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Intercomparison between Lagrangian and Eulerian simulations of the development of mid-latitude streamers as observed by CRISTA

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Abstract. During the CRISTA-1 mission three pronounced fingerlike structures reaching from the lower latitudes to the mid-latitudes, so-called streamers, were observed in the measurements of several trace gases in early November 1994. A simulation of these streamers in previous studies employing the KASIMA (Karlsruhe Simulation Model of the Middle Atmosphere) and ROSE (Research on Ozone in the Stratosphere and its Evolution) model, both being Eulerian models, show that their formation is due to adiabatic transport processes. Here, the impact of mixing on the development of these streamers is investigated. These streamers were simulated with the CLaMS model (Chemical Lagrangian Model of the Stratosphere), a Lagrangian model, using N_2O as long-lived tracer. Using several different initialisations the results were compared to the KASIMA simulations and CRISTA (Cryogenic Infrared Spectrometer and Telescope for the Atmosphere) observations. Further, since the KASIMA model was employed to derive a 9-year climatology, the quality of the reproduction of streamers from such a study was tested by the comparison of the KASIMA results with CLaMS and CRISTA. The streamers are reproduced well for the Northern Hemisphere in the simulations of CLaMS and KASIMA for the 6 November 1994. However, in the CLaMS simulation a stronger filamentation is found while larger discrepancies between KASIMA and CRISTA were found especially for the Southern Hemisphere. Further, compared to the CRISTA observations the mixing ratios of N_2O are in general underestimated in the KASIMA simulations. An improvement of the simulations with KASIMA was obtained for a simulation time according to the length of the CLaMS simulation. To quantify the differences between the simulations with CLaMS and KASIMA, and the CRISTA observations, the probability density function technique (PDF) is used to interpret the tracer distributions. While in the PDF of the KASIMA simulation the small scale structures observed by CRISTA are smoothed out due to the numerical diffusion in the model, the PDFs derived from CRISTA observations can be reproduced by CLaMS by optimising the mixing parameterisation. Further, this procedure gives information on small-scale variabilities not resolved by the CRISTA observations.

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1 Introduction

While the transport of air masses from the troposphere into the stratosphere occurs mainly in the tropics (Holton et al., 1995) the exchange in the stratosphere between the mid-latitudes and the tropics is hindered by a subtropical transport barrier (e.g. Trepte et al., 1993; Plumb, 1996). However, observations of long-lived chemical compounds and analyses of conserved meteorological quantities such as Ertel's potential vorticity (Ertel, 1942) indicate that some transport between the mid-latitudes and the tropics does occur in the form of so-called streamers (e.g. Waugh, 1993; Randel et al., 1993). These streamers are pronounced fingerlike structures which reach from the lower latitudes into the mid-latitudes. Streamers have been identified at all altitudes from the tropopause to the middle stratosphere. Waugh (1993, 1996) showed that these streamers are linked to disturbances of the polar vortex caused by planetary wave activity. A rather pronounced streamer caused by large planetary-wave activity and the associated vortex displacement was observed during the CRISTA-2 mission in the Southern Hemisphere (Riese et al., 2002).

The CRISTA instrument was flown first during the CRISTA-1 mission on board the Space Shuttle from 4 to 12 November 1994 (Offermann et al., 1999; Riese et al., 1999a). During the CRISTA-1 mission in early November 1994 three streamers were observed (Offermann et al., 1999; Riese et al., 1999b). Two of the observed streamers were located in

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the Northern Hemisphere while the third was located in the Southern Hemisphere. The three pronounced streamers observed by the CRISTA experiment on 6 November 1994 were simulated previously by Riese et al. (1999b) and Kouker et al. (1999) employing Eulerian models, the ROSE and the KASIMA model, respectively. Eyring et al. (2003) employed the KASIMA model nudged with ECMWF analyses in T42 resolution and the coupled chemistry-climate model ECHAM4.L39(DLR)/CHEM (E39/C) to establish streamer climatologies. They derived a 9-year climatology (1990-1998) with each of both models by counting all streamer events between 21 and 25 km. By comparing the streamer climatologies derived with the KASIMA model and the E39/C model they showed that both climatologies were qualitatively in agreement and that in both models the highest streamer frequencies occurred in the Northern Hemisphere in winter. The aim of the study by Eyring et al. (2003) was to use the KASIMA model, driven by ECMWF meteorological analysis, as a reference to check the abilities and deficiencies of E39/C with respect to the temporal and spatial distribution of streamers in the model.

Here, we employ the CLaMS model (McKenna et al., 2002a,b) to test the quality of reproduction of streamers in the results of the KASIMA model. This is done in the frame of a specific case study for which CRISTA observations are available to perform a model validation. Thus, we focus on the streamers observed by CRISTA in early November 1994. We compare the results of the 9-year model run and two short term sensitivity runs of KASIMA obtained for the streamers on 6 November 1994 with the results obtained with CLaMS for the same date. In this way, an intercomparison between Eulerian and Lagrangian simulations of the development of mid-latitude streamers will be given here. Further, we establish a link between the pure model study of Eyring et al. (2003) and the CRISTA observations which allows to discuss to which extent the simulated streamers in the climatology are supported by observations. Finally, we calculate probability density functions (PDF) of the N_2O fields measured by CRISTA and simulated by the CLaMS and KASIMA model. These PDF's are used to quantify differences between the different model types (Eulerian and Lagrangian), differences due to different model resolutions used in KASIMA (T42 and T106) and differences between the derived model fields and CRISTA measurements. However, differences between KASIMA and CLaMS are also expected due to the fact that the vertical coordinate of the two models are different.

2 Model descriptions

2.1 The Chemical Transport Model KASIMA

The KASIMA model is a global circulation model including stratospheric chemistry for the simulation of the behaviour of physical and chemical processes in the middle atmosphere (Reddmann et al., 2001; Ruhnke et al., 1999a). The meteorological component is based on a spectral architecture with the pressure altitude $z=-H\ln(p/p_0)$ as vertical coordinate where H=7 km is a constant atmospheric scale height, p is the pressure, and p_0=1013.25 hPa is a constant reference pressure. The meteorology module of the KASIMA model consists of three versions: the diagnostic model, the prognostic model and the nudged model which combines the prognostic and diagnostic model (Kouker et al., 1999).

