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Evaluation of the transport in the GSFC 3D chemical transport model using the "Equivalent Length" diagnostic.

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Abstract.
Transport and mixing in the extratropical stratosphere of the NASA GSFC 3D chemical transport model (CTM) is evaluated using the modified Lagrangian-mean diagnostic. The normalized equivalent length squared (ξ) has been calculated from simulated N_2O and CH_4 distributions using two different wind data sets and 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 CTMs 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 CTMs show regions of high ξ in the extratropics that are not observed in ξ from CLAES. These high values occur where there is small-scale variability in N_2O in regions with very weak meridional gradients. Comparison of ξ from isentropic tracer simulations using the same wind fields as used in the 3D CTM show good agreement except during the summer. The isentropic tracers do not have as much small-scale variability as the 3D CTM tracer fields, indicating that the enhanced small-scale structures in the CTM N_2O, and high values of ξ, are produced by small-scale horizontal variability in the vertical motions. The fact that vertical motions can influence summer values of ξ means that care needs to be applied when interpreting these ξ fields in terms of isentropic mixing.

1. Introduction

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.

The recently developed modified Lagrangian-mean (MLM) analysis of *Nakamura* [1995, 1996] provides such diagnostics. Within this framework the equivalent length is defined to provide a measure of the geometric complexity of tracer contours. Equivalent length can be used identify mixing regions and barriers to transport (see next section for further discussion). The equivalent length can be calculated directly from a tracer distribution without knowledge of the wind field, and can be calculated from either observed or simulated fields. 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 isentropic simulations of passive, artificial tracer [*Haynes and Shuckburgh,* 2000a, 2000b; *Allen and Nakamura* 2001; *Shuckburgh et al.*, 2001].

In this paper, we use the equivalent length diagnostic to evaluate the transport in the NASA Goddard Space Flight Center (GSFC) 3D 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 those 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 N_2O 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 3D CTM simulations. Unfortunately, the CLAES data are for a different

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period (September 1991 to May 1993) than the winds used in the GSFC 3D CTM simulations (1997 to 1999), which complicates the comparison as differences may be due interannual variability rather than model deficiencies. However, the CLAES data is the only multi-year dataset with daily hemispheric coverage of long-lived tracers, and this coverage is needed for the calculation of the equivalent length. (*Lingenfelser and Grose* [2002] have recently calculated the equivalent length from HALOE observations of CH_4 using analyzed potential vorticity fields to form daily hemispheric fields. It may be possible to use this equivalent length data for further model evaluations.)

To determine the role of vertical motions in producing features in the tracer and equivalent length fields we also perform two-dimensional (2D) 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 source of the winds and the advection scheme are the same as that in the GSFC 3D CTM, so comparisons between the 2D and 3D simulations isolates the role of vertical motions.

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 calculation from CLAES measurements of N_2O and CH_4. The equivalent length of N_2O from GSFC CTM simulations is then analyzed and compared with that from CLAES N_2O in section 4. In Section 5 we calculate the equivalent length from isentropic tracer simulations, and compare with the equivalent length from the 3D CTM N_2O. A summary of this work is presented in the final section.

2. MLM diagnostics

The modified Lagrangian-mean (MLM) diagnostics used in this study 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.

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" ϕ_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 then quantified by calculating the equivalent length L_e

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

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 $(\hat{\cdot})$ 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), and can be related to the efficiency of mixing on isentropic surfaces. A more complex geometric structure corresponds to larger stretching / folding of tracer contours and greater mixing.

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

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

where D is the constant microscale diffusion coefficient. From this it can seen that the "effective horizontal diffusivity" is proportional to L_e^2, and hence L_e^2 is a measure of the efficiency of cross-mass transport of tracer. 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.

In the following analysis we use the non-dimensional number

$$\xi = \ln(L_e^2/L_0^2), \qquad (3)$$

(where $L_0(\phi_e) = 2\pi a \cos\phi_e$, is the length of a zonal circle at latitude ϕ_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 ξ to identify regions of strong mixing and small ξ to identify weak mixing (mixing barriers).

