

**Implementation  
issues in chemistry  
and transport models**

S. E. Strahan and  
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# Implementation issues in chemistry and transport models

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Received: 2 September 2005 – Accepted: 28 September 2005 – Published: 21 October 2005

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Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

EGU

## Abstract

Offline chemistry and transport models (CTMs) are versatile tools for studying composition and climate issues requiring multi-decadal simulations. They are computationally fast compared to coupled chemistry climate models, making them well-suited for integrating sensitivity experiments necessary for understanding model performance and interpreting results. The archived meteorological fields used by CTMs can be implemented with lower horizontal or vertical resolution than the original meteorological fields in order to shorten integration time, but the effects of these shortcuts on transport processes must be understood if the CTM is to have credibility. In this paper we present a series of CTM experiments, each differing from another by a single feature of the implementation. Transport effects arising from changes in resolution and model lid height are evaluated using process-oriented diagnostics that intercompare CH<sub>4</sub>, O<sub>3</sub>, and age tracer carried in the simulations. Some of the diagnostics used are derived from observations and are shown as a reality check for the model. Processes evaluated include the tropical ascent, tropical-midlatitude exchange, the poleward circulation in the upper stratosphere, and the development of the Antarctic vortex. We find that faithful representation of stratospheric transport in this CTM using Lin and Rood advection is possible with a full mesosphere, ~1 km resolution in the lower stratosphere, and relatively low vertical resolution (>4 km spacing) in the middle stratosphere and above, but lowering the lid from the upper to lower mesosphere leads to less realistic constituent distributions in the upper stratosphere. Ultimately, this affects the polar lower stratosphere, but the effects are greater for the Antarctic than the Arctic. The fidelity of lower stratospheric transport requires realistic tropical and high latitude mixing barriers which are produced at 2° × 2.5°, but not lower resolution. At 2° × 2.5° resolution, the CTM produces a vortex capable of isolating perturbed chemistry (e.g. high Cl<sub>y</sub> and low NO<sub>y</sub>) required for simulating polar ozone loss.

ACPD

5, 10217–10258, 2005

## Implementation issues in chemistry and transport models

S. E. Strahan and  
B. C. Polansky

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

## 1. Introduction

In recent years, coupled chemistry climate models have been used to study complex atmospheric phenomena such as the recovery of the Antarctic ozone hole (Austin and Butchart, 2003; Tian and Chipperfield, 2005). The models' chemistry, dynamics, and radiation are fully coupled allowing the radiative properties of the constituents to feed-back into the radiation calculation, the radiation to affect the dynamics, the updated dynamics to then transport the constituents, and so on. Model experiments attempting to reproduce past observations or predict future climate states require multi-decadal simulations, which, for a coupled climate model at reasonably high resolution, is computationally expensive. The time and cost to perform additional sensitivity experiments with a coupled model, necessary for understanding its behavior, may be prohibitive.

An offline chemistry transport model (CTM) is a frequently used tool that simplifies model calculations by using archived meteorological fields, making multi-decadal simulations tractable. Meteorological fields, generated from a general circulation model (GCM) or data assimilation system (DAS), are input into the CTM and updated several times per model day. The CTM lacks the ability to simulate feedbacks between the constituents, radiation, and dynamics, which may be large for ozone loss in the polar vortex (MacKenzie and Harwood, 2000). However, radiative coupling with ozone will not automatically lead to a more realistic simulation of ozone loss if the GCM has a cold pole problem, as the coupling would strengthen the already too strong polar vortex (Austin, 2002). A CTM has the advantage of being integrated much more quickly than a coupled model, which also allows – even encourages – its users to conduct sensitivity studies that increase the understanding of the model performance (e.g., sensitivity to boundary conditions, input wind fields, resolution, etc.). Constituent transport in a GCM will also be sensitive to resolution, but that sensitivity cannot readily be tested because physical parameterizations in the GCM are tuned to a particular resolution. The assessment of CTM performance and sensitivity to inputs has been the hallmark of the Global Modeling Initiative (GMI) project; see, for example, Douglass et al. (1999)

### Implementation issues in chemistry and transport models

S. E. Strahan and  
B. C. Polansky

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

and Rotman et al. (2001).

