcia 1994). There is a considerable level of interhemispherical asymmetry in the $K_{yy}$ winter structures derived from the OT experiments with the MACCM2 and STRATAN-DAS winds (cf. the January
and July $K_{yy}$ distributions in Figs. 2, 3, and 5). Both wind datasets indicate a narrow and intensive mixing region in the SH from May to September centered between 25° and 45°S, while in the northern winter hemisphere the broad area of stratospheric mixing is shifted to middle and high latitudes, and rapidly changes position over the months, indicating the high level of wave activity variations through the year in the NH. Similar interhemispherical asymmetries in the winter mixing are seen from the $K_{yy}$ distributions derived from the PV fields (Fig. 6). However, the areal extent of the regions associated with high mixing in the polar stratosphere is broader than is found with the OT technique (Fig. 5).

Using the MACCM2 temperature and wind fields, we have calculated the PV, eddy PV fluxes, and the meridional rms winds, and we have estimated the linear dissipation rate $\beta$ implied by the PWs with the zonal wave-numbers 1–6, in regions where Garcia’s (1991) criterion for PW breaking is satisfied. Based on these parameters and following the strategy of Randel and Garcia (1994), we have estimated $K_{yy}$ due to wave breaking and calculated the probability of barotropic instability occur-

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**Fig. 4.** The Eulerian (first column), TEM (second), and transport (third) meridional streamfunctions derived from the sixth year of the MACCM2 simulations. The first row shows results for Jan; the second row presents results for Jul. The dashed streamfunction contours designate the clockwise mass transport (from south to north); solid lines show the counterclockwise mass transport.
Fig. 5. Latitude-height cross sections for $K_{yy} \times 10^5$ m$^2$/s$^2$ for a passive tracer derived from the sixth year of MACCM2 simulations for January, April, July, and November. The dashed lines correspond to the zero, $+5$, $-5$, and mean zonal winds. Values of $K_{yy}$ higher than $10^6$ m$^2$/s$^2$ are shaded.

Fig. 6. Latitude-height cross sections for $K_{yy} \times 10^5$ m$^2$/s$^2$ for PV derived from the MACCM2 simulations for January, April, July, and November. The dashed lines indicate zero, $+5$, $-5$, and mean zonal winds. Values of $K_{yy}$ higher than $10^6$ m$^2$/s$^2$ are shaded.
Fig. 7. Latitude–height cross sections for the probability of the barotropic instability occurrences \( \gamma \) derived from the sixth year of MACCM2 simulations for Jan, Apr, Jul, and Nov. The dashed lines indicate zero, +5, −5 mean zonal winds. Values of \( \gamma \) higher than 0.6 are shaded.

Fig. 8. Latitude–height cross sections for \( K_{yy} \times 10^6 \text{ m}^2 \text{ s}^{-1} \), calculated from the planetary wave breaking parameterization. The PW amplitudes, phases, zonal mean wind, and the time-scales of dissipation were derived from the sixth year of MACCM2 simulations for Jan, Apr, Jul, and Nov. The dashed lines correspond to zero, +5, −5 mean zonal winds. The values of \( K_{yy} \) higher than \( 10^6 \text{ m}^2 \text{ s}^{-1} \) are shaded.
Figure 9. Latitude–height cross sections for $K_{yy} \times 10^5$ m$^2$ s$^{-1}$ derived by the OT approach from the (a) MACCM2, (b) CCM3, (c) GFDL-PM87, and (d) STRATAN-DAS in Oct. The dashed lines correspond to the zero, $+5$, $-5$ mean zonal winds. The values of $K_{yy}$ higher than $10^6$ m$^2$ s$^{-1}$ are shaded.

Figures 7 and 8 illustrate the height–latitude distribution of $g$ (the areas with $g$ higher than 60% are shaded). Figure 8 shows the $K_{yy}$ distributions estimated by the PW breaking parameterization. In order to obtain a more or less continuous distribution of $K_{yy}$ associated with the breaking of stationary and traveling PWs, we assumed propagation of nine PW modes with horizontal phase speed velocities $C_x$ in the range between $-8$ and $8$ m s$^{-1}$ for every zonal wavenumber $m$ ($m = 1, 2, \ldots, 6$). It should be noted that in such a simple implementation of this PW breaking parameterization for calculations of $K_{yy}$, there is no feedback between the mean flow, specifically in the polar region during the summer and equinox months. All these methods of $K_{yy}$ estimation show high values of mixing (Figs. 5, 6, 8) inside the shaded areas of $g > 60\%$ (Fig. 7) in the winter stratosphere above 20 km.

To show that various GCMs and DAS predict different large-scale horizontal mixing, we plot the October $K_{yy}$ distribution derived by the OT method from MACCM2 (Fig. 9a), CCM3 (Fig. 9b), GFDL (from the PM87 study, Fig. 9c), and the STRATAN-DAS (Fig. 9d). From comparison of these figures, we see considerable differences in the $K_{yy}$ magnitudes, and the position of the surf zones above the tropopause at mid-latitudes.

