Evaluation of the transport in the Goddard Space Flight Center three-dimensional chemical transport model using the equivalent length diagnostic

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Received 5 March 2002; revised 30 August 2002; accepted 16 December 2002; published 29 March 2003.

[1] Transport and mixing in the extratropical stratosphere of the NASA Goddard Space Flight Center (GSFC) three-dimensional (3-D) chemical transport model (CTM) are evaluated using the modified Lagrangian-mean diagnostic. The normalized equivalent length squared ($\xi^2$) has been calculated from simulated N$_2$O and CH$_4$ distributions using two different wind data sets and has been compared with that calculated from observations by the CLAES satellite instrument. There is generally good agreement, indicating that the CTM realistically simulates the location and seasonal evolution of mixing regions/barriers in the extratropical lower and middle stratosphere. Differences that occur between the CTM fields and observations at high latitudes in winter and spring can be attributed to interannual variability in polar meteorology. There are also some differences in northern summer: the CTM series shows regions of high $\xi$ in the extratropics that are not observed in $\xi$ from CLAES. These high values occur where there is small-scale variability in N$_2$O in regions with very weak meridional gradients. Comparison of $\xi$ from isentropic tracer simulations using the same wind fields as used in the 3-D CTM show good agreement except during the summer. The isentropic tracers do not have as much small-scale variability as the 3-D CTM tracer fields, indicating that the enhanced small-scale structures in the CTM N$_2$O, and high values of $\xi$, are produced by small-scale horizontal variability in the vertical motions. The fact that vertical motions can influence summer values of $\xi$ means that these $\xi$ fields cannot be interpreted in terms of quasi-horizontal mixing.

INDEX TERMS: 0341 Atmospheric Composition and Structure: Middle atmosphere—constituent transport and chemistry (3334); 3334 Meteorology and Atmospheric Dynamics: Middle atmosphere dynamics (0341, 0342); 3337 Meteorology and Atmospheric Dynamics: Numerical modeling and data assimilation; KEYWORDS: modified Lagrangian mean, equivalent length, CLAES, chemical transport model, transport, mixing


1. Introduction

[2] Three-dimensional chemical transport models (CTMs) play an important role in understanding the distribution of ozone and other trace constituents, and are used for assessing future changes in atmospheric composition. However, a major issue with CTMs is the realism of the transport in these models [e.g., Park et al., 1999; Kawa et al., 1999]. Because of these concerns it is important to evaluate the transport within these models. To do this it is necessary to have quantitative diagnostics of transport and mixing that can be derived from models and observations. [3] The recently developed modified Lagrangian-mean (MLM) analysis of Nakamura [1995, 1996] provides such a diagnostic. Within this framework the equivalent length is defined to provide a measure of the geometric complexity of tracer contours. Equivalent length can be used to identify mixing regions and barriers to transport (see next section for further discussion). The equivalent length can be calculated directly from either observed or simulated tracer distributions without knowledge of the wind field. The MLM diagnostics have previously been applied to long-lived tracer fields from satellite observations [Nakamura and Ma, 1997; Allen et al., 1999; Lingenfelser and Grose, 2002] and three-dimensional models [Nakamura, 1995; Nakamura and Ma, 1997; Shuckburgh et al., 2001]. The equivalent length (or the “effective diffusivity,” which is
proportional to the square of the equivalent length, see next section) has also been calculated from two-dimensional (isentropic) simulations of passive, artificial tracer [Haynes and Shuckburgh, 2000a, 2000b; Allen and Nakamura, 2001; Shuckburgh et al., 2001].

[4] In this paper, we use the equivalent length diagnostic to evaluate the transport in the NASA Goddard Space Flight Center (GSFC) 3-D CTM [Douglass et al., 1997; Douglass and Kawa, 1999]. The equivalent length is calculated from long-lived tracer fields from this model and compared with that calculated from observations of the same tracers by the Cryogenic Limb Array Etalon Spectrometer (CLAES) instrument on the Upper Atmosphere Research Satellite (UARS) [Roche et al., 1996]. The MLM diagnostics have previously been applied to N2O from CLAES [Nakamura and Ma, 1997] (hereinafter “NM97”), and we revisit the equivalent length fields from CLAES focusing on the seasonal evolution of mixing regions and barriers in the extratropical stratosphere, and compare the location and evolution of these features with those in GSFC 3-D CTM simulations. Unfortunately, the CLAES data are for a different period (September 1991 to May 1993) than the winds used in the GSFC 3-D CTM simulations (1997 to 1999), which complicates the comparison as differences may be due interannual variability rather than model deficiencies. However, the CLAES instrument provides the only multiyear data set with daily hemispheric coverage of long-lived tracers, and this coverage is needed for the calculation of the equivalent length. (Lingenfelser and Gröse [2002] have recently calculated the equivalent length from HALOE observations of CH4 using analyzed potential vorticity fields to form daily hemispheric fields. It may be possible to use this equivalent length data for further model evaluations.)