The magnitude of ξ 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 ξ 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 ξ, and in particular the identification of regions with strong or weak mixing, is insensitive to data resolution, and so it is possible to use ξ to compare regions of strong/weak mixing between models and data of different resolution.

ξ can be calculated from the distribution of any conserved (or quasi-conserved) tracer that has monotonic meridional gradients. Nitrous oxide (N_2O) and methane (CH_4) are two long-lived stratospheric tracers with tropospheric sources and middle and upper stratospheric sinks. As a result, both exhibit monotonically decreasing zonal mean isentropic distributions from equator to both poles, and can be mapped into the ϕ_e space in each hemisphere. Here we use the maximum tracer isopleth to define the equivalent equator, and calculate ξ separately for isopleths north and south of this isopleth (see *Ma* [1999] for details).

3. UARS CLAES measurements

In this paper we use CLAES version 9 N_2O and CH_4 data. CLAES version 7 data was used in the previous MLM analysis of CLAES N_2O by NM97, and the differences in the MLM diagnostics between the two versions are minor.

A full description of the CLAES instrument and data is given in *Roche et al.* [1993] and *Roche et al.* [1996], and the data are only briefly discussed here. The CLAES instrument made measurements of N_2O and CH_4 (and other trace constituents) 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.

Roche et al. [1996] compared CLAES measurements with non-satellite measurements. 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_2O measurements have a lower systematic error with similar random errors. *Roche et al.* noted that the spatial and temporal correlation between N_2O 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. These initial differences are most likely due to contamination by the large aerosol loading from the eruption of Mt Pinatubo.

3.1. Comparison of ξ from N_2O and CH_4

Before examining the seasonal variation of ξ from CLAES measurements, we examine the differences between ξ calculated from the CLAES measurements of N_2O and CH_4. As both tracers are long-lived they should yield similar values of ξ (as we aim to use ξ as a diagnostic of mixing the calculated ξ field should not be sensitive to tracer from which it is calculated).

Plate 1 shows ξ calculated from N_2O and CH_4 (together with the tracer fields) for two periods exactly a year apart (January 25-27, 1992 and 1993). There is good agreement between ξ from CH_4 and N_2O in 1993, but there are notable differences at low altitudes in 1992. These differences are quantified in Figure 1, which shows the mean difference between ξ calculated from N_2O and CH_4 at three isentropic surfaces. (As shown below there are large spatial and temporal variations in the values of ξ, with the value varying between near zero to over three.) In the middle and upper stratosphere (800K and 1000K) the differences are of similar magnitude (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 the higher altitudes by the middle of the data record.

The tracer contours in Plate 1 show large differences in January 1992 with suspicious features in the CH_4 distribution in the lower stratosphere (e.g., local minimum in CH_4 around 600 K in January 1992 distribution). This indicates that the large differences in ξ in the lower stratosphere may be due to errors in the CH_4 data. Furthermore, the decay of the differences with time indicates 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 to the CLAES measurements and that CLAES CH_4 has a larger error than CLAES N_2O in the lower stratosphere.

Because of the uncertainty in the CLAES measurements in the lower stratosphere during the early part of the data record and the larger CH_4 errors, we focus our analysis ξ from N_2O for the last year of data (i.e. April 1992 to March 1993). Note that the overall small difference between ξ obtained from the two different tracers, after the first 100 days, adds to our confidence of utilizing the CLAES data to evaluate of the models.

3.2. Seasonal evolution of ξ

In NM97 potential temperature – equivalent latitude cross-sections of ξ were examined for given dates, whereas here we focus on the temporal evolution of ξ on isentropic surfaces. ξ has been calculated on a range of isentropic surfaces covering lower to upper stratosphere. We focus here on the evolution of ξ on the 600K, 800K, and 1000K isentropic surfaces (approximately 24.5, 29, and 35 km). Unless otherwise stated ξ is calculated from N_2O.