Figure 10 compares previously published estimates of $K_{yy}$ for the January stratosphere (between 20 and 30
km) obtained from different observational datasets (Lyjak et al. 1987; Newman et al. 1988; Yang et al. 1990; Sassi et al. 1990; Randel and Garcia 1994; Stanford et al. 1993) and models. All predictions of horizontal mixing show a more or less similar latitudinal dependence of $K_{yy}$; however, the magnitudes of $K_{yy}$ vary significantly. The different GCMs, datasets and methods, as seen from Figs. 9 and 10, predict different intensities of large-scale mixing. Perhaps, the level of interannual variability in the stratospheric $K_{yy}$ values obtained by other authors from different datasets.

The derivation of the vertical diffusivity above the boundary layer from data is a poorly known area and is based on the estimation of the diabatic vertical velocities calculated using the observed temperature, ozone, and water vapor fields. The global distribution of $K_{zz}$ in the troposphere and stratosphere has been discussed only by PM87 for 2D transport simulation needs. Lyjak (1987) has presented the Lagrangian estimates of stratospheric $K_{zz}$ using the NH winter 1978/79 LIMS temperature and constituent data. Recently, Sparling et al. (1997) presented their Lagrangian estimates of $K_{zz}$ in the lower stratosphere.

Figure 11 shows the typical structure of $K_{zz}$ obtained by the OT technique driven by the MACCM2, CCM3 and GFDL OT transport experiments (PM87) for October. All of these GCMs have comparable vertical and horizontal resolution in the troposphere, but they use different numerical schemes for advection of constituents, temperature, and horizontal winds, and have different physical formulations. The tracers in the MACCM2 and CCM3 were transported using the same SLT scheme. Transport calculations in PM87 were carried by using the semi-implicit leapfrog scheme. Advection of wind and temperature fields in the MACCM2, CCM3, and GFDL were performed by the semi-implicit leapfrog scheme. The differences in the numerical formulation of CCM3 compared to MACCM2 include a change to the form of the hydrostatic matrix (Kiehl et al. 1996), which follows the approach described in Williamson and Olson (1994). This change ensures consistency between $\omega$ and the discrete form of the continuity equation.

The most dominating feature in the $K_{zz}$ structures derived from the GCMs is the large vertical diffusivity in the tropical troposphere between 2 and 10 km. Maximum magnitudes of $K_{zz}$ (due to resolved GCM eddies), as large as 40 m$^2$ s$^{-1}$ in the upper troposphere, correspond to a mixing timescale in the tropical troposphere of about 1–2 weeks. It is shorter than other dynamical timescales in the 2D transport problem, as was remarked in PM87. In PM87, these high values of $K_{zz}$ were not discussed in detail. Plumb and Mahlman (1987) just emphasized that, outside the tropical troposphere, the $K_{zz}$ due to resolved model motions was not well structured in their tracer experiments. They also mentioned that their determination of $K_{zz}$, based on the FGR, was ill-conditioned in the regions where the vertical eddy fluxes are dominated by advection. Except for some events in the polar region of the stratosphere, our tracer experiments did not reveal problems in the derivation of $K_{zz}$ outside the tropical troposphere. Perhaps, the possible explanation for these different conclusions about the determination of $K_{zz}$ may be found in the use of modern numerical transport schemes in the present study rather than the leapfrog transport scheme used by PM87 10 years ago.

To understand the nature of the high values of tropical $K_{zz}$, we performed analysis of the vertical wind rms, eddy vertical fluxes of momentum, heat, and tracers, but could not find a clear answer, except for a possible breakdown of the FGR for parameterization of the eddy vertical fluxes in the tropical region. On the other hand, our 2D transport experiments with these large values of $K_{zz}$ in the Tropics tended to underestimate the total ozone amounts in the Tropics [250 Dobson units (DU)] in comparison with the Total Ozone Mapping Spectrometer (TOMS) total ozone observations (260 DU) (Fig. 16), and our simulations with more moderate values of tropical values of $K_{zz}$ (less than 20 m$^2$ s$^{-1}$, Fig. 15d).

B. A. Boville (1997, personal communication) has shown that if the semi-Lagrangian formulation for vertical advection is used for advective transport of vor-
ticity, divergence, and heat instead of the second-order finite differencing scheme used in these GCM simulations, then the equivalent vertical diffusion of the zonal wind component in the tropical troposphere due to resolved motions is considerably suppressed. B. A. Boville (1997, personal communication) has suggested that our derived high values of \( K_{zz} \) in the tropical troposphere are a reflection of numerical diffusion associated with the advective numerical scheme employed in the MACCM2 simulation (Boville 1995). Perhaps, some influence of numerical schemes is seen from comparison between our \( K_{zz} \) estimates derived from the transport experiments driven by the MACCM2 and CCM3 (Figs. 11a,b), although there are also some differences in the wind fields simulated by MACCM2 and CCM3 due to the different physical parameterizations and position of the upper boundaries in these GCMs. Williamson and Olson (1994) have compared Eulerian and semi-Lagrangian CCM2 formulation. They reported that the principal differences between these two numerical formulations arose because the semi-Lagrangian vertical approximations seem to be more accurate. They suggested that, in the vertical, the semi-Lagrangian approximations produce less damping, dispersion, or diffusion of the tropical tropopause temperature than the other finite-difference approximations. These possible explanations for the high tropical values of \( K_{zz} \) due to numerical diffusion are beyond the scope of this paper.
Another way to understand these considerable values of $K_{zz}$ (20–40 m$^2$ s$^{-1}$) in the Tropics is to check the validity of the FGR, which is our starting point for calculations of the $K$-tensor. In order to validate the FGR in the tropical troposphere we can write the tendency equations for the vertical eddy flux, assuming the decomposition of variables into the zonally averaged means and nonzonal eddy terms:

\[
\frac{\partial}{\partial t} q' W' + H_s = -\langle W \rangle W' \frac{\partial}{\partial z} \langle q \rangle - W' W' \frac{\partial}{\partial z} \langle q \rangle - W' W' \frac{\partial}{\partial z} q',
\]

where $q$ is mixing ratio, $W$ is vertical velocity, $z$ is the log pressure coordinate, and $t$ is time. The prime denotes a departure from the zonal average magnitudes, which are marked by $\langle \rangle$. Here $H_s$ represents the influence of the horizontal eddy transport terms. The eddy terms on the right side determine the evolution of the vertical structure of the eddy flux $F_z = q' W'$, and they are written explicitly. Because $\langle W \rangle \ll W'$, the first term is negligible in comparison with the second and third terms. For weak eddy amplitudes, the second term is larger than the third, and in this case the FGR is valid, and $K_{zz}$ values, proportional to $\langle W' W' \rangle$, can be determined using the OT technique. For finite-eddy amplitudes, the justification of the FGR depends on the competition between the second-order and third-order eddy terms. The first two rows of Fig. 12 illustrate the vertical profiles (at selected latitudes) and longitudinal structures (around the position of the $K_{zz}$ maxima) for the vertically stratified tracer at two selected latitudes (28°S and 1°N). The dashed lines in the first row show the $K_{zz}$ profiles calculated on the assumption that the FGR is valid. The third row of Fig. 12 shows the longitudinal structure and zonally averaged means of the second-order (dashed lines) and third-order (solid line) eddy terms in Eq. (1) at 8 km. All these magnitudes were derived from the tracer experiments driven by the CCM3 winds in which the influence of numerical diffusion is probably less than in the other GCMs. From comparison of the right and left columns of Fig. 12 we can see that the use of the FGR appears to be valid in the extratropical troposphere and above the equatorial tropopause, while below 16 km in the Tropics the third-order eddy term in Eq. (1) is responsible for the evolution of the eddy vertical fluxes because of the strong longitudinal variation of $q'$. This leads to a breakdown of the FGR for parameterization of the eddy vertical fluxes of passive tracers in the tropical troposphere. It is worthwhile to carry out some additional study of the FGR validation, implementing different numerical schemes in the 3D transport experiments and another strategy for estimating $K_{zz}$ based on the Lagrangian dispersion of particles similar to those performed by Sparling et al. (1997) in the lower stratosphere. It should be recognized, however, that the initialization of the material tubes by particles in the equatorial troposphere, in order to obtain the zonally averaged $K_{zz}$ estimates, is probably a complex task due to the strong longitudinal variation of the resolved eddy fluxes.

In order to obtain reasonable values of the tropical total ozone in our 2D simulations, with the transport parameters derived from the OT experiments driven by the MACCM2 winds (section 4), we put a 20 m$^2$ s$^{-1}$ limit on the value of $K_{zz}$ in the tropical troposphere.

In the lower stratosphere (Fig. 11), the values of $K_{zz}$ are relatively small (less than 0.2 m$^2$ s$^{-1}$), during the whole year. In particular, our January values of $K_{zz}$ (not shown) are consistent with the diabatic cross-isentropic dispersion in the lower stratosphere that was estimated by Sparling et al. (1997), based on trajectory calculations driven by the January–February 1993 winds from the NASA GSFC and United Kingdom Meteorological Office DASs. Their two-month trajectory results, confined by the 440- and 560-K isentropes, showed that diabatic dispersion is weak at high latitudes in the polar vortex and in the Tropics, while the largest vertical mixing is seen at middle and high latitudes in the Southern Hemisphere. Their main conclusion was that the diabatic cross-isentropic dispersion deduced from both DASs depends on the position of the large-scale transport barriers. During NH winter, these barriers schematically split the winter lower stratosphere into four regions: the SH extratropics, the Tropics, the NH surf zone, and the polar vortex. Our derived structures for $K_{zz}$ in the winter lower stratosphere also revealed a similar correlation with large-scale horizontal mixing, as parameterized by $K_{zz}$. It means that both techniques for obtaining the vertical diffusivity estimates [based on the Lagrangian particle ensembles of Sparling et al. (1997) and our OT simulations with the MACCM2 and CCM3 winds] give qualitatively similar results in the lower stratosphere. The transport experiments with the STRATAN-DAS winds reveal the same correlation of $K_{zz}$ and $K_{zz}$, but the values of $K_{zz}$ in the stratosphere are higher by an order of magnitude than the values obtained from the MACCM2 transport experiments and reported by Sparling et al. (1997). A possible explanation for this discrepancy is that, in the assimilative simulations, the eddy vertical velocity $W'$, calculated from the continuity equation, is considerably higher than the $W'$ from GCMs and the $W'$, estimated from the diabatic heating rates, used in the trajectory calculations of Sparling et al. (1997).