For the simulation of the streamers observed by CRISTA on 6 November 1994 the nudged model version is used. In this version, the model is nudged towards the ECMWF re-analyses (ERA-15, until 1994) and operational analyses thereafter. A correction is solely applied to the temperature field after integrating the primitive equations in the prognostic model. That is, the calculated temperature is nudged towards the ECMWF analysed temperature using a Newtonian cooling like algorithm. The setup of the nudging coefficient is taken from the experience obtained from sensitivity studies (Kouker et al., 1999). A horizontal resolution of T42 ($2.8°\times2.8°$) and 63 vertical levels between 10 and 120 km altitude with a resolution of 750 m in the middle stratosphere are used. The model is initialised in 1990 with an atmosphere at rest and a barotropic temperature field taken from the U.S. Standard Atmosphere (1976). The model runs continuously until 1998. In the KASIMA model an idealised tracer representing stratospheric N_2O is transported by the model winds. The tracer has a source region in the equatorial lower stratosphere and a loss through photolysis depending on altitude and solar zenith angle only (Eyring et al., 2003). The KASIMA transport algorithm is formulated as a two step flux corrected algorithm (Zalesak, 1979). A first order upwind scheme from Courant et al. (1962) is used which is followed by an antidiffusive step based on the difference between the scheme of Lax and Wendroff (1960) and the first order scheme multiplied by a limiter function given by Roe and Baines (1982).

2.2 The Chemical Lagrangian Model CLaMS

The CLaMS model is a chemistry transport model which simulates the dynamics and chemistry of the atmosphere along trajectories of multiple air parcels (McKenna et al., 2002a,b). Trajectories are calculated using a fourth-order Runge-Kutta scheme (Sutton et al., 1994) with a 30-min time step. Here, wind fields were taken from the United Kingdom Meteorological Office (UKMO) Stratosphere-Troposphere Data Assimilation System (Swinbank and O'Neill, 1994). The UKMO data have a meridional and zonal resolution of 2.5° and 3.75°, respectively. The vertical coverage is from 1000 to 0.316 hPa with 22 quasi-logarithmic levels. Analyses are available every day at 12:00 UT.

The mixing of different air masses, that means the interaction between neighbouring air parcels, is introduced by both combining air parcels and adding new air parcels under

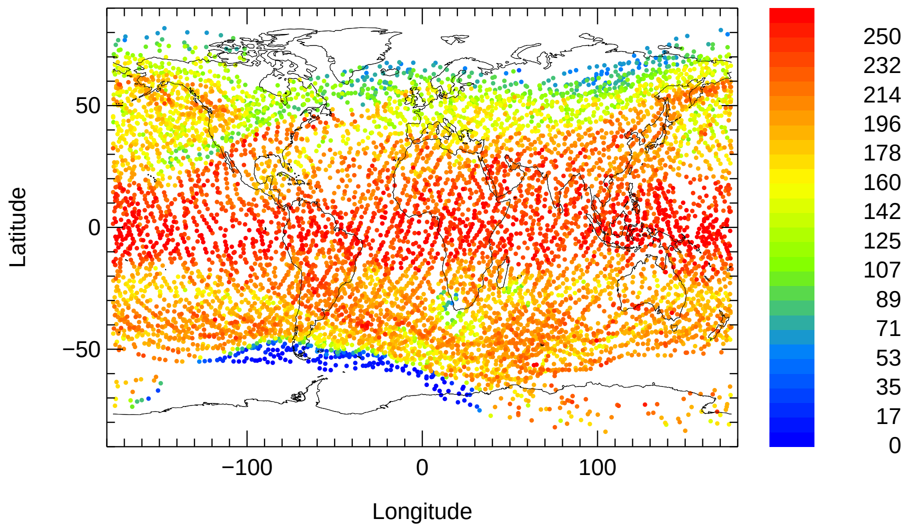

Fig. 1. CRISTA observations of N_2O between 4 November 1994, 21:00 UT and 6 November 1994, 12:00 UT at Θ=675±25 K transformed to a synoptic time (6 November 12:00 UTC) by trajectory calculations.

certain conditions determined by the deformation of the flow (McKenna et al., 2002b; Konopka et al., 2003). The intensity of mixing is controlled by the Lyapunov exponent λ for a given spatial resolution r_0 and a given mixing time step Δt. The Lyapunov exponent is a measure of the deformation rate of the horizontal wind field and switches on mixing in the flow regions where λ exceeds the critical Lyapunov exponent λ_c, that is, in flow regions for which the deformation of the flow is strong enough (Konopka et al., 2003). The CLaMS simulations suggest a temporally and spatially inhomogeneous mixing in the lower stratosphere with a lateral (across the wind) effective diffusion coefficient of the order of $10^3 m^2 s^{-1}$. Optimised mixing parameters were deduced as an mixing time step of Δt=24 h and a critical Lyapunov exponent λ_c ranging between 0.8 and 1.2 d^{-1} by Konopka et al. (2003) from the comparison of simulations of CLaMS with spatially highly resolved ER-2 observations. However, we will show below that if coarsely resolved satellite data is considered the best results are obtained with slightly different mixing values of λ_c=1.5 d^{-1} and Δt=12 h as recently discussed in Konopka et al. (2005) for the simulation of CRISTA observations.

3 CRISTA observations

CRISTA is a limb scanning instrument which measures the thermal emission (4–71 μm) of 15 trace gases, and of aerosols and clouds. CRISTA has a high spatial resolution in all three dimensions (typically 6° in longitude, 3° in latitude and 2 km vertical). The horizontal distance of two adjacent measurement points is about 200 km along the flight track and 650 km across the flight track. The CRISTA-1 mission was conducted from 4–12 November 1994 and the CRISTA instrument was launched aboard the NASA Space Shuttle "Atlantis" into a 300 km, 57° orbit. The CRISTA instrument was mounted on the CRISTA Shuttle Pallet Satellite (SPAS) platform which operates at a distance of 20–100 km behind the shuttle. Several different photochemically active gases like O_3, $ClONO_2$, HNO_3, NO_2, N_2O_5 as well as the long-lived tracers CFC-11, N_2O and CH_4 have been measured (Offermann et al., 1999; Riese et al., 1999a). Here, we focus on the CRISTA measurements of N_2O. The systematic and statistical errors are 26% and 3%, respectively, at 25 km and 23% and 3.5%, respectively, at 30 km (Version 3 data). A description of the CRISTA error analysis can be found in Riese et al. (1999a).