Plate 2 shows the evolution of ξ on the 600, 800, and 1000K surfaces over the last year of CLAES data. Also shown (contours) is 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 ξ (blue regions) and high ξ (yellow-red regions), which have strong seasonal variations. The seasonal evolution of these regions is similar in both hemispheres and on different isentropic surfaces. In mid-summer there is low ξ in low latitudes and high ξ in high latitudes, see northern hemisphere (NH) in July-August and southern hemisphere (SH) in January in Plate 2 (see also Plates 2a, 3a, 4d, and 5d of NM97). During late summer / fall the area of low ξ at low latitudes decreases and at the same time another region of low ξ develops at high latitudes (October in NH and April in SH). This region of low ξ at the high latitudes becomes more pronounced in the winter and, as can be seen from comparison with the zonal winds, corresponds to the edge of the winter polar vortices. As the region of low ξ at high latitudes develops, the area of subtropical low ξ reduces to its minimal value and the mid-latitude values of ξ increase in magnitude. The winter hemisphere is then characterized by an area of high ξ in mid-latitudes between two regions of low ξ (December-March in NH and June-September in SH in Plate 2; see also Plates 2d, 3d, 4a, and 5a of NM97). In spring, both regions of low ξ move toward the pole, until the high latitude low ξ completely disappears (along with the polar night jet) and the hemispheric distribution of ξ returns to the summer configuration.

Nakamura 1996], the above seasonal variation of ξ can be related to the formation and destruction of mixing regions and mixing barriers. In particular, Plate 2 show the formation and destruction of mixing barriers at the edge of the polar winter in fall and spring, respectively, together with a perennial barrier zone in the subtropics with seasonally varying meridional width [*Plumb* 1996], and strong mixing in wintertime mid-latitude "surf zones" [*McIntyre and Palmer* 1984] as well as at summer high latitudes. The high values of ξ 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], and are consistent with recent observational evidence of wave activity in the summer [e.g. *Wagner and Bowman* 2000, *Hoppel et al.,* 2001]. Plate 2 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 ξ in southern high latitudes at 1000K but low ξ are only starting to develop at 600K. 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 1000 K the southern barrier is equatorward of $\phi_e = -50°$ in August, whereas the northern barrier is always poleward of $\phi_e = 55°$. Both these differences are climatological features of the vortices [*Waugh and Randel* 1999].

Plate 2 also indicates different origins for polar barriers in the upper and lower stratosphere, especially in the southern hemisphere. At 600 K the Antarctic polar barrier (low ξ)

first appears in the polar region, then moves equatorward to $\phi_e = -45°$ in late June, and then moves back towards the pole during September, and finally disappears by the end of November. At 1000K, the mid-latitude mixing zone (high ξ) is interrupted around April, and a second transport barrier (region of low ξ) originates in the subtropics and merges with the developing polar barrier. This dual origin of the polar barrier may also take place at 800K but it is clear because of the missing data in May.

4. GSFC 3D chemical transport model

4.1. Model description

We now examine tracers simulated by the GSFC 3D chemical transport model (CTM) [*Douglass and Kawa*, 1999]. This off-line 3D 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 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).

We consider N_2O from two simulations. The "1997/98 simulation" covers the period 18 March 1997 to 31 March 1998, whereas the "1998/99 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. Unfortunately, the meteorological fields used in the two GSFC simulations are from different assimilation systems: The 1997/98 simulation is driven by fields from the GEOS-1 assimilation, whereas 1998/99 simulation is driven by fields from the GEOS-2 assimilation. There are many differences between the two assimilation systems, including different vertical co-ordinates (GEOS-1 used 46 vertical hybrid pressure levels with six sigma levels at the bottom, whereas GEOS-2 used 70 terrain-following sigma levels) and different analysis procedure (optimal interpolation was used GEOS 1 whereas physical-space statistical analysis was used in GEOS-2) [*Shubert et al.*, 1995, *da Silva and Guo*, 1996]. Hence some apparent year-to-year variations may be due to changes in the assimilation system.