The effects of vertical mixing and advection in the tropical lower stratosphere have also been quantified to some extent in the recent studies (Mote et al. 1996, 1998; Hall and Waugh 1997b; Hall et al. 1998) based on the constituent observations. Using the characteristics of propagation of the annual cycle of water vapor and methane, derived from HALOE measurements, together with the estimates of mean age, derived from the aircraft and balloon measurements of SF$_6$, Hall and
Fig. 12. (first row) The vertical profiles of the passive tracer (logo-isobaric height, in km) at different longitudes (solid lines) and estimated $K_{zz}$, m$^2$s$^{-1}$, from the FGR (dashed lines); (second row) the longitudinal distributions of the passive tracer around the position of the $K_{zz}$ maxima: 8 km is the solid line, 10 km is the dot-dot-dashed line, 6 km is the dashed line, and the zonal mean values of tracer are shown by the thick long-dashed lines; (third row) the longitudinal variations and zonal mean values of the second-order (dashed lines) and third-order (solid lines) eddy terms in Eq. (1). The left part shows results at 28$^\circ$S; the right part presents results at 1$^\circ$N.

Waugh (1997b) obtained a best estimate of 0.01 m$^2$s$^{-1}$ for the $K_{zz}$ in the tropical lower stratosphere, assuming the validity of the tropical leaky pipe conceptual model. Mote et al. (1998) found noticeable vertical variations of mixing with the $K_{zz}$ values being larger above 24 km ($K_{zz}$ $\sim$ 0.1 m$^2$s$^{-1}$) than below ($K_{zz}$ $\sim$ 0.02–0.04 m$^2$s$^{-1}$). Comparison of these observational estimates for the vertical mixing with our derived values for the large-scale $K_{zz}$ from MACCM2 and CCM3 (Fig. 11, top row) shows that above 24 km our $K_{zz}$ diagnostic results are close to those reported by Mote et al. (1998). However, between 16 and 24 km, our derived values of mixing
from both of the NCAR GCMs are in disagreement with the observational values suggested by Hall and Waugh (1997b) and Mote et al. (1998). We do not know the exact reason for this disagreement. Perhaps, the same possible explanations could be suggested that we discussed above interpreting our tropospheric values of $K_{zz}$. One of them is the influence of the numerical “mixing” associated with the dynamical core of GCMs, another reason could be the spreading of the tropospheric FGR breakdown into the lowermost stratosphere. The possible consequences of such errors for model transport evaluation in the tropical lower stratosphere have been discussed by Hall et al. (1999).

5. Zonally averaged model results and comparison with tracer transport from the parent GCM

As has been remarked in PM87, the calculation of GCM-based transport parameters gives an opportunity to assess the validity of the FGR as a basis for the parameterization of eddy transport in 2D CTMs. Although the FGR is formally justified only in the small-amplitude limit and, as shown above, might break down in some regions, the qualitative agreement between the 2D and 3D tracer experiments shown in PM87 and discussed below supports its practical application, in part, for large-scale transport by finite-amplitude eddies. In this section, we describe our comparisons between 2D and 3D results for the long-lived species CH$_4$ and N$_2$O that have tropospheric sources and O$_3$, which has its photochemical source in the stratosphere. These constituent simulations were driven by transport parameters obtained from the MACCM2. The 2D transport experiments were driven by the monthly mean TEM meridional circulation and the symmetric part of the $K$-tensor as discussed in the previous section. Production and loss rates of CH$_4$, N$_2$O, and O$_3$ have been obtained from the 2D photochemical model described in Smyshlyaev and Yudin (1995) and Smyshlyaev et al. (1998).

Figure 13 illustrates a comparison of our 2D transport experiments after four years of simulation (solid lines) against the zonally averaged 3D results (dashed lines) after two years of simulation, which have been described in Rasch et al. (1995) for CH$_4$ in January, April, July, and September. This comparison shows that the 2D transport parameters derived from the parent GCM reproduce reasonably well the combined effects of large-scale advection and mixing during the equinoxes and solstices on a monthly averaged timescale. In the southern winter–fall hemisphere the 2D simulated slopes of CH$_4$ clearly show the existence of four different transport regions in the stratosphere that are seen in the 3D simulations: the winter polar vortex, the well-mixed SH midlatitudes and subtropics, the Tropics, and an almost advectively controlled summer stratosphere above 25 km. The same schematic competition of advection and mixing in the formation of 2D slopes of CH$_4$ is seen in the NH winter (January) [see also the discussion in Mahlman (1985)]. As seen from both the 2D and 3D tracer simulations, the area occupied by the NH polar vortex is considerably less than that of the SH winter polar vortex; the subtropical surf zones in the winter SH have deeper vertical extent through the entire stratosphere, while in the NH winters, subtropical large-scale mixing is only effective in the 25–35-km region. In order to illustrate why it is important to derive self-consistent horizontal mixing and advective circulation for 2D modeling, we ran the 2D CH$_4$ and N$_2$O transport experiments with the set of $K_{zz}$ estimated from the PV eddy fluxes instead of with the OT-derived values. A comparison of results from these runs for CH$_4$ against 3D simulations is illustrated in Fig. 14. From the comparison of Figs. 13 and 14, we see that the level of disagreement between the 2D and 3D results is larger, especially in the winters, when the $K_{zz}$-PV distribution was used rather than the $K_{zz}$-OT values.