Previous studies have examined the differences in stratospheric tracer transport between online and offline calculations. Rasch et al. (1994) used daily averaged winds from the Middle Atmosphere Community Climate Model 2 (MACCM2) to transport simple tracers in an offline model and reported a significant speed up over the online calculation. They found that many aspects of tracer transport were well represented, but mixing out of the tropics was much slower than in the online calculation. This was attributed to using daily averaging of winds that eliminated large transients in vertical velocities. They found that using winds every 6 h greatly reduced online-offline differences in a tropospheric simulation. Waugh et al. (1997) experimented with temporal sampling of meteorological fields used in offline simulations and concluded that to obtain good agreement with the online calculation, multi-year CTM simulations would require winds sampled at least every 6 h.

Computational expediency is important for studies of phenomena occurring on decadal timescales, such as ozone recovery and effects of increasing greenhouse gases on climate, and for assessments. Such simulations involve many atmospheric processes, and in order to understand and interpret long-term simulations, a number of model sensitivity studies should be performed. For example, to understand a CTM's response to the Mt. Pinatubo eruption requires simulations with and without volcanic effects, and with different levels of chlorine-loading (Stolarski et al., 2005). CTMs are also widely used for assessments because their rapid integration time makes it possible to run the many required scenarios (e.g. IPCC, 2001). The choice of implementation, or usage, of archived winds in a CTM affects the computational time. Compromises to the meteorological fields, such as halving the horizontal resolution – for example, putting the  $2^\circ \times 2.5^\circ$  input fields on a  $4^\circ \times 5^\circ$  grid – will speed up the advection calculation by a factor of 8. Computational time can also be shortened by reducing the number of vertical levels, including lowering the top level of the CTM. Parameterization of chemistry is another approximation that can be used to decrease a simulation's integration time.

---

**Implementation  
issues in chemistry  
and transport models**

S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

---

**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

---

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

Each compromise, or “shortcut”, will give results different from a CTM simulation run with the full resolution of the input meteorological fields. It is vital that we determine the extent to which the compromises we make corrupt the representation of transport processes seen at full resolution. In this paper we systematically explore a variety of meteorological field implementations and evaluate their effects on transport using methane (CH<sub>4</sub>), ozone (O<sub>3</sub>), and an age tracer. First, the differences between the offline and online calculation at the same resolution are presented. Analyses of CH<sub>4</sub> and age tracer from different CTM implementations are compared to assess how various stratospheric processes are affected by the “shortcuts”. Some observations are used to assess the realism of the simulations. We conclude with recommendations for implementations that have minimal impact on constituent distributions.

## 2. Model description

Implementation experiments were conducted using an updated version of the Goddard Space Flight Center (GSFC) three-dimensional CTM used in Douglass et al. (2003). The advection core of the CTM uses a flux form semi-Lagrangian transport code with a quasi-Lagrangian vertical coordinate (Lin, 2004; Lin and Rood, 1996). All CTM experiments began on 1 July and used a five-year sequence of meteorological fields from a 50-year integration of the Finite Volume General Circulation Model (FVGCM) that had interannually varying sea surface temperatures. Additional details of the FVGCM can be found in Stolarski et al. (2005). The native resolution of the FVGCM fields is 2° latitude × 2.5° longitude (~220 km × ~275 km at the equator) with 55 layers between the surface and 0.01 hPa. Horizontal winds and temperature are updated in the CTM every 6 h using 6-hourly averages, as recommended by previous offline/online transport comparisons (Waugh et al., 1997). Meteorological fields from a previous version of the FVGCM were used in full chemistry simulations with the GSFC CTM (Douglass et al., 2003) and the GMI CTM, which also uses a Lin and Rood advection scheme. Observationally-based diagnostics, used to evaluate the GMI CTM, demon-

strated the credibility of some aspects of stratospheric transport with FVGCM winds at  $4^\circ \times 5^\circ$  ( $\sim 440 \text{ km} \times \sim 550 \text{ km}$ ) resolution (Strahan and Douglass, 2004; Considine et al., 2004).