[5] To determine the role of vertical motions in producing features in the tracer and equivalent length fields we also perform two-dimensional (2-D) tracer simulations. As in the calculations of Haynes and Shuckburgh [2000a] and Allen and Nakamura [2001], these calculations use isentropic winds and the tracer is conserved. The winds and the advection scheme are the same as are used in the GSFC 3-D CTM, so comparisons between the 2-D and 3-D simulations isolates the role of vertical motions.

[6] The MLM diagnostics, in particular the equivalent length, are briefly described in section 2. In section 3, MLM analysis of UARS CLAES measurements are revisited, focusing on seasonal evolutions of the equivalent length. We also compare the equivalent length calculations from CLAES measurements of N2O and CH4. The equivalent length of N2O from GSFC CTM simulations is analyzed and compared with that from CLAES N2O in section 4. In section 5 we compare the equivalent length from isentropic tracer simulations with the equivalent length from the 3-D CTM N2O. A summary of this work is presented in the final section.

2. MLM Diagnostics

[7] The modified Lagrangian-mean (MLM) diagnostics were introduced by Nakamura [1995, 1996], and we refer readers to these studies for full details. Only a brief outline of the diagnostics is given here.

[8] In the MLM framework the three-dimensional distribution of a long-lived tracer is decomposed onto isentropic layers, and the area enclosed by tracer contours on each isentropic surface is used to define an “equivalent latitude” $\phi_e$ which replaces the geographic latitude as the meridional coordinate ($\phi_e = \sin^{-1}(1 - A/2\pi a^2)$, where $A$ is the area enclosed by the contour and $a$ the Earth’s radius). The mixing on each isentropic surface is quantified by calculating the equivalent length $L_e$:

$$L_e^2(A,t) = \left| (\nabla q)^2 / (\partial q / \partial t)^2 \right| \tag{1}$$

where $q$ is the concentration of a tracer, $A$ is the area occupied by all tracer with concentration less (or greater, depending on the tracer’s pole-to-equator trend) than or equal to $q$, and $t$ is the average of any scalar around the tracer contour. $L_e$ is a measure of the geometric complexity of a contour Haynes and Shuckburgh [2000a] showed that the perimeter of the tracer contour is a lower bound for $L_e$. $L_e$ can be related to the efficiency of mixing on isentropic surfaces. A more complex geometric structure corresponds to larger stretching/slowing of tracer contours and greater mixing.

[9] Nakamura [1996] showed that a conserved tracer obeys the following two dimensional advection diffusion equation (in the area coordinate on an isentrope):

$$\frac{\partial}{\partial t} q(A,t) = \frac{\partial}{\partial A} \left( D L_e^2 \frac{\partial q}{\partial A} \right) \tag{2}$$

where $D$ is the constant microscale diffusion coefficient. From this it can be seen that the “effective horizontal diffusivity” is proportional to $L_e^2$, and hence $L_e^2$ is a measure of the efficiency of tracer transport across material isosurfaces. Mixing is large in regions where $L_e^2$ is large, and is weak where $L_e^2$ is small. Hence, relative maxima and minima in $L_e^2$ correspond to mixing regions and mixing barriers (weak mixing regions), respectively.

[10] In the following analysis we use the non-dimensional number

$$\xi = \ln(L_e^2 / L_0^2), \tag{3}$$

(where $L_0(\phi_e) = 2\pi a \cos \phi_e$ is the length of a zonal circle at latitude $\phi_e$) to diagnose the mixing properties of the real and modeled stratosphere. $\xi = 0$ for zonal tracer contours, and increases with the geometric complexity of the contour. Below we use large $\xi$ to identify regions of strong mixing and small $\xi$ to identify weak mixing (mixing barriers).

[11] The magnitude of $\xi$ depends on the resolution of the tracer field from which it was calculated, and so it is not possible to quantitatively compare the magnitudes of $\xi$ from data with differing horizontal resolution. This is the case here; the CLAES data and GSFC CTM differ in resolution. However, NM97 showed that spatial structure of $\xi$ and the use of $\xi$ to identify regions of strong or weak mixing are insensitive to data resolution. Thus it is possible to use $\xi$ to compare regions of strong/weak mixing between models and data of different resolution.