The N_2O distribution on the 675±25 K isentropic surface observed by CRISTA on 6 November 1994 is shown in Fig. 1. Here, asynoptic profiles observed between 4 November and 6 November were transformed to the synoptic time on 6 November, 12:00 UTC, by using isentropic forward trajectories. The 675±25 K level has been chosen since at this level streamers are most pronounced. The measurements show a typical distribution with high N_2O mixing ratios in the tropics and low mixing ratios towards the polar regions. The southern hemispheric polar vortex is noticeable as a region with very low mixing ratios centered near 70° W and 60° S due to the strong descent of air masses inside the polar vortex.

At mid-latitudes, the N_2O distribution exhibits three narrow tongues (streamers) showing tropical values of N_2O in the mid-latitude regions. Two of these three streamers are located in the Northern Hemisphere while the third one is located in the Southern Hemisphere. The first streamer is originating at about 120° W, 30° N pointing northeast to about

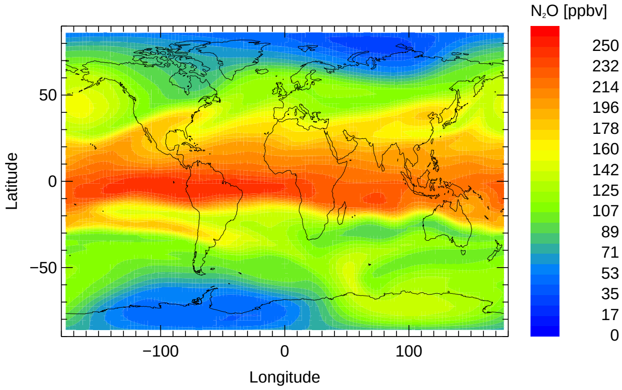

Fig. 2. Result of the KASIMA 9-year run for the 6 November 1994.

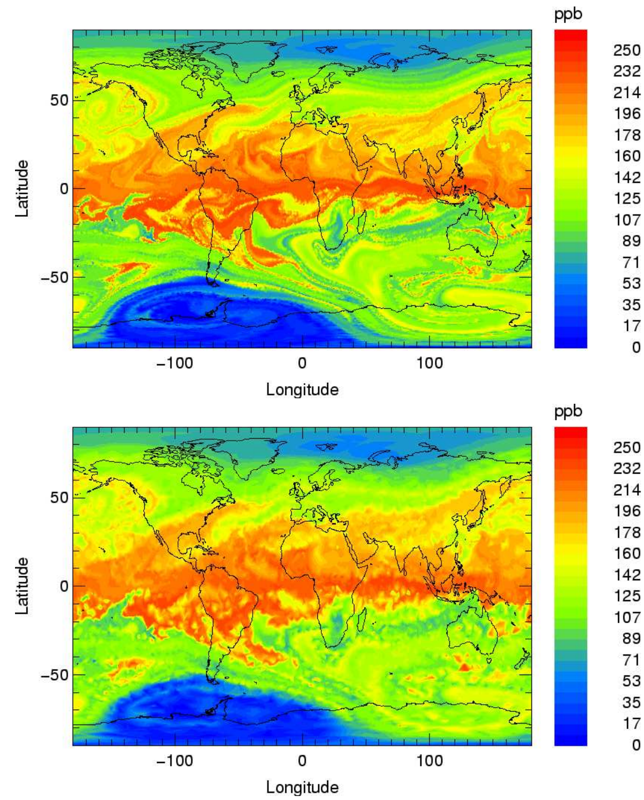

Fig. 3. CLaMS simulation with high resolution (top) and low resolution (bottom) for the 6 November 1994 (Table 1, case B). The CLaMS simulation was initialised on 20 October 1994 with KASIMA model results (Θ=675 K).

0° E, 60° N while the second one is originating at about 90° E, 30° N pointing northeast to about 180° E, 60° N. The southern hemispheric streamer is originating at 90° W, 20° S pointing southeast to about 20° E, 45° S. Following Offermann et al. (1999) these three streamers will hereinafter referred to as the (1) Atlantic streamer, (2) the east Asian streamer, and (3) the Southern Hemisphere streamer. The Southern Hemisphere streamer, however, is much weaker pronounced than those in the Northern Hemisphere as can be observed in the weak gradient of N_2O.

4 Model simulations

4.1 Model setup of the CLaMS simulations

To obtain a meaningful comparison of the results of CLaMS and KASIMA, the CLaMS simulation was initialised with the results of the 9-year run of KASIMA (Eyring et al., 2003). That is, both model simulations start with the same initial conditions. The CLaMS simulation was initialised for 20 October and was run until 6 November 1994. The simulation time of 17 days should be sufficient to investigate the influence of mixing processes on the N_2O distribution and on the development of streamers, since this length of simulation time is about the time scale where mixing processes become important (Konopka et al., 2005).

We also performed simulations with a shorter simulation time (8 days, not shown) initialising the CLaMS simulation on 29 October; the date used by Kouker et al. (1999) for their KASIMA simulations. In general, with both the 8-day and 17-day simulation, similar results were achieved. In the shorter run (8 days) the three streamers are already distinguishable. However, in the longer model run (17 days) a more distinctive filamentation is found showing that the longer run is on a time scale which is more suitable for studying mixing processes as already stated in Konopka et al. (2005).