4.2. Equivalent length diagnostic

Plates 3 and 4 show the evolution of ξ calculated from the model N_2O from the 1997/98 and 1998/99 simulations. The ξ fields are shown from April to March to aid comparison with the CLAES ξ. Comparison with Plate 2 reveals that the majority of the features in the CLAES ξ are captured by both model simulations. (Note because the resolutions of the CTM and CLAES N_2O differ the magnitudes of ξ from the CTM and CLAES cannot be quantitatively compared.) ξ from both models show the development of polar barriers (minima in ξ at high latitudes) in autumn and decay in late winter / early spring, with large mixing (ξ) in the mid-latitude surf zone during winter and at high latitudes during summer. They also show high ξ inside the Antarctic polar vortex, and the movement of high ξ 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 ξ indicates that the isentropic mixing in the extratropical lower and middle stratosphere is realistic. There are, however, some areas of disagreement between ξ calculated from simulated and CLAES N_2O.

Some of these differences are related to the different winters, with differing Arctic meteorology, covered by the simulations, and not problems with the simulations. First, there are differences in the strength of the Arctic polar barriers: These barriers are not as clear and consistent in ξ from either GSFC simulation as in ξ from CLAES N_2O. The largest difference occurs in December 1998, where there a sudden and large increase in ξ poleward of $\phi_e = 60^o$ at all levels (see Plate 4). These high values of ξ 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 ξ at high latitudes resume in January when the polar jet recovers from the warming, but there is a second increase in ξ at high latitudes in late February / March 1999 when the final warming occurred. Although there was no major warming during the 1997/98 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 ξ at high latitudes in the 1997/98 simulation. In contrast, zonal winds during 1992/93 winter show that the polar vortex persisted without a significant disturbance.

There are also differences in both hemispheres in the decay of the polar barriers. Although the low ξ 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 ξ at 600 K 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 1997/98 simulation, and in mid-December and mid-March for the 1998/99 simulation. Although not shown, the 1997/98 simulation also included the northern winter-summer transition for 1997 which occurred in early May. The above model-data differences are also due to the different years simulated. The transition from low to high ξ 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].

Other differences are, however, 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 ξ south of 50N. In the 1997/98 simulation the high values are confined to a narrow region around 30N, whereas in the 1998/99 simulation there are high ξ from the subtropics to the pole (at 1000K there is a narrow region of low ξ around 40-50°N). There is also less dramatic difference between simulations and CLAES in the southern summer.

Examination of the northern summer N_2O 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_2O meridional gradients around 30N, whereas the simulations, and in particular July 1999, have only weak gradients, see Figure 2. The regions of high ξ are also shown in Figure 2 (shading), and it can be seen that the higher values of ξ occur where there are much weaker meridional N_2O gradients. It therefore appears that the differences in the large-scale N_2O are contributing to the differences in ξ.

The higher ξ in regions of weaker gradients shown in Figure 2 can be understood by considering that L_e^2 is equal to the ratio of small-scale ('local') variability in the tracer field ($|\hat{\nabla} q|^2$) to the large-scale meridional gradient ($(\partial q/\partial A)^2$). So if there is comparable small-scale structure in the N_2O fields, the existence of weaker meridional gradients results in enhanced values of ξ. Examination of the simulated N_2O fields shows comparable small-scale structure in the simulations, see Figure 3. So the differences in ξ in the northern summer appear to be related in the difference of the meridional gradients of N_2O.

It is not known whether the differences in N_2O gradients between the simulations and 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) (see *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, so it does not appear that the QBO can explain all the differences between the 1997 and 1999 simulations.

Figure 3 shows not only comparable small-scale structure in the simulated summer N_2O summer fields, but also shows that there is a large amount of small-structure. Given that the large-scale gradients are weak this large small-scale variability will result in very large values of ξ. The small-scale structure (and hence large ξ) could be produced by quasi-horizontal mixing or by vertical advection on small horizontal scales (or by a combination of these processes). Examination of 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 in *Haynes and Shuckburgh* [2000a,b] and *Allen and Nakamura* [2001], which have no vertical advection and compare the resulting ξ with that from the 3D CTM.