[12] $\xi$ can be calculated from the distribution of any conserved (or quasi-conserved) tracer that has near mono-
tonic meridional gradients. Nitrous oxide (N$_2$O) and methane (CH$_4$) are two long-lived stratospheric tracers with tropospheric sources and middle and upper stratospheric sinks. Both exhibit monotonically decreasing zonal mean isentropic distributions from equator to both poles, and can be mapped into the $\phi$ space in each hemisphere. Here we use the maximum tracer isopleth to define the equivalent equator, and calculate $\xi$ separately for isopleths north and south of this isopleth (see Ma [1999] for details).

3. UARS CLAES Measurements

[13] In this paper we use CLAES version 9 N$_2$O and CH$_4$ data. CLAES version 7 data was used in the previous MLM analysis of CLAES N$_2$O by NM97, and the differences in the MLM diagnostics between the two versions are minor.

[14] Full descriptions of the CLAES instrument and data are given by Roche et al. [1993, 1996]. CLAES instrument made measurements of N$_2$O and CH$_4$ from September 1991 to early May 1993. During this period CLAES provided near-continuous daily coverage of a single hemisphere (from 80 degrees in one hemisphere to 34 degrees in the other). The satellite was yawed to view the opposite hemisphere approximately every 36 days.

[15] Roche et al. [1996] compared CLAES measurements with correlative observations from instruments on other platforms. In the lower and middle stratosphere CLAES CH$_4$ has a systematic error of about 15% with CLAES biased high, and a random error of around 7%. The CLAES N$_2$O measurements have a lower systematic error with similar random errors. Roche et al. noted that the spatial and temporal correlation between N$_2$O and CH$_4$ is good, except at southern high latitudes in August–September 1992 and in the tropics. Also, initially there is a “bulge” in the concentration of both tracers in the tropics between 40 hPa and 20 hPa, which gradually disappears. The “bulge” is most likely due to contamination by the large aerosol loading from the eruption of Mt Pinatubo.

3.1. Comparison of $\xi$ From N$_2$O and CH$_4$

[16] Before examining the seasonal variation of $\xi$ from CLAES measurements, we examine the differences between $\xi$ calculated from the CLAES measurements of N$_2$O and CH$_4$. As both tracers are long-lived they should yield similar values of $\xi$ (as we intend to use $\xi$ as a diagnostic of mixing the calculated $\xi$ field should not be sensitive to tracer from which it is calculated).

[17] Figure 1 shows $\xi$ calculated from N$_2$O and CH$_4$ (together with the tracer fields) for two periods exactly a year apart (25–27 January 1992 and 1993). There is good agreement between $\xi$ from CH$_4$ and N$_2$O in 1993, but there are notable differences below about 750K in 1992. These differences are quantified in Figure 2, which shows the mean difference between $\xi$ calculated from N$_2$O and CH$_4$ at three isentropic surfaces. As shown below there are large spatial and temporal variations in the values of $\xi$, with the value varying between near zero to over three. In the middle and upper stratosphere (800K and 1000K) the differences are less than 0.5 for the complete data record, except perhaps for the first 2 months when there are slightly larger differences. At 600K there are large differences at the beginning of the data record, and these gradually decrease to values comparable with those found at the higher altitudes by the middle of the data record.

[18] The tracer contours in Figure 1 show large differences in January 1992 with suspicious features in the CH$_4$ distribution in the lower stratosphere (e.g., the local minimum in CH$_4$ around 600K in January 1992 distribution). This indicates that the large differences in $\xi$ in the lower stratosphere may be due to errors in the CH$_4$ data. Furthermore, the decay of the differences with time suggests that these errors are related to the elevated levels of sulfate aerosols following the eruption of Mt. Pinatubo. This is consistent with analysis of Roche et al. [1996], who noted the possible influence of a sulfate layer on the CLAES measurements and that CLAES CH$_4$ has a larger error than CLAES N$_2$O in the lower stratosphere.

[19] Because of the uncertainty in the CLAES measurements in the lower stratosphere during the early part of the data record and the larger errors in CH$_4$, we focus our analysis on $\xi$ from N$_2$O for the last year of data (i.e., April 1992 to March 1993). Note that the overall small difference between $\xi$ obtained from the two different tracers after the first 100 days adds to our confidence in utilizing the CLAES data to evaluate of the models.

3.2. Seasonal Evolution of $\xi$

[20] In NM97 potential temperature-equivalent latitude cross-sections of $\xi$ were examined for given dates. Here we focus on the temporal evolution of $\xi$ on isentropic surfaces. $\xi$ has been calculated on a range of isentropic surfaces covering lower to upper stratosphere. We focus on the evolution of $\xi$ on the 600K, 800K, and 1000K isentropic surfaces (approximately 24.5, 29, and 35 km). Unless otherwise stated $\xi$ is calculated from N$_2$O.