The CLaMS simulations were made on an isentropic level of $\Theta=675$ K negelecting diabatic effects, using UKMO data to drive the model, an mixing time step of $\Delta t=24$ h and a Lyapunov exponent of $\lambda=1.2$ (in-situ optimised mixing, (Konopka et al., 2003)). The isentropic level of $\Theta=675$ K ($\approx$27 km) was chosen since N_2O is a good dynamical tracer at this level. Further, the streamers are most pronounced at these altitudes in the CRISTA measurements (Offermann et al., 1999; Riese et al., 1999b; Kouker et al., 1999). While in the CLaMS simulation around 50 000 air parcels are used, in the KASIMA simulation only 8000 grid boxes per level are used. To allow an assessment of the impact of the spatial resolution of the model simulations to KASIMA, the simulation of CLaMS was repeated with a resolution corresponding to KASIMA (approximately 8000 air parcels).

4.2 Comparison of CLaMS and KASIMA results

The results of the KASIMA (T42) model calculations derived for the 6 November 1994 are shown in Fig. 2 and the results of the CLaMS calculation (17 days) for the same day in Fig. 3. The low resolution simulation with CLaMS (approximately 8000 air parcels) corresponds to the T42 simulation

Table 1. Mixing time steps and critical Lyapunov exponents used for the CLaMS simulations initialised with KASIMA.

Case	Δt, h	λ_c, d^{-1}	mixing intensity
A	24	2.0	reduced
B	24	1.2	in-situ optimised
C	12	1.5	satellite optimised
D	6	1.2	enhanced

of KASIMA (Fig. 3, bottom panel) while the high resolution simulation (approximately 50 000 air parcels) has a considerably greater spatial resolution. Both models reproduce the two northern hemispheric streamers, the Asian and the Atlantic streamer, well. However, in the CLaMS simulation the streamers are much more distinctive than in the simulation with KASIMA (Fig. 2).

The conditions in the Southern Hemisphere are not well reproduced by KASIMA. Significant differences between the KASIMA model results (Fig. 2) and the CRISTA measurements (Fig. 1) are evident. The location of the Southern Hemisphere streamer is not well reproduced by the KASIMA model. A possible explanation of this failure may be found in the weak pronounced features of the streamer in the CRISTA data. Small errors in KASIMA e.g. in the reproduction of the residual circulation may lead to errors in the N_2O distribution in the polar vortex that in turn may affect the gradients in the streamers. This issue is known and has already been discussed in detail by Kouker et al. (1999). However, an overall correctness of the residual circulation in KASIMA has been shown in Ruhnke et al. (1999b) and Reddmann et al. (2001).

Further, using the low resolution model simulation of CLaMS (approximately 8000 air parcels) which is corresponding to the KASIMA resolution, the streamers are, as in the high resolution simulation, much more pronounced in the CLaMS simulation. In general, in the CLaMS simulation a much greater filamentation is simulated even in the simulation with the low resolution. Further, the elongated extension of the Atlantic streamer which spun up the globe measured by CRISTA is simulated in both CLaMS simulations, with high and low resolution, but not with KASIMA.

Both model simulations show high N_2O values in the region centered around 140° W and 50° N. This appears to be in an anticylconic circulation, which is likely part of the planetary wave event that caused the east Asian streamer. Further, both models show a swirling pattern centered near 120° E and 70° S which appears to be associated to the anticyclone that was involved in the development of the Southern Hemisphere streamer.

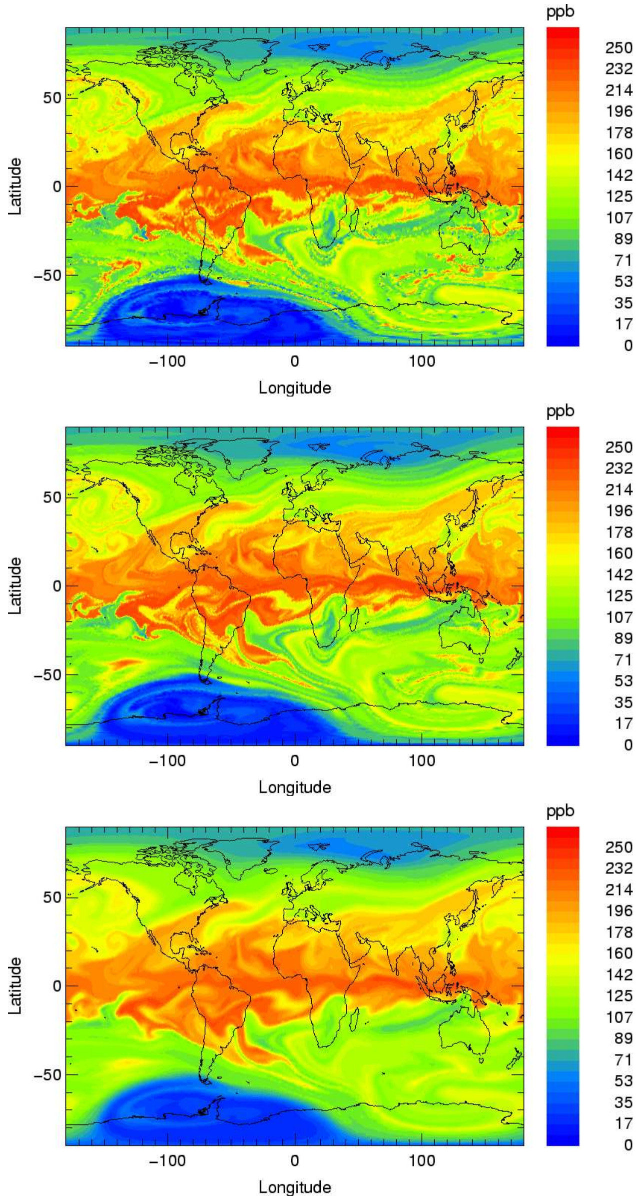

Fig. 4. CLaMS simulations with different mixing intensities for the 6 November 1994 initialised on 20 October 1994 (Θ=675 K) with KASIMA. Reduced mixing (top, case A), satellite optimised mixing (middle, case C) and enhanced mixing (bottom, case D).

4.3 Influence of different mixing parameterisations on the development of streamers within ClaMS

The influence of different mixing parameterisations on the filamentary structure in chemical tracer fields in CLaMS was previously investigated by Konopka et al. (2003). For a more precise estimation of the influence of the mixing parameterisation on the formation of the streamer the CLaMS simulations for the initialisation on 20 October 1994 (17 day model run, approximately 50 000 air parcels) were repeated using different mixing intensities, that is, different mixing

Table 2. Mixing time steps and critical Lyapunov exponents used for the CLaMS simulations initialised with CRISTA.