5. Artificial tracer experiments

We have performed a series of two-dimensional (2D) transport calculations in which conserved tracers are advected with isentropic winds. We use the same assimilated wind fields, advection scheme, and horizontal resolution as used in the 3D CTM. The tracer is initialized as either as the sine function of geographic latitude, as in *Haynes and Shuckburgh* [2000a, 2000b] and *Allen and Nakamura* [2001], or as the N_2O from the 3D CTM. The resulting ξ is very similar between the calculation using different initial conditions (see Figure 4 below), and we focus on calculations initialized with the N_2O field.

Plate 5 shows the ξ calculated from the 2D tracer simulations on the 800K isentropic surface for (a) 1997/98 and (b) 1998/99. The results for the first month should be disregarded, see [*Allen and Nakamura*, 2001] and [*Haynes and Shuckburgh*, 2000] for discussions of dependence on initial conditions. The general structure and evolution of ξ shown in Plate 5 agrees well with the ξ from the 3D CTM N_2O (Plates 3b and 4b) (and also the calculations of *Haynes and Shuckburgh* [2000a] and *Allen and Nakamura* [2001]): the ξ fields from both 2D and 3D simulations show strong latitudinal and seasonal variations, with, for example, formation of polar barrier in fall and destruction in spring. There are however differences between the 2D and 3D simulations in the summer hemisphere (and in particular the northern summer).

ξ from the 2D simulation of June-August 1997 has low values at polar latitudes, high values in mid- to high latitudes, and low values in subtropics, whereas the ξ from the 3D CTM has high values at polar latitudes and subtropics. The differences are even larger in June-August 1999, where the 2D ξ has low values in middle latitudes as opposed to the high values in the 3D ξ. These differences can be clearly seen in Figure 4 which shows the latitudinal variation of ξ in mid-July for the various simulations. Note that Figure 4 also shows good agreement between the two 2D simulations with different initial fields and between all simulations in the winter (southern) hemisphere.

Comparisons of the summer tracer fields from the 2D and 3D simulations show dramatic differences with regard to the small-scale horizontal variability. As shown in Figure 3, the fields from the 2D simulation vary smoothly with little small-scale structure whereas the 3D CTM N_2O fields contain many small-scale "blobs". The lack of small-scale tracer structures in the isentropic simulations (together with the strong variability of the vertical velocities on small horizontal scales) indicates that the small-scale structures in the 3D CTM N_2O are produced by vertical advection on small horizontal scales. It therefore may be erroneous to attribute the large summer values of ξ from the CTM N_2O to large quasi-horizontal mixing.

Although there is much less small-scale variability in the summer fields from the 2D simulations there are still regions of high ξ in the extratropics (see Plate 5 and Figure 4). As for the 3D CTM calculations, these high ξ tend to occur in regions with weak meridional gradients. However, the high summer ξ are at different latitudes in the 2D calculations because of differences in the meridional gradients (and in particular the latitudes with very weak gradients) between the two types of calculation.

Given that the high summer values occur in region of weak gradients it is not clear that, even in the 2D calculations, they can be attributed to large horizontal mixing. *Shuckburgh and Haynes* [2002] have recently shown that the equivalent length calculation may not be robust when there are weak gradients. Furthermore, calculations of ξ from 2D simulations using the same winds as above but a van Leer advection scheme [*van Leer*, 1977] (as used by *Allen and Nakamura* [2001]) agree well with those in Plate 5 except during the summer, indicating that the summer values of ξ are not robust.

6. Summary

In this study, we have used the equivalent length (ξ) diagnostic to evaluate transport in the extratropical stratosphere of the NASA GSFC 3D CTM. ξ 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"). ξ has been calculated from N_2O and CH_4 distributions from two different GSFC 3D CTM simulations (March 1997 to March 1998; October 1998 to December 1999), and compared with the corresponding ξ from CLAES observations of these long-lived tracers (for April 1992 to March 1993).