[21] Figure 3 shows the evolution of $\xi$ on the 600, 800, and 1000K surfaces over the last year of CLAES data. The contours are the zonal wind from the National Center for Environmental Prediction (NCEP) Climate Prediction Center (CPC) stratospheric analyses [Gelman et al., 1996]. These plots show pronounced regions of low $\xi$ (blue regions) and high $\xi$ (yellow-red regions) with strong seasonal variations. The seasonal evolution of these regions is similar in both hemispheres and on different isentropic surfaces. In midsummer there is low $\xi$ at low latitudes and high $\xi$ at high latitudes. (See Northern Hemisphere (NH) in July August and Southern Hemisphere (SH) in January in Figure 3; see also Plates 2a, 3a, 4d, and 5d of NM97). During later summer/fall the area of low $\xi$ at low latitudes decreases and at the same time another region of low $\xi$ develops at high latitudes (October in NH and April in SH). This region of low $\xi$ at the high latitudes becomes more pronounced in the winter and corresponds to the edge of the winter polar vortices, as can be seen from comparison with zonal winds. As the region of low $\xi$ at high latitudes develops, the area of subtropical low $\xi$ reduces to its minimal value and the midlatitude values of $\xi$ increase in magnitude. The winter hemisphere is then characterized by an area of high $\xi$ in midlatitudes between two regions of low $\xi$ (December–March in NH and June–September in SH in Figure 3; see also Plates 2d, 3d, 4a, and 5a of NM97). In spring, both regions of low $\xi$ move toward the pole, until the high latitude low $\xi$ completely disappears along with the polar night jet, and the hemispheric distribution of $\xi$ returns to the summer configuration.
Taking $\xi$ as indication of the strength of mixing [Nakamura, 1996] related the above seasonal variation of $\xi$ to the formation and destruction of mixing regions and mixing barriers. In particular, Figure 3 shows the fall formation and spring destruction of mixing barriers at the edge of the polar vortex. Also seen are a perennial barrier zone in the subtropics with seasonally varying meridional width [Plumb, 1996], strong mixing in wintertime midlatitude “surf zones” [McIntyre and Palmer, 1984], and strong mixing at summer high latitudes. The high values of $\xi$ in the summer, which are often larger than the winter surf zone values have also been diagnosed by others [Allen and Nakamura, 2001; Haynes and Shuckburgh, 2000a]. These are consistent with recent observational evidence of wave activity in the summer [e.g., Wagner and Bowman, 2000; Hoppel et al., 1999].

Figure 3 also reveals differences between the Arctic and Antarctic polar barriers. First, the mixing barrier at the edge of the Antarctic vortex (as indicated by the dark blue track in the high latitudes) appears and disappears in the upper stratosphere first, e.g., in April there are very low values of $\xi$ in southern high latitudes at 1000K but low $\xi$ are only starting to develop at 600K (see also Plates 3 and 5 of NM97). This top-down formation and decay of the polar barrier is not seen in the Northern Hemisphere. Second, the Antarctic polar barrier is generally further from the pole.
than the Arctic polar barrier, i.e., at 1000K the southern barrier is equatorward of $\phi_e = -50^\circ$ in August, whereas the northern barrier is always poleward of $\phi_e = -55^\circ$. Both these differences are climatological features of the vortices [Waugh and Randel, 1999].

4. GSFC 3-D Chemical Transport Model

4.1. Model Description

[24] We now examine tracers simulated by the GSFC 3-D chemical transport model (CTM) [Douglass and Kawa, 1999]. This off-line 3-D CTM includes a full chemistry module and constituents are transported using the advection scheme of Lin and Rood [1996]. The CTM is driven by winds and temperatures from recent versions of the Goddard Earth Observing System Data Assimilation System (GEOS DAS) [Schubert et al., 1993]. The vertical winds used in the CTM are calculated from the horizontal winds assuming mass continuity. The horizontal resolution is 2° latitude by 2.5° longitude, and there are 28 vertical levels between the surface and around 1 hPa. The vertical spacing is around 1.5 km up to 20 km and then gradually increases to around 2.7 km above 30 km.