Despite good qualitative agreement between the 2D and 3D simulations (Fig. 13), there are some serious quantitative differences between them. The most serious shortcomings of our 2D transport formulation, seen from the CH$_4$ and N$_2$O (not shown) experiments, are the following. In the tropical stratosphere, our 2D transport parameterizations underestimate the tracer upwelling in comparison with the 3D simulation and gives a broadening of the tracer’s ascent into the subtropics. This 2D failure to reproduce the 3D tracer simulation has been discussed in PM87 for the vertically stratified tracer experiment (see their Fig. 13). They were trying to interpret such failure in terms of the excessive $K_{zz}$ values adopted in their 2D model. However, their additional simulations with reduced values of $K_{zz}$ worsened the agreement between the 2D and 3D simulations, rather than improved it. Our explanation for the differences between the 2D and 3D results in the tropical regions is based on the inability of the OT technique to derive the “true” values of the vertical diffusivity in the Tropics, due to the FGR breakdown. As a consequence, we cannot calculate the transport meridional streamfunction introduced in PM87 and have to use the TEM formulation for the meridional circulation, which is probably only a “relaxed” approximation to the GCM advection in the 2D framework.

Another drawback of the 2D formulation in comparison with 3D simulations is the discrepancy in the winter polar region of the upper troposphere and lower stratosphere. Day-to-day variability of the eddy fluxes and the zonally averaged vertical and meridional tracer gradients in these regions during winters, along with weak horizontal mixing and strong vertical advection, allow us to estimate only the monthly averaged values of the transport parameters. An increase of the relaxation rates in the polar region in order to stabilize the behavior of the orthogonal tracers leads to considerable artificial intensification of horizontal mixing for a passive tracer inside the polar vortex due to the large “chemical” eddy diffusion (Newman et al. 1988; Juckes 1989).
Fig. 13. Comparison of the 3D (dashed) and 2D (solid lines) transport model results for CH$_4$. The 2D transport experiment is driven by the TEM circulation and symmetric part of $K$-tensor derived from the MACCM2 by the OT technique.

Fig. 14. The same as in Fig. 13 but in the 2D transport experiment the employed $K_y$ distribution is derived from the PV eddy fluxes.
We have made attempts similar to those described in PM87 to adjust our values of $K_{yy}$ and $K_{zz}$ in order to improve our agreement in the stratosphere. However, a “crude” adjustment did not significantly improve our simulation. More comprehensive iterative tuning of the derived transport parameters, based on the adjoint of the transport equation and parameter estimation theory, might be a possible tool for analyses of the 2D–3D discrepancies and transport diagnostics in the future studies. For instance, using independent 3D tracer experiments, we can calculate monthly mean or day-by-day zonally averaged true tracer structures and study the sensitivity of our tracer simulation to the variation in the derived zonally averaged transport parameters.

Figure 15 illustrates comparisons of the total ozone distributions generated by our 2D CTM with different transport specifications: (a) result with the TEM circulation and $K$-tensor derived by the OT technique driven by the MACCM2 winds; (b) results when the (a) transport parameters have been used, except that the $K_{yy}$ distributions are estimated from the PV eddy fluxes; (c) simulation with a constant value of $K_{yy} = 3 \times 10^3$ m$^2$ s$^{-1}$; (d) result with a latitudinally and yearly averaged specification of the $K_{yy}$.
formulations of the horizontal and vertical mixing. We see that a self-consistent specification of the annual cycle of $K_{yy}$ (Figs. 15a,b,d) allows us to simulate the observed annual variation of the total ozone (Fig. 16) in the Tropics and subtropics, while simulation with constant $K_{yy}$ (Fig. 15c) does not replicate the observed annual total ozone variations. It is likely that the observed interannual variability of the total ozone in the Tropics and subtropics (Fig. 16) is a reflection of the year-to-year variability of the large-scale mixing in the upper troposphere and lower stratosphere. Partial support for this comes from the different behavior of the TEM circulation and $K_{yy}$ derived from the transport experiments with the 1992 and 1993 GEOS-DAS assimilative winds. The major differences in the total ozone distribution between cases of Fig. 15a and Fig. 15b, when we replaced the $K_{yy}$-OT with $K_{yy}$-PV, are at high latitudes. In particular, case (b) gives smaller values for the total ozone around the NH spring months. Figure 15d presents the results of a total ozone simulation with latitudinally and yearly averaged value of $K_{zz}$. Neglect of the annual and latitudinal variability in $K_{zz}$ changes con-
siderably the values of the total ozone around the equa-
tor and at high latitudes, while keeping the annual var-
ation in the subtropics.

The 2D model results (Fig. 15a) also reproduce rea-
sonably well the zonal mean results of the 3D total
ozone simulations (Fig. 16 in Rasch et al. 1995). Quan-
titative differences between the 2D and 3D total ozone
simulations might be traced, in part, to the differences
in the photochemical codes employed in Rasch et al.
(1995) and the present study. Changes of the upper limit
of $K_{zz}$ in the tropical troposphere, used in our 2D CTM,
also significantly affect total ozone amounts in the Trop-
ics.