These comparisons indicate that the GSFC 3D CTM realistically simulates the location and seasonal evolution of mixing regions and mixing barriers in the extratropical lower and middle stratosphere. ξ from CLAES and from both GSFC CTM simulations show the same development of polar barriers (minima in ξ at high latitudes) in autumn and decay in late winter / early spring, with large mixing (ξ) in the mid-latitude surf zone during winter. They also show high ξ inside the Antarctic polar vortex, and the movement of high ξ to polar latitudes in the summer.

However there are some differences. There strength and persistence of the region of low ξ at northern high latitudes during winter, as well as the timing of the disappearance of these low ξ 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.

There are also differences during northern summer. The CLAES data for June-August 1993 show high ξ in high latitudes and low values south of 50N, whereas the 1997 simulation has a region of high ξ around 30N and the 1999 simulation has high ξ throughout the extratropics. These differences in ξ appear to be related to differences in the subtropical tracer gradients. The high values of ξ in summer occur when small-scale structure is superimposed on weak large-scale meridional gradients, and there are large difference in the meridional gradients between the different simulations and CLAES (with very weak gradients 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.

Isentropic tracer simulations, using the same GEOS DAS wind fields and advection scheme as used in the 3D CTM, do not produce as much small-scale structure in the summer, indicating that the small-scale structure in the 3D CTM N_2O fields is produced by variability in the vertical motions on small horizontal scales. ξ calculated from the 2D tracer simulations agrees well with that from the CTM fields, except in the summer hemisphere.

The fact that vertical motions can influence ξ means that care needs to be applied when interpreting these ξ fields in terms of isentropic mixing, i.e., the summer high values of ξ from N_2O may not imply strong isentropic mixing. However, calculations of ξ from N_2O (or other tracers) are still very useful for evaluation of three dimensional models, as the values can be directly compared with those calculated from observations (from UARS or future satellites).

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Figure 1. Temporal variation of mean difference of equivalent length between CLAES N_2O and CH_4, on the 600, 800, and 1000K isentropic surfaces.

Figure 2. Potential temperature - equivalent latitude cross section of N_2O mixing ratio (contours in ppb) and high values of ξ (shaded regions) for July 17 from (a) 1997 simulation, (b) 1999 simulation, and (c) CLAES 1992 measurements. The shaded regions correspond to regions with ξ greater than 2.0 for the simulations and 1.5 for the observations.

Figure 3. Contour plots of 800 K fields for N_2O from 3D CTM simulations of (a) 17 July 1997 and (b) 17 July 1999, and isentropic simulations of (c) 17 July 1997 and (d) 17 July 1999. Contour interval is 5 ppb.

Figure 4. Variation of ξ with equivalent latitude for 2D and 3D simulations averaged over 10-20 July. Upper plot shows simulations of 1997 and lower plot of 1999.

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Plate 1. Potential temperature and equivalent latitude cross section of ξ from CLAES measurements: (a) N_2O during January 25-27, 1992, (b) N_2O during January 25-27, 1993, (c) CH_4 during January 25-27, 1992, (d) CH_4 during January 25-27, 1993. Contours show average true isopleths in equivalent latitude space.

Plate 2. Variation of ξ from CLAES N_2O (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 ϕ_e contours calculated from NCEP potential vorticity data).

Plate 3. As in Plate 2 except ξ from GSFC CTM simulation and zonal wind from GOES DAS for March 1997 to March 1998.

Plate 4. As in Plate 3 except for the 1998-1999 simulation. Note that the simulation was from October 1998 to December 1999, but for consistency with Plates 2 and 3 April to Nov 1999 and then December 98 to March 99 are shown.

Plate 5. Variation of ξ from isentropic N_2O simulation (color) and zonal wind from GEOS DAS(contours) on the 800 K isentropic surface for (a) 1997/1998 and (b) 1998/1999. Compare with Plates 3(b) and 4(b) respectively.