[25] We have examined N$_2$O and CH$_4$ from two simulations. The “1997/1998 simulation” covers the period 18 March 1997 to 31 March 1998, whereas the “1998/1999 simulation” is for the period 7 October 1998 to 19 December 1999. The two simulations considered cover more than two years and therefore some year-to-year variation can be observed. The meteorological fields used in the two GSFC simulations are from different assimilation systems: The 1997/1998 simulation is driven by fields from the GEOS-1 assimilation; the 1998/1999 simulation is driven by fields from the GEOS-2 assimilation. There are many differences between the two assimilation systems. The GEOS-1 hybrid vertical grid contained 6 terrain following sigma levels at the bottom and 40 pressure surfaces above. GEOS-2 had 70 levels and used the terrain following sigma coordinate throughout the domain. The GEOS-1 analysis procedure was optimal interpolation [Schubert et al., 1995]. This was replaced by the physical space statistical analysis system in GEOS-2 [da Silva and Guo, 1996]. Hence some apparent year-to-year variations may be due to changes in the assimilation system.

[26] Comparisons between tracer observations and CTM results are a routine part of model evaluation for the three dimensional models [Rasch et al., 1995; Douglass et al., 1997]. Disagreement between observations and the CTM representation of such features as the horizontal gradients between the tropics and middle latitudes are readily apparent, and suggest deficiencies in the some combination of the mean circulation and horizontal and vertical mixing [Weaver et al., 1993, 2000]. Application of the equivalent length diagnostic as described in the following section provides a more quantitative assessment of the CTM horizontal mixing than can be achieved by such phenomenological comparisons as observed with modeled tracer gradients or seasonal cycles.

4.2. Equivalent Length Diagnostic

[27] Figures 4 and 5 show the evolution of $\xi$ calculated from the model N$_2$O from the 1997/1998 and 1998/1999 simulations. The $\xi$ fields are shown from April to March to aid comparison with the CLAES $\xi$. Comparison with Figure 3 reveals that the majority of the features in the CLAES $\xi$ are captured by both model simulations. Note because the resolutions of the CTM and CLAES N$_2$O differ, the magnitudes of $\xi$ from the CTM and CLAES cannot be quantitatively compared. $\xi$ from both model runs shows the development of polar barriers (minima in $\xi$ at high latitudes) in autumn and decay in late winter/early spring, with large mixing (large $\xi$) in the midlatitude surf zone during winter and at high latitudes during summer. They also show high $\xi$ inside the Antarctic polar vortex, and the movement of high $\xi$ to polar latitudes in the summer. Furthermore, in both simulations the Antarctic polar barrier forms and decays at upper levels before lower levels. The good agreement with the CLAES $\xi$ indicates that the isentropic mixing in the extratropical lower and middle stratosphere is realistic. There are, however, some areas of disagreement between $\xi$ calculated from simulated N$_2$O and that calculated from CLAES N$_2$O. Comparisons between $\xi$ calculated CH$_4$ show similar agreement and disagreement between the CTM simulations and the CLAES observations.

[28] Some of these differences are related to the different Arctic meteorology in the winters covered by the simulations, and not problems with the simulations themselves. First, there are differences in the strength of the Arctic polar barriers: These barriers are not as clear and consistent in $\xi$ from either GSFC simulation as in $\xi$ from CLAES N$_2$O. The largest difference is found in December 1998, when there is a
sudden and large increase in $\xi$ poleward of $\phi_e = 60^\circ$ at all levels (see Figure 5). These high values of $\xi$ closely follow the reversal of the polar jet winds, and correspond to the occurrence of a major sudden warming [e.g., Manney et al., 1999]. Low values of $\xi$ at high latitudes resume in January when the polar jet recovers from the warming, and there is a second increase in $\xi$ at high latitudes in late February/March 1999 when the final warming occurred. Although there was no major warming during the 1997/1998 winter this was also an active winter with a weak polar night jet and relatively high polar temperatures [Pawson and Naujokat, 1999]. Consistent with this there are frequent interruptions to the region of low $\xi$ at high latitudes in the 1997/1998 simulation.

In contrast, zonal winds during 1992/1993 winter show that the polar vortex persisted without a significant disturbance. [29] There are also differences in both hemispheres in the decay of the polar barriers. Although the low $\xi$ at high latitude from CLAES and the simulations increase rapidly in spring, the timing of this increase varies. CLAES data shows that the Southern Hemisphere (SH) transition from low to high $\xi$ at 600K occurred in December 1992 while the Northern Hemisphere (NH) transition occurred in April 1993. The corresponding transitions occur in mid-November and early April for the 1997/1998 simulation, and in mid-December and mid-March for the 1998/1999 simulation. Although not shown, the 1997/1998 simulation also

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**Figure 3.** Variation of $\xi$ from CLAES N$_2$O (color) and zonal wind from NCEP CPC analyses (contours) between April 1992 and March 1993, on the (a) 1000K, (b) 800K, and (c) 600K isentropic surfaces. The zonal wind is the average around $\phi_e$ contours calculated from NCEP potential vorticity data). See color version of this figure at back of this issue.
included the northern winter-summer transition for 1997 which occurred in early May. The above differences between observations and models are also due to the different years simulated. The transition from low to high $\xi$ at high latitudes corresponds to the breakdown of the polar vortex and the mixing barrier at its edge, and the above variations are consistent with the interannual variability in the timing of the breakup of the Antarctic and Arctic vortices [Waugh et al., 1999].