Case	Δt, h	λ_c, d^{-1}	mixing intensity
A	24	1.2	in-situ optimised
B	12	1.5	satellite optimised
C	6	1.2	enhanced

time steps and critical Lyapunov exponents (Konopka et al., 2003). The mixing intensity was once stronlgy reduced and once strongly enhanced. Further, we use the mixing values proposed by Konopka et al. (2005) for the simulation of coarsely resolved satellite data like the CRISTA observations (Section 2.2). Thus, the following configurations of the mixing parameterisation are used: strongly reduced (Δt=24 h, λ_c=2.0 d^{-1}), satellite optimised (Δt=12 h, λ_c=1.2 d^{-1}) and strongly enhanced (Δt=6 h, λ_c=1.2 d^{-1}). An overview of the employed mixing time steps and critical Lyapunov exponents are given in Table 1.

The simulations with different mixing time steps and Lyapunov exponents shows that the intensity of mixing in the CLaMS model has no significant influence on the formation of the streamers (Fig. 4). Thus, the formation of the streamers is primarily caused by large-scale advection of air masses out of the tropics (Riese et al., 1999b) corroborating the conclusions of the model studies by Kouker et al. (1999) and Eyring et al. (2003). However, in the Southern Hemisphere some differences become noticeable. For example, with increasing mixing intensity in the model, the structures are smoothed and some of the smaller filaments disappear. This is similarly observed in the Northern Hemisphere but to a somewhat smaller degree.

4.4 Comparison of the simulations with CRISTA measurements

The comparison of the KASIMA model results with CRISTA shows an underestimation of the KASIMA N_2O values in general, especially in the Southern Hemisphere (Figs. 1 and 2). The simulated gradients in the Southern Hemisphere are too strong in the subtropics (about 20° S) and too weak at the edge of the polar vortex. Since the CLaMS simulations were initialised with the KASIMA distribution on 20 October these features are also found in the CLaMS result (Figs. 3 and 4). The location and the spatial extent of the Atlantic and east Asian streamer are well reproduced by KASIMA. However, the location and spatial extent of the Southern Hemisphere streamer is not well reproduced. The differences between the N_2O mixing ratios simulated by KASIMA and the N_2O mixing ratios measured by CRISTA are possibly due to the simplified N_2O chemistry in the KASIMA model. However, comparisons are limited by uncertainties of the N_2O measurements of CRISTA (Riese et al., 1999a).

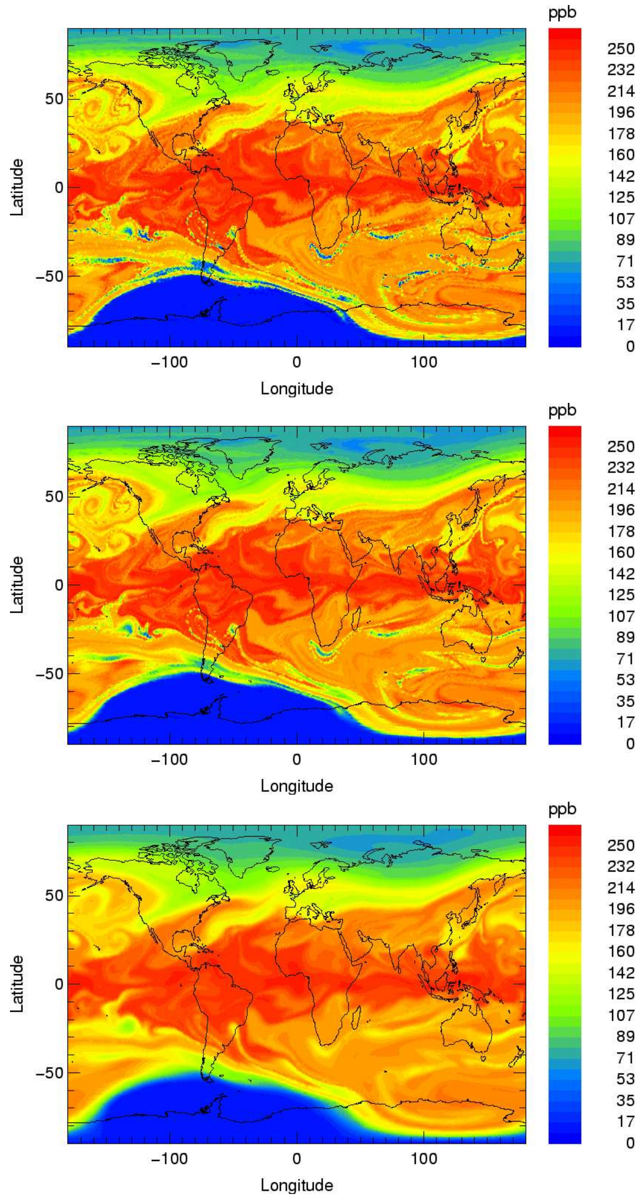

Fig. 5. CLaMS simulations with different mixing intensities for the 6 November 1994 initialised on 20 October 1994 with PV/N_2O correlation (Θ=675 K) derived from the CRISTA observations. In-situ optimised mixing (top, case B), satellite optimised mixing (middle, case C) and enhanced mixing (bottom, case D).

4.4.1 CLaMS simulation initialised with a N_2O-PV correlation from CRISTA observations

To improve the comparison of the model results with the CRISTA observations the CLaMS model was initialised with a N_2O-PV correlation which was deduced from the CRISTA data (McKenna et al., 2002a). The simulation was started on 20 October 1994 with a high spatial resolution (approximately 50 000 air parcels). To investigate the influence of mixing processes on the formation of the streamer, as in the previous section, different mixing time steps and critical Lyapunov exponents were used for the simulations (Table 2): in-situ optimised mixing (Δt=24 h, λ_c=1.2 d^{-1}), satellite optimised mixing (Δt=12 h, λ_c=1.5 d^{-1}) and enhanced mixing (Δt=6 h, λ_c=1.2 d^{-1}).