The relationship between cumulus transport, vertical
advection, horizontal, and vertical mixing in the Tropics
is presumably one of the main factors that controls
stratosphere–troposphere mass exchange (Holton et al.
1995). Recently, Hall et al. (1999) evaluated the trans-
port properties of the number of 2D and 3D CTMs that
participated in the NASA “Model and Measurements
2” study by comparing simulations of the mean age and
age spectra to estimates of the transport characteristics
from in situ and satellite tracer observations. They con-
cluded that there is large variation in transport among
2D and 3D models. For instance, the model-to-model
transport differences produce mean age distributions
that vary by more than a factor of 2. Two of the 3D
CTM AOA results (GMI-NCAR and MONASH2) anal-
alyzed by Hall et al. (1998) were obtained with the
archived MACCM2 winds. The MONASH2 AOA simu-
lation was performed with the same offline 3D CTM
(Rasch et al. 1997) that was used in this study, to derive
our 2D transport parameters from MACCM2 dynamics.

As an additional test of our derived 2D transport pa-
rameters, we calculate AOA spectra and compare them
to the MONASH2 3D AOA results (Hall et al. 1998).
Figure 17 presents the AOA spectra at 18, 22, 26, and
30 km for 5°, 45° and 75°S. The solid line presents the
3D MONASH2 results. The dashed line illustrates our
2D CTM calculations obtained with monthly averaged
transport parameters, while the dashed–dotted line rep-
resents the AOA spectra, calculated with the monthly
averaged specification for $K$-tensor and daily averaged es-
estimates for the TEM meridional circulation. There is
a reasonable agreement between the 2D and 3D AOA
spectra in the stratosphere for middle and high latitudes
(second and third columns of Fig. 17). The exponential
decays of the AOA spectra after several years are almost
identical for 2D and 3D results, confirming that the
global diffusive properties of 2D and 3D CTMs are the
same.

An important difference between the 2D and 3D AOA
results is seen in the equatorial region during the first
years (first column of Fig. 17) when the signal from the
tropospheric “delta source” penetrates into the strato-
sphere. We found that the use of the daily averaged TEM
in our 2D CTM gave a bit better agreement between
2D and 3D AOA spectra below 22 km. However, the
use of daily averaged TEM does not improve agreement
between the 2D and 3D AOA spectra in the Tropics
above 22 km. We cannot interpret this disagreement
between our 2D and 3D MONASH2 results with con-
fidence. We can list the differences between the MO-
HASH2 3D CTM and our 2D CTM performances that
might be responsible for this discrepancy: 1) the 3D
CTM used convective transports while no convective
transports were included in 2D CTM; 2) the 2D and 3D
AOA simulations employed different transport numerical
schemes; and 3) MONASH2 used 3D winds stored
every 6 h, while the 2D CTM was based on the monthly
averaged specification of the $K$-tensor.

These differences, as well as the FGR breakdown in
the tropical troposphere, plus certain simplifications in
the 2D description of the large-scale 3D wave transport
by the zonal mean $K$-tensor could be the cause of dis-
agreement between the 2D and 3D AOA spectra. Spe-
cifically, during the first months of the AOA simula-
tions, when the initial delta source creates the broad
frequency spectrum of the solution, it would be worth-
while to study the influence of the convective transports
and the numerical schemes on the formation of the equa-
torial stratospheric AOA spectra. It is interesting to note
that the major discrepancies between the mean age re-
sults generated by GMI-NCAR and MONASH2 3D
CTMs (both driven by MACCM2 winds) were confined
to the Tropics (see Fig. 11 in Hall et al. 1998).

To illustrate the sensitivity of the mean AOA ($\Gamma$)
distribution to the specification of the large-scale mixing
and meridional circulation in the 2D AOA experiments,
we performed additional simulations and compared
them with the 3D MONASH2 $\Gamma$ distribution [Fig. 18a,
case (a)]. Figure 18 presents the zonal mean structures
of AOA for the following transport cases: (b) the trans-
pore transport parameters from the GCM, and $K_{yy}$
derived from the PV eddy fluxes. From Fig. 18 we see
that the self-consistent determination of the transport
parameters (Fig. 18b) allows us to reproduce reasonably
well the 3D mean age results, while inconsistent selec-
tion of mixing (Figs. 18c,d) fails to reproduce the 3D
AOA distribution. For instance, use of the $K_{yy}$ derived
from the PV eddy fluxes in the troposphere and lower
stratosphere cannot describe adequately the competition
between strong horizontal mixing and vertical advection
in the tropical and subtropical regions. In general, in
these regions, the $K_{yy}$-PV fields are not well-structured
and their values are less than the $K_{yy}$-OT values (Figs.
5, 6) As a result, the mean age fields calculated with
arbitrarily specified weak horizontal mixing (Figs.
18c,d) are younger compared to the results (Fig. 18a)
calculated with the self-consistent specification (strong
horizontal mixing). Under the same specification for the vertical transport parameters it simply means that weakening of the horizontal mixing in the equatorial troposphere and lower stratosphere helps vertical advection to establish relatively fast air exchange between layers.

6. Summary and conclusions

The success of the 2D CTM with transport parameters estimated from the 3D orthogonal tracer (OT) experiments proposed by Plumb and Mahlman (1987) in re-
producing the transport properties of the parent GCM gives a certain level of credibility to the use of the flux-gradient relationship (FGR) to represent large-scale transports of passive tracers in zonally averaged models of the troposphere and middle atmosphere, except in the tropical troposphere. In this region, the FGR breaks down and other accurate transport diagnostics of the large-scale mixing due to the model resolved motions are needed in future studies.