However, other differences are not so obviously due to the different years considered. In particular, there are differences during Northern Hemisphere summer. The simulations and CLAES all show high values at high latitudes, but whereas CLAES has low values south of 50N the simulations show regions of high $\xi$ south of 50N. In the 1997/1998 simulation the high values are confined to a narrow region around 30N, whereas in the 1998/1999 simulation there are high $\xi$ from the subtropics to the pole (at 1000K there is a narrow region of low $\xi$ around 40–50°N). Differences between simulations and CLAES are similar in character but smaller in magnitude during the southern summer.

Examination of the northern summer N$_2$O fields from the simulations and CLAES also reveals significant differences between the simulations and the CLAES data. The CLAES July 1993 data show strong N$_2$O meridional gradients around 30N, whereas the simulations have weak gradients particularly during July 1999 (Figure 6). The regions of high $\xi$ are also shown in Figure 6 (shading), and it can be seen that the higher values of $\xi$ occur where there are much weaker meridional N$_2$O gradients.

The higher $\xi$ in regions of weaker gradients shown in Figure 6 can be understood by considering that $L_x^2$ is equal to the ratio of small-scale ("local") variability in the tracer field ($\nabla q^2$) to the large-scale meridional gradient ($\partial q/\partial \lambda$). If there is comparable small-scale structure in the N$_2$O fields, the weaker meridional gradients result in enhanced values of $\xi$. The simulated N$_2$O fields exhibit comparable small-scale structure (Figure 7, left panels). So

![Figure 4.](image-url)
the differences in \( \xi \) in the northern summer appear to be related in the difference of the meridional gradients of N\(_2\)O. \[33\] It is not known whether the differences in N\(_2\)O gradients between the simulations and with CLAES are due to real interannual variability or due to differences in the assimilation procedures. Some interannual variability in the tropics and subtropics is expected because of the quasi-biennial oscillation (QBO) \cite{Shuckburgh et al. 2001} for an analysis of QBO induced variability in tropical and subtropical mixing using MLM diagnostics. However, July 1997 and 1999 are both in westerly phase of the QBO (and July 1992 is in easterly phase), so it does not appear that the

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5}
\caption{As in Figure 4 except for the 1998–1999 simulation. Note that the simulation was from October 1998 to December 1999, but for consistency with Figures 3 and 4 April to November 1999 and then December 1998 to March 1999 are shown. See color version of this figure at back of this issue.}
\end{figure}
QBO can explain all the differences between the 1997 and 1999 simulations.

[34] Figure 7 shows not only comparable small-scale structure in the simulated summer N2O summer fields, but also shows that there is a large amount of small-structure. Given that the large-scale gradients are weak this small-scale variability results in very large values of $\xi$. The small-scale structure (and hence large $\xi$) could be produced by quasi-horizontal mixing or by vertical advection on small horizontal scales (or by a combination of these processes). The vertical velocities used in the CTM show strong variability on small horizontal scales, suggesting that vertical advection on small horizontal scales does play a role. To examine this further we perform isentropic tracer calculations, as did Haynes and Shuckburgh [2000a, 2000b] and Allen and Nakamura [2001], and compare the resulting $\xi$ with that from the 3-D CTM.

5. Artificial Tracer Experiments

[35] We have performed a series of two-dimensional (2-D) transport calculations in which conserved tracers are advected with the same assimilated wind fields, advection scheme, and horizontal resolution as used in the 3-D CTM. Although the 3-D CTM uses hybrid-pressure as its vertical coordinate the 2-D simulations are done on isentropic surfaces. The tracer is initialized either as the sine function of geographic latitude, as did Haynes and Shuckburgh [2000a, 2000b] and Allen and Nakamura [2001], or as the N2O from the 3-D CTM. The resulting $\xi$ is nearly independent of the initial conditions (see Figure 8 below), and we focus on calculations initialized with the N2O field.

[36] Figure 9 shows the $\xi$ calculated from the 2-D tracer simulations on the 800K isentropic surface for (a) 1997/1998 and (b) 1998/1999. The results for the first month should be disregarded, (see Allen and Nakamura [2001] and Haynes and Shuckburgh [2000a] for discussions of dependence on initial conditions). The general structure and evolution of $\xi$ shown in Figure 9 agrees well with the $\xi$ from the 3-D CTM N2O (Figures 4b and 5b), and also the calculations of Haynes and Shuckburgh [2000a] and Allen and Nakamura [2001]. The $\xi$ fields from both 2-D and 3-D simulations show strong latitudinal and seasonal variations, with, for example, formation of polar barrier in fall and...
destruction in spring. However, there are differences between the 2-D and 3-D simulations in the summer hemisphere; these are most pronounced during northern summer.

The $\xi$ from the 2-D simulation of June–August 1997 has low values at polar latitudes, high values in middle to high latitudes, and low values in subtropics, whereas the $\xi$ from the 3-D CTM has high values at polar latitudes and subtropics. The differences are even larger in June–August 1999, where the 2-D $\xi$ has low values in middle latitudes as opposed to the high values in the 3-D $\xi$. These differences can be clearly seen in Figure 8 which shows the latitudinal variation of $\xi$ in mid-July for the various simulations. Note that Figure 8 also shows good agreement between the two 2-D simulations with different initial fields and between all simulations in the winter (southern) hemisphere.

The summer tracer fields from the 2-D and 3-D simulations show dramatic differences with regard to the small-scale horizontal variability. As shown in Figure 7, the fields from the 2-D simulation vary smoothly with little small-scale structure whereas the 3-D CTM N$_2$O fields contain many small-scale “blobs.” The lack of small-scale tracer structures in the isentropic simulations, and the strong variability of the vertical velocities on small horizontal scales indicate that the small-scale structures in the 3-D CTM N$_2$O are produced by vertical advection on small horizontal scales. It is unclear whether this vertical advection is an artifact of the vertical winds used in the CTM or due to real atmospheric motion. However, regardless of this, the formation of small horizontal scales and large values of $\xi$ in the CTM by vertical motion means that it is erroneous to attribute the large summer values of $\xi$ from the CTM N$_2$O to large scale quasi-horizontal mixing.

Although there is much less small-scale variability in the summer fields from the 2-D simulations there are still regions of high $\xi$ in the extratropics (see Figures 8 and 9). It is not clear that the high summer values of $\xi$ can be attributed to large horizontal mixing even in the 2-D calculations. As for the 3-D CTM calculations, these high $\xi$ tend to occur in regions with weak meridional gradients;
because of differences in the latitudes with very weak gradients the high summer $\xi$ are at different latitudes in the 2-D calculations. E. Shuckburgh and P. Haynes (Diagnosing transport and mixing using a tracer-based coordinate system, submitted to Physics of Fluids, 2001) have recently shown that the equivalent length calculation may not be robust when there are weak large-scale gradients. Also, calculations of $\xi$ from 2-D simulations using the same winds as above but a van Leer advection scheme \cite{van Leer1977} (as used by Allen and Nakamura \cite{Allen2001}) agree well with those in Figure 9 except during the summer, indicating that the summer values of $\xi$ are not robust. Finally, the $\xi$ in summer is larger than the values in the wintertime surf zone which, if $\xi$ is a diagnostic of quasi-horizontal mixing, implies that the mixing in the summer is as strong as that in the winter. This is not consistent with other diagnostics \cite[e.g., Waugh and Rong, 2002]{Waugh2002}. Taken together the above suggest that $\xi$ is not a robust diagnostic of quasi-horizontal mixing in the summer hemisphere.

6. Summary

[46] In this study, we have used the equivalent length ($\xi$) diagnostic to evaluate transport in the extratropical stratosphere of the NASA GSFC 3-D CTM. The $\xi$ can be calculated from tracer distributions without knowledge of the wind fields, and can be used to identify and quantify regions of strong mixing and weak mixing ("mixing barriers"). The $\xi$ has been calculated from $N_2O$ and $CH_4$ distributions from two different GSFC 3-D CTM simula-

Figure 8. Variation of $\xi$ with equivalent latitude for 2-D and 3-D simulations averaged over 10–20 July. Upper plot shows simulations of 1997 and lower plot of 1999.

Figure 9. Variation of $\xi$ from isentropic $N_2O$ simulation (color) and zonal wind from GEOS DAS(contours) on the 800K isentropic surface for (a) 1997/1998 and (b) 1998/1999. Compare with Figures 4b and 5b, respectively. See color version of this figure at back of this issue.
tions (March 1997 to March 1998; October 1998 to December 1999), and compared with the corresponding $\xi$ from CLAES observations of these long-lived tracers (for April 1992 to March 1993).

[41] The fact that the CLAES data are for a different period than the winds used in the GSFC 3-D CTM simulations complicates the comparisons as differences may be interannual variability, model deficiencies, measurement problems, or a combination of these. However, it is still possible to compare general features, and other studies and data can be used to provide some information on interannual variability.

[42] These comparisons indicate that the GSFC 3-D CTM realistically simulates the location and seasonal evolution of mixing regions and mixing barriers in the extratropical lower and middle stratosphere. The $\xi$ from CLAES and from both GSFC CTM simulations show the same development of polar barriers (minima in $\xi$ at high latitudes) in autumn and decay in late winter/early spring. Large values of $\xi$ in the midlatitude surf zone during winter indicate mixing. High $\xi$ from CTM fields and observations are found inside the Antarctic polar vortex, and the high $\xi$ values move to polar latitudes in the summer.

[43] However there are some differences. The strength and persistence of the region of low $\xi$ at northern high latitudes during winter, as well as the timing of the disappearance of these low $\xi$ in both Northern and Southern Hemisphere varies between simulations and observations. These differences appear to be due to interannual variability in the strength and persistence of the Arctic and Antarctic polar vortices rather than model deficiencies.

[44] There are also differences during northern summer. The CLAES data for June–August 1993 show high $\xi$ in high latitudes and low values south of 50$^\circ$N, whereas the 1997 simulation has a region of high $\xi$ around 30$^\circ$N and the 1999 simulation has high $\xi$ throughout the extratropics. These differences in $\xi$ are shown to be related to differences in the subtropical tracer gradients. The high values of $\xi$ in summer occur when small-scale structure is superimposed on weak large-scale meridional gradients, and the meridional gradients from the simulations are much weaker than observed by CLAES, particularly in the 1999 simulation. The cause of these differences in the large-scale meridional gradients is unclear, and may be due to problems with the GEOS winds or the CTM rather than actual interannual variability in atmosphere. Several previous studies have shown that CTMs driven by assimilated winds do not correctly simulate subtropical tracer gradients [Douglas et al., 1997; Chipperfield, 1999].

[45] The $\xi$ calculated from isentropic tracer calculations, using the same GEOS DAS wind fields and advection scheme as used in the 3-D CTM, agrees well with that from the CTM fields, except in the summer hemisphere. This casts doubt on whether the $\xi$ in summer, particularly that calculated from $N_2O$ fields, is a robust diagnostic of quasi-horizontal mixing. Comparisons between the isentropic and 3-D calculations indicate that the small-scale structure in the 3-D CTM $N_2O$ fields is produced by variability in the vertical motions on small horizontal scales. This variability in the vertical motion may be a model artifact, but even if it is the fact that small-scale structure produced by vertical motion contributes to the large values of $\xi$ means that the summer high values of $\xi$ from $N_2O$ do not necessarily imply strong isentropic mixing.

[46] Although there are issues with the interpretation of the values in the summer hemisphere, calculations of $\xi$ from $N_2O$ and other tracers are useful for evaluation of transport in three dimensional models, in that values can be directly compared with those calculated from observations from UARS or other satellites.

[47] Acknowledgments. We thank K. Yeh for assistance with the 2-D Lin-Rood advection code. This work was supported by the NASA Atmospheric Chemistry and Modeling Program.


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Figure 1. Potential temperature and equivalent latitude cross section of \( \xi \) from CLAES measurements: (a) \( \text{N}_2\text{O} \) during 25–27 January 1992, (b) \( \text{N}_2\text{O} \) during 25–27 January 1993, (c) \( \text{CH}_4 \) during 25–27 January 1992, (d) \( \text{CH}_4 \) during 25–27 January 1993. Contours show average true isopleths in equivalent latitude space.
Figure 3. Variation of $\xi$ from CLAES N$_2$O (color) and zonal wind from NCEP CPC analyses (contours) between April 1992 and March 1993, on the (a) 1000K, (b) 800K, and (c) 600K isentropic surfaces. The zonal wind is the average around $\phi_e$ contours calculated from NCEP potential vorticity data.)
Figure 4. As in Figure 3 except $\xi$ from GSFC CTM simulation and zonal wind from GOES DAS for March 1997 to March 1998.
Figure 5. As in Figure 4 except for the 1998–1999 simulation. Note that the simulation was from October 1998 to December 1999, but for consistency with Figures 3 and 4 April to November 1999 and then December 1998 to March 1999 are shown.
Figure 9. Variation of $\xi$ from isentropic N$_2$O simulation (color) and zonal wind from GEOS DAS (contours) on the 800K isentropic surface for (a) 1997/1998 and (b) 1998/1999. Compare with Figures 4b and 5b, respectively.