Parameterized chemistry for  $\text{O}_3$  and  $\text{CH}_4$  were calculated using production and loss rates from the 2-D simulations of Fleming et al. (1999). These did not interact with the model's radiation code. A fixed surface boundary condition for the  $\text{CH}_4$  tropospheric source was imposed at the three lowest model levels to eliminate the need for boundary layer mixing. Initial conditions for each species come from a previous long-term CTM simulation with FVGCM winds. Each experiment also has an age tracer initialized in the manner of Hall et al. (1999): it is emitted between  $10^\circ \text{S}$  and  $10^\circ \text{N}$  for only the first month of the simulation and lost through surface deposition. All CTM simulations, except the one with  $1^\circ \times 1.25^\circ$  horizontal resolution, were run for 5 years.

### 3. CTM sensitivity to meteorological implementation

#### 3.1. The implementation issues

Previous studies have investigated the effects of different CTM implementations on transport. Bregman et al. (2001) compared simulations of lower stratospheric  $\text{O}_3$  from three CTMs using the same advection scheme but different horizontal and vertical interpolations of ECMWF winds (top level of 10 hPa). They attributed the significant differences in performance to the interpolation of original spectral horizontal winds to different grids, which may have lead to inaccuracies in the vertical winds. However, each CTM came from a different institution and there was more than one difference between the simulations, for example both horizontal regridding and time between meteorological updates differed, making the determination of the cause(s) of the differences inexact. Van den Broek et al. (2003) used a CTM with a finite-differencing advection scheme at 3 horizontal resolutions to investigate the effect on tracer profiles in the Arctic vortex. They concluded that  $6^\circ \times 9^\circ$  resolution was too coarse to represent the vortex,

---

## Implementation issues in chemistry and transport models

S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

---

**Implementation  
issues in chemistry  
and transport models**

S. E. Strahan and  
B. C. Polansky

---

but that  $3^\circ \times 2^\circ$  and  $1^\circ \times 1^\circ$  resolution performed equally well and better than  $6^\circ \times 9^\circ$  resolution. But using a CTM with the Prather (1986) second order moments advection scheme, Searle et al. (1998) found no sensitivity in diffusiveness at the vortex edge to horizontal resolution even at  $5.6^\circ \times 5.6^\circ$ . It is vital to understand a model's sensitivity to resolution because of the serious consequences it may have on its ability to maintain high  $Cl_y$  levels in the vortex and to disperse ozone-depleted air to the midlatitudes.

In this study we perform a series of experiments that test different implementations of the input meteorological fields in a CTM. Each experiment is designed to test the effect of a single change, for example, the horizontal resolution. Some observations will be used to establish the realism of the simulation's behavior, but most of the comparisons will be between experiments, with the goal of understanding how one differs from another.

The model intercomparisons presented address several questions:

- How does the vertical resolution of the input wind fields affect the CTM transport circulation?
- What is the impact on the stratosphere of lowering the CTM lid?
- How does horizontal resolution affect tracer transport?

Table 1 lists 7 experiments performed. Each experiment contains a single implementation change relative to another, usually the experiment above it in the table. For example, experiment “Low Lid” is identical to “High Lid” except that the top 5 vertical levels have been removed, lowering the lid to 0.4 hPa. A comparison of experiments “High Res” ( $1^\circ \times 1.25^\circ$ ) and “Low Lid” ( $2^\circ \times 2.5^\circ$ ) examines the effect of change in horizontal resolution while the scale of the wind forcing is the same. This tests the effect of resolution on advection, independent of the wave forcing in the wind fields. Experiments “Low Res” ( $4^\circ \times 5^\circ$ ) and “Smoothed” ( $2^\circ \times 2.5^\circ$ ) also test the advection calculation but at lower resolution.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