The results of the simulation show that the simulated N_2O mixing ratios are greater for this simulation than for the simulation using the results of the KASIMA 9-year run as initialisation (Fig. 5). The simulated N_2O values are in good agreement with the CRISTA observations. The observed gradients in the Southern Hemisphere are well reproduced by CLaMS. Even some vortex remnants in the mid-latitudes characterised by low N_2O values were reproduced. However, in the CLaMS simulation some filaments are present which were not measured by CRISTA. This may be due to the fact that the spatial resolution of the CLaMS simulation is higher than the resolution of CRISTA. CRISTA has a resolution of 200 km×650 km while in the CLaMS simulation a resolution of r_0=100 km was used.

The simulations with different mixing time steps and Lyapunov exponents are not significantly different from each other. However, some differences occur in the Southern Hemisphere. Small filaments which are partly evident in the CRISTA measurement disappear due to the enhanced intensity of mixing (Table 2, case C). The best agreement with the CRISTA observations was achieved with an mixing time step of Δt=12 h and a Lyapunov exponent of λ_c=1.5 d^{-1} (satellite optimised case).

4.5 Impact of different meteorological analyses on CLaMS results

In the present study, KASIMA is driven by ECMWF analyses and CLaMS by UKMO analyses. To investigate in how far differences in the KASIMA and CLaMS simulations are caused by differences in the employed meteorological analyses, we conducted CLaMS simulations driven by ECMWF (ERA-40) analyses for case B (Table 1) initialised with the results of the 9-year run of KASIMA (Fig. 6, top panel) and initialised with a N_2O-PV correlation from CRISTA (Fig. 6, bottom panel). The CLaMS simulations were initialised on 20 October 1994 and were run until 6 November 1994.

The results based on ECMWF and UKMO analyses show similar structures. However, there are some differences in the details of the simulated filamentary patterns, that are particularly noticeable for the Southern Hemisphere. Nonetheless, the use of different meteorological analyses is not the major cause for the differences between CLaMS and KASIMA simulations.

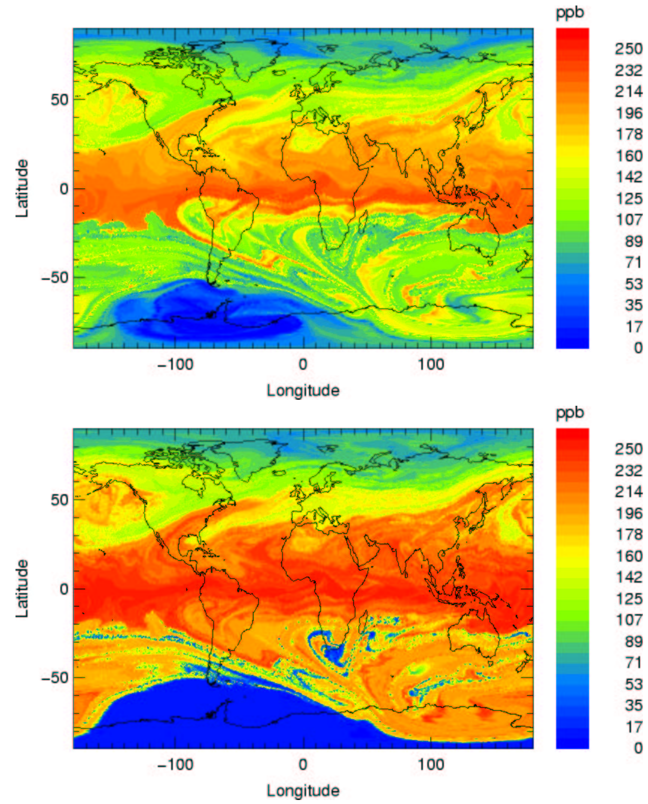

Fig. 6. CLaMS simulations for the 6 November 1994 driven by ECMWF analyses to study the impact of different meteorolgical analyses on CLaMS results. The CLaMS simulations were initialised on 20 October 1994. Top panel: As Fig. 3, top panel, but CLaMS driven by ECMWF analyses instead of UKMO analyses. Bottom panel: As Fig. 5, top panel, but CLaMS driven by ECMWF analyses instead of UKMO analyses.

4.6 Impact of spatial resolution and temporal coverage on KASIMA results

To assess the impact of the spatial resolution of the KASIMA model on the model results, the simulations were repeated using a resolution of T42 and T106 (2.8°×2.8° and 1.125°×1.125° (250×250 km and 110×110 km), roughly corresponding to 8000 and 50.000 air parcels (with a resolution of 250 km and 100 km), respectively). For these simulations the model was initialised with an atmosphere at rest and a barotropic temperature field taken from the U.S. Standard Atmosphere (1976) at 15 October 1994. As in the previous KASIMA simulations the nudging technique is used. The model is nudged to the ECMWF re-analyses (ERA-40, see chapter 2.1). The N_2O field was initialised by an idealised tracer representing stratospheric N_2O which is transported by the model winds. The tracer has a source region in the equatorial lower stratosphere (equator-wards of 15 latitude and at altitudes below 100 hPa) and a prescribed photoly-

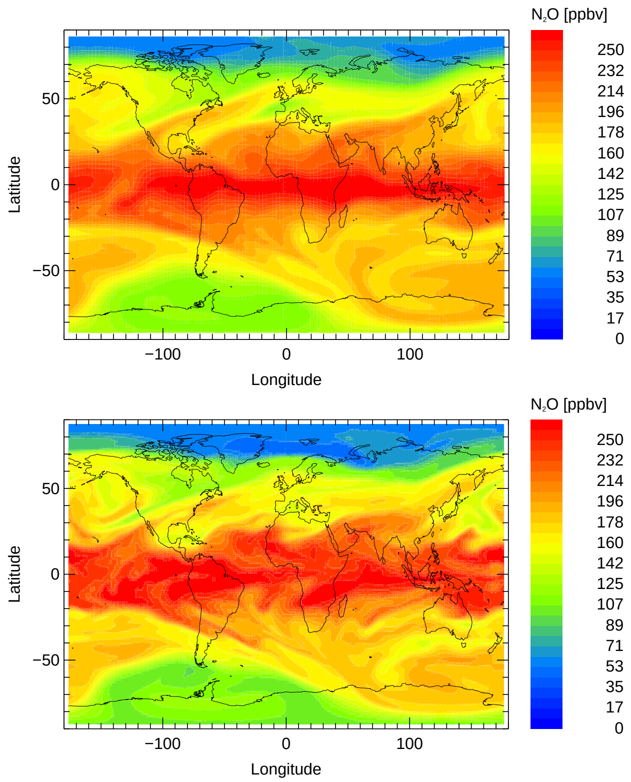

Fig. 7. KASIMA simulations for T42 (top) and T106 (bottom) resolution for the 6 November 1994 initialised on 15 October 1994.