The set of 2D transport experiments with CH$_4$, N$_2$O, O$_3$, and age of air (AOA) showed that the 2D transport formulation (e.g., monthly mean TEM meridional circulation plus the symmetric part of the $K$-tensor in vertical pressure coordinates) is a reasonable approximation...
and can account for the major transport properties of the MACCM2. These include the interhemispherical asymmetries in the polar stratospheric transport and subtropical surf zone mixing in the winter hemispheres.

The annual evolution of $K_{zz}$ in the troposphere and stratosphere clearly follows the seasonal changes in the behavior of the near-zero mean zonal winds. This indicates that the generation of mixing is mainly driven by tropospheric wave activity and depends on the wave propagation in the stratosphere. The estimates of the large-scale vertical diffusivity ($K_{zz}$) in the tropical upper troposphere with the OT approach revealed a breakdown of the FGR in that region. In the stratosphere, the derived low values of $K_{zz}$ are consistent with previous estimates of vertical mixing obtained from the Lagrangian dispersion of particles.

A reasonable agreement between the zonally averaged mean age distribution calculated by our 2D CTM and the 3D MONASH2 simulations (Hall et al. 1998) in part confirmed that the adopted 2D transport formulation can be used as 2D diagnostic supplement for long-term assessment simulations of the effects of future human activity on ozone and other constituents, representing qualitatively the 3D transport properties of the parent GCM or other 3D datasets.

Diagnostics of the transport properties of the GEOS-STRATAN (Coy et al. 1994) data assimilative system (DAS) revealed interesting features of the interannual variability of the TEM meridional circulation and large-scale mixing during 1992–93. Diagnostics of the DAS shows that there is correlation between the following quantities in the stratosphere: the phase of the QBO, the variability of the TEM meridional circulation and large-scale vertical diffusivity ($K_{zz}$). To derive these four components of the $K$-tensor from a knowledge of the zonally averaged eddy fluxes and mean tracer gradients, generated by the 3D CTM, we used the orthogonal tracer (OT) experiments following the strategy of PM87. The 3D tracer experiments were run offline with winds stored every 6 h for 1 yr from a previous GCM experiment. The initial conditions for the orthogonal tracers are identical to the experiments 3 and 4 of PM87. The horizontally stratified tracer is sin$\theta$, and the vertically stratified tracer is the log pressure height. The 3D experiments were run for about 14 months. To preserve nonzero and nonparallel tracer gradients throughout the course of these numerical experiments, the tracer distributions were relaxed back toward their zonally averaged values; for example, the loss and sink terms in the 3D OT experiments were specified as follows:

$$F_y = -K_{yy} \frac{\partial q}{\partial y} - K_{yz} \frac{\partial q}{\partial z},$$

$$F_z = -K_{yy} \frac{\partial q}{\partial y} - K_{zz} \frac{\partial q}{\partial z},$$

where $K_{yy}$ and $K_{zz}$ are diagonal components, and $K_{yy}$ and $K_{yz}$ are off-diagonal components of the $K$-tensor. The zonally averaged continuity equation for a quasi-conserved constituent with mixing ratio $q$ can be written in log pressure coordinates as

$$\frac{\partial q}{\partial t} = -\nabla \cdot (q \nabla q) - \frac{1}{\cos \theta} \frac{\partial}{\partial y} (\cos \theta q' w') - \frac{\partial}{\partial z} (\nu w q') + P - Lq,$$

where $\nabla = a \partial \theta / \partial \phi$, $\phi$ is latitude, $a$ is the earth’s radius, $z$ is the log pressure coordinate, and $P - Lq$ represents sources and sinks. We define $F_y = q' w'$ and $F_z = q' w''$ as the eddy fluxes. In order to obtain a zonally averaged closure of (A1) the eddy fluxes must be parameterized in terms of zonally averaged quantities. Assuming the validity of the flux gradient relationship we represent $F_y$ and $F_z$ as follows:

$$F_y = -K_{yy} \frac{\partial q}{\partial y} - K_{yz} \frac{\partial q}{\partial z},$$

$$F_z = -K_{yy} \frac{\partial q}{\partial y} - K_{zz} \frac{\partial q}{\partial z},$$

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APPENDIX

Numerical Experiments with Orthogonal Tracers

The zonally averaged continuity equation for a quasi-conserved constituent with mixing ratio $q$ can be written in log pressure coordinates as

$$\frac{\partial q}{\partial t} = -\nabla \cdot (q \nabla q) - \frac{1}{\cos \theta} \frac{\partial}{\partial y} (\cos \theta q' w') - \frac{\partial}{\partial z} (\nu w q') + P - Lq,$$

where $\nabla = a \partial \theta / \partial \phi$, $\phi$ is latitude, $a$ is the earth’s radius, $z$ is the log pressure coordinate, and $P - Lq$ represents sources and sinks. We define $F_y = q' w'$ and $F_z = q' w''$ as the eddy fluxes. In order to obtain a zonally averaged closure of (A1) the eddy fluxes must be parameterized in terms of zonally averaged quantities. Assuming the validity of the flux gradient relationship we represent $F_y$ and $F_z$ as follows:

$$F_y = -K_{yy} \frac{\partial q}{\partial y} - K_{yz} \frac{\partial q}{\partial z},$$

$$F_z = -K_{yy} \frac{\partial q}{\partial y} - K_{zz} \frac{\partial q}{\partial z},$$

where $K_{yy}$ and $K_{zz}$ are diagonal components, and $K_{yy}$ and $K_{yz}$ are off-diagonal components of the $K$-tensor. To derive these four components of the $K$-tensor from a knowledge of the zonally averaged eddy fluxes and mean tracer gradients, generated by the 3D CTM, we used the orthogonal tracer (OT) experiments following the strategy of PM87. The 3D tracer experiments were run offline with winds stored every 6 h for 1 yr from a previous GCM experiment. The initial conditions for the orthogonal tracers are identical to the experiments 3 and 4 of PM87. The horizontally stratified tracer is sin$\theta$, and the vertically stratified tracer is the log pressure height. The 3D experiments were run for about 14 months. To preserve nonzero and nonparallel tracer gradients throughout the course of these numerical experiments, the tracer distributions were relaxed back toward their zonally averaged values; for example, the loss and sink terms in the 3D OT experiments were specified as follows:

$$P - Lq = -L(\theta, z)[q(\lambda, \theta, z) - \overline{q}(\theta, z)].$$

The selection of $L$ was based on the following requirements: 1) $L$ had to be large enough to conserve the zonally averaged tracer gradients; and 2) $L$ had to be small enough to keep the tracer almost passive.

The first criterion was quantified by determining the approximate timescale on which tracer gradients were destroyed in the 3D experiments with the zero relaxation
rates. Numerical experiments with the “almost-zero” (and the zero) relaxation rates showed that it is possible to obtain the monthly averaged distribution of the $K$-tensor by initializing tracer every month. Numerical effects of the tracer initialization (tracer adjustment to the transport) on the derived values of mixing can be excluded by eliminating the first few days integration from the period of averaging in order to obtain the monthly average eddy fluxes of tracer. The first and second columns of Fig. 1 illustrate the selected comparisons of the derived values of $K_{yy}$. The first column corresponds to the OT experiments with the almost-zero relaxation rates and with new initialization of tracers every month; the second column presents results with “nonzero” relaxation rates and with continuous integration of tracer through 1 yr. These derivations for the seasonal behavior of $K_{yy}$ (Fig. 1) showed that two OT experiments gave the similar results, although use of stronger relaxation rates in the continuous OT experiments gives more mixing in comparison with the weak relaxation due to chem-
ical eddy effects. For another check of the independence of our $K$-tensor calculations from the initial conditions, we compared the calculated values of $K$-tensor derived from first and second years of continuous integration. The difference between the calculated diffusivities for the first and 13th months were relatively small (mostly less than 10%).

The second criterion on the selection of relaxation rates in term of the timescale $T_d = 1/L$ that we used to conduct the OT experiments can be written

$$T_d = 1/L \gg 1/R,$$

$$R = |\partial \ln(q^{T/2})/\partial t| = \left(\frac{q^2}{q}\right)^{-1} \left[ \frac{\partial q}{\partial y} + \frac{\partial q}{\partial z} + \frac{\partial q^2/2}{\partial y} + \frac{\partial q^2/2}{\partial z} \right].$$

(A4)

Briefly, this states that employed chemical relaxation rates that we use to keep the nonzero tracer gradients should be much less than the dispersion of the passive tracer induced by the eddy mixing. Derivation of (A4) is based on the linearized version of the continuity equation. It also assumes that the third-order eddy terms [in Eq. (1), section 4) are negligible in comparison to the second-order eddy terms. As shown above, it is not valid in the tropical upper troposphere, where strong longitudinal asymmetries in tracer distribution are observed. However, to make a continuous integration of the OT through 1 yr we employed (A4) to estimate $R$ on the basis of the 3D transport experiments with zero relaxation rates.

Our calculations of $R$ values for different months and regions showed that their vertical structure and magnitudes are quite different for horizontally (h-tracer) and vertically (z-tracer) stratified tracers. Except for some points in the tropical troposphere, the adopted values of $L$ were generally less than the order of $R$. Typical vertical profiles of $L$ and $R$ at midlatitudes and the equator for equinox conditions (October), latitudinally averaged profiles of these inverse timescales ($L$) and ($R$), and the maximum and minimum relaxation rate profiles used in the PM87 study are shown in Fig. A1. Basically, the latitudinally averaged values of the inverse timescales $R^{-1}$ for h and z tracers in the OT experiments with MACCM2 winds are in the range of 1–4 days in the troposphere and in the range of 3–7 days in the stratosphere. It is, perhaps, reasonable confirmation that the longitudinal asymmetries in the tracer fields are well developed one week after initialization. This range of $(R)$ seems to be also a possible explanation for why our estimates for the large-scale mixing in the continuous OT experiments (second column of Fig. 1) and in the OT simulations, initialized every month (first column of Fig. 1), are close to each other. Depending on the month, the values of $T_d$ used in our OT experiments are in the range of 20–200 days with higher $L$ in zones of strongest large-scale mixing.

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