### 3.2. Model analysis tools

Evaluation of transport sensitivity requires constituents that have significant vertical or horizontal gradients and relatively long photochemical lifetimes. Methane and ozone are long-lived in much of the stratosphere. Methane has a surface source and destruction in the upper stratosphere, while ozone is produced and destroyed primarily in the middle and upper stratosphere. The locations of large gradients in CH<sub>4</sub> and O<sub>3</sub> are different because of the differences in their sources and sinks, but used together their gradients show sensitivity to transport over much of the stratosphere. Their vertical and horizontal gradients, shown in Fig. 1, indicate where each constituent has the greatest transport sensitivity. Examples of zonal mean CH<sub>4</sub> and O<sub>3</sub> fields can be found in Fig. 2. Model gradients are used in the figures because their stratospheric distributions are quite realistic compared to the UARS reference atmosphere plots (see <http://code916.gsfc.nasa.gov/Public/Analysis/UARS/urap/home.html>). Ozone has large sensitivity to transport across the subtropics in the lower stratosphere and that CH<sub>4</sub> will be especially sensitive to vertical motions at high latitudes. Ozone gradients are similar in all seasons while CH<sub>4</sub> gradients tend to be largest at the mid and high latitudes during the cold seasons. Smaller transport sensitivity is seen for O<sub>3</sub> above ~20 hPa where its distribution is strongly influenced by photochemistry.

These species are also well suited for model evaluation because they have been extensively measured by aircraft and satellite instruments. Long-term, global data sets of CH<sub>4</sub> and O<sub>3</sub> are available from the Halogen Occultation Experiment (HALOE) (Park et al., 1996) and the Cryogenic Limb Array Etalon Spectrometer (CLAES) (Roche et al., 1996) on the Upper Atmosphere Research Satellite (UARS). This study uses process-oriented diagnostics derived from HALOE and CLAES measurements to evaluate how well physical processes are represented by the models. Similar diagnostics were used to evaluate transport in GMI CTM simulations (Douglass et al., 1999; Strahan and Douglass, 2004).

---

## Implementation issues in chemistry and transport models

S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion



#### 4. Offline and online calculations

The CTM and FVGCM have been integrated with the same parameterized CH<sub>4</sub> loss and surface boundary conditions but do not produce the same results. Figure 3 shows the differences between the FVGCM and the CTM simulation “Full Vert”, which was integrated with the same winds and grid as the FVGCM. The differences, shown for the 5th year of the CTM simulation, have reached a steady state. In the annual mean, stratospheric CH<sub>4</sub> in the CTM is 1–5% lower than the FVGCM, with the differences increasing with height due to faster photochemistry and shorter transport timescales. Previous studies have suggested that offline transport differences arise from the differences between the vertical wind calculated in the CTM (from the 6-hourly averaged u and v fields using continuity) and the vertical wind calculated in the GCM (Rasch et al., 1994; Waugh et al., 1997).

The other panels of Fig. 3 show the differences between online and offline during the seasons of greatest vertical transport (adiabatic descent) in each hemisphere, where CH<sub>4</sub> has large sensitivity to vertical transport. Photochemical loss is negligible at high latitudes during fall and is unlikely to be the cause of the differences. Horizontal maps (not shown) have the greatest differences during periods of strong wave activity, which is usually accompanied by vertical motions, with near zero differences during quiescent periods. Rasch et al. (1994) and Waugh et al. (1997) reason that the use of 6-hourly averaged u and v in the CTM leads to smaller calculated vertical velocity because large vertical transients will be averaged out. This would result in slower tropical ascent in the CTM and for a CH<sub>4</sub>-like tracer would produce differences with the same sign as shown here.

#### 5. Results of CTM implementation experiments

In each section below, a pair of simulations is compared to determine how the change in implementation affects stratospheric transport processes. An overview of the circu-

### Implementation issues in chemistry and transport models

S. E. Strahan and  
B. C. Polansky

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

lation differences is presented first. Then, a series of process-oriented comparisons is made that examines tropical ascent, exchange between the tropics and midlatitudes, poleward transport of tropical air in the upper stratosphere, and the behavior of the lower stratospheric