sis coefficient depending on altitude and zenith angle only (Eyring et al., 2003). From many experiments it has been shown, that this combination of meteorological and chemical initialisation reveals a 3-d distribution of N_2O after several days typically observed in the lower stratosphere. A simulation time of 20 days was used, thus allowing a three day model spin up before the 17 day simulation period for which CLaMS and KASIMA are being compared.

In general, with these KASIMA simulations a better agreement with the CRISTA observations was found for both the Southern and Northern Hemisphere (Fig. 7). In the Northern Hemisphere the elongated extention of the Atlantic streamer which spun up the globe is now reproduced by KASIMA. Further, the location of the Southern Hemisphere streamer is now better simulated though there is still a slight displacement. The absolute values of the N_2O mixing ratios are better reproduced, except in the Southern Hemisphere at the location of the polar vortex where the KASIMA values are too high. In the T106 simulation more spatial structure and a stronger filamentation is found compared to the T42 simulation. However, some structures, like the Atlantic streamer, are smeared out.

4.7 Probability density functions (PDFs) of the observed and the simulated N_2O distributions

The study of the PDFs (probability density functions) of tracer differences between APs (air parcels) separated by a prescribed distance offers an effective way to analyse the variability of tracer distributions (e.g. Sparling, 2000; Hu and Pierrehumbert, 2001, 2002). In turbulent flows, anomalously high probability of extreme spatial concentration fluctuations, termed "intermittency", is expected and, consequently, the corresponding PDFs are characterised by a Gaussian core and non-Gaussian tails (e.g. Shraiman and Siggia, 2000). Konopka et al. (2005) used this technique to quantify the statistics of N_2O variability both in CRISTA observations and in CLaMS simulations, and to determine the critical flow deformation and thus the critical Lyapunov exponent in CLaMS that triggers the mixing algorithm in CLaMS. Here, we apply this method in order to quantify the differences between the CRISTA observations and the simulations carried out with the Eulerian model KASIMA and the Lagrangian model CLaMS.

The PDFs on the 675 K isentropic surface are calculated for all pairs of grid points separated by distances between 100 and 300 km and, owing to the limited coverage of the CRISTA observations, with latitudes between 60° S and 70° N. By numbering the APs (air parcels) from north to south, only pairs with $i<j$ are considered to avoid double counting (thus, the PDFs are not necessarily symmetric). The PDFs were calculated for the time period of the CRISTA campaign (4–12 November 1994) and the results are shown in Fig. 8, where the CLaMS PDFs are obtained from the simulated N_2O-distributions initialised either from the KASIMA distribution (top panel) or from the PV/N_2O-correlation deduced from CRISTA observations (bottom panel). The PDFs were also calculated for the KASIMA simulations initialised on 15 October 1994 using both a T42 and a T106 resolution. However, for the KASIMA T42 simulation only 25% of the distances between the next neighbours achieved the prescribed distance of 100 and 300 km making thus the statistic unusable. Therefore, only the PDF for the KASIMA T106 simulation is shown in Fig. 8 (top panel). For this configuration, about 85% of the distances between the next neighbours vary between 100 and 300 km with lowest and highest values in the tropics and polar regions, respectively (note that this meridional bias is not present in the PDFs derived from the CLaMS distributions). In principle, the form of a PDF is not scale independent, that is it is not independent of the spatial resolution of the model in question (Hu and Pierrehumbert, 2001). However, Konopka et al. (2005), have shown (in their Fig. 6) that only a weak increase occurs in the width of the PDFs for a fourfold increase in the CLaMS model resolution. Therefore this issue can be neglected in our further discussion here.

The PDF derived from CRISTA observations (gray thick line in both panels of Fig. 8) is characterised by a Gaussian core, that is most likely due to instrumental precision, and non-Gaussian tails, the so-called "fat tails", indicating an anomalously high probability of events with steep N_2O gradients. These strong gradients occur mainly at the edges of the polar vortices and across streamers, filaments and vortex remnants which were sampled by CRISTA. The tails of the PDF derived from the KASIMA distributions are steeper (i.e. more Gaussian) than the CRISTA observations. This indicates that numerical diffusion in the KASIMA model smoothes out the small-scale structures with strong tracer gradients observed by CRISTA.

The PDFs derived from the CLaMS simulations of the N_2O-distribution strongly depend on the choice of the mixing parameters. The tails of these PDFs are most pronounced in the run with a reduced mixing intensity and are increasingly smoothed out for higher mixing intensities. The satellite optimised configuration approximates fairly well the PDF derived from CRISTA whereas the CLaMS distributions obtained with the in-situ optimised and enhanced mixing parameterisation over- and underestimate the observed N_2O variability, respectively. Even the CLaMS simulation with enhanced mixing shows slightly more pronounced PDF tails, thus, higher N_2O variability than the KASIMA simulation. In the lower panel of Fig. 8, the same kind of sensitivity study is shown carried out for the N_2O variability in CLaMS by initialising the model with CRISTA observations. The satellite optimised configuration approximates the PDF obtained from CRISTA better than the N_2O distribution derived with in-situ optimised mixing. Further, the PDFs derived from CLaMS simulations driven by ECMWF analyses (not shown) are very similar to those derived from the CLaMS simulations driven by UKMO analyses.

As Konopka et al. (2005) argued, physical structures with scales smaller than the horizontal and vertical weighting functions of CRISTA (about 200 km and 2 km, respectively) are smoothed out in the observations ("optical mixing"). Indeed, Sparling and Bacmeister (2001) have shown that the width of PDFs derived from in-situ observations increases with the spatial resolution of the data. Therefore, the CRISTA observations may underestimate the true atmospheric variability of N_2O, i.e. the tails in the corresponding PDFs are expected to be more pronounced in reality and may therefore better agree with the PDF obtained from the in-situ optimised simulation.

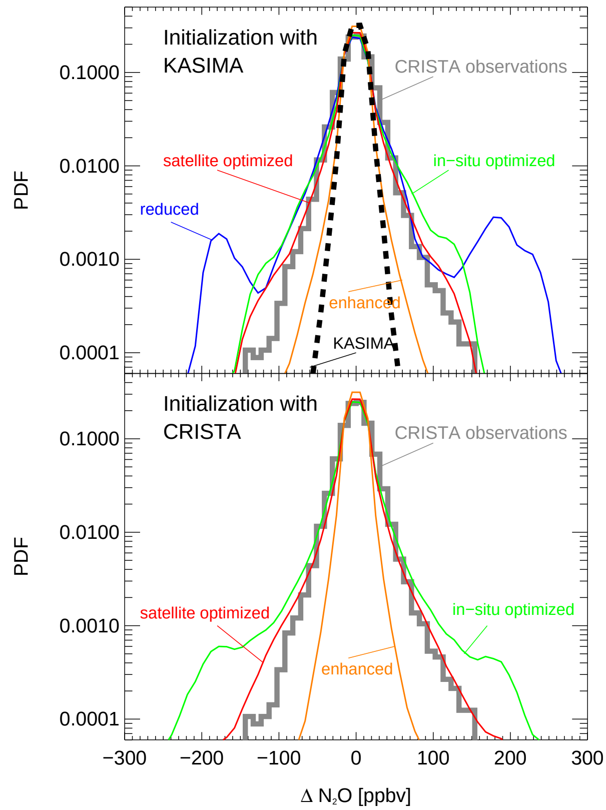

Fig. 8. PDFs of N_2O distribution on Θ=675 K observed by CRISTA (gray solid line) and calculated from the KASIMA (black dotted line) and CLaMS simulations using different mixing parameterisations (enhanced mixing (orange), in-situ optimised mixing (green), satellite optimised mixing (red) and reduced mixing (blue)) for the time period of CRISTA measurements (4–12 November 1994). Top: CRISTA versus KASIMA (T106) versus CLaMS for CLaMS initialised on 20 October 1994 with KASIMA. Bottom: CRISTA versus CLaMS for CLaMS initialised with the PV/N_2O-correlation deduced from CRISTA observations.

5 Conclusions

We investigated the formation and the development of the three streamers that were observed by the CRISTA-1 experiment on 6 November 1994. We compared the results obtained with the CLaMS model to the results of the 9-year simulation by Eyring et al. (2003) conducted with the KASIMA model. For the CLaMS simulation the N_2O distribution on 20 October obtained with the 9-year simulation conducted with KASIMA was used as initialisation. Further, the results from both models were compared to the CRISTA observations.

The CLaMS model as well as the KASIMA model reproduces the streamers observed on 6 November 1994 well. However, a stronger filamentation than in KASIMA is present in all CLaMS simulations, both in the high resolution (approximately 50.000 air parcels) and in the low resolution (approximately 8000 air parcels) simulations. In the Southern Hemisphere, the observed gradients in N_2O are underestimated by KASIMA. In general, the N_2O values simulated by KASIMA are lower in both hemispheres than measured by CRISTA. This is possibly caused by the employed initialisation of the 9-year run of KASIMA or by the fact that the simulation was made for a time period of 9-years and therefore that a simplified N_2O chemistry had to be implemented. However, uncertainties in the CRISTA N_2O measurements have to be taken into account.

To improve the results of the CLaMS simulations we also used a N_2O-PV correlation derived from CRISTA measurements as initialisation. For this comparison a better agreement between measurements and model results was obtained. In contrast to the initialisation with the KASIMA model results, the N_2O gradients in the Southern Hemisphere were well reproduced by CLaMS. Therefore, our results show that the initialisation used for the model simulation significantly influences the results of the simulation. Thus, an initialisation based on measurements is essential for a realistic model simulation.

Further, whether an Eulerian or a Lagrangian model is more adequate for the simulation depends on the intention of the scientific studies. In case of a streamer climatology as in Eyring et al. (2003) an Eulerian model is particularly suitable since such models require much less computer effort than Lagrangian models. This is a significant advantage for long-term simulation studies over several years. In the study of Eyring et al. (2003) a streamer climatology was derived with KASIMA and compared to the ECHAM4.L39(DLR)/CHEM (E39/C) model showing a good agreement between both models. Although from a case study as the one presented here no conclusions on the validity of a climatology can be drawn, the agreement between the principle features of the CLaMS and KASIMA simulations with the streamer structures observed by CRISTA gives confidence in the ability of KASIMA to simulate the large scale structure of streamers. However, if the intention is to investigate the development and fine scale structure of certain streamers a high resolution Lagrangian model, such as the CLaMS model, seems more appropriate.

However, simulations with KASIMA on a shorter time scale corresponding to that of the CLaMS simulations, and the usage of different spatial resolutions showed an improvement of the KASIMA results. A better agreement with the CRISTA measurements was found in both hemispheres. Further, an improvement of the absolute values of N_2O mixing ratios was achieved.

PDFs (probability density functions) were calculated in order to quantify the differences in N_2O variability between the CRISTA observations and the simulations carried out with the CLaMS and KASIMA model. The PDF derived from the KASIMA simulations indicates that the small scale structures observed by CRISTA are smoothed out in this model as a result of relatively high numerical diffusion. The PDFs derived from the CLaMS simulation depend strongly on the mixing parameterisation showing that the satellite optimised configuration is in good agreement with the CRISTA observation. However, in the CRISTA observations, physical structures are smoothed out due to "optical mixing". Thus, through the PDFs additional information on atmospheric variability is given indicating that in-situ observations are necessary to quantify the real mixing intensity of the stratosphere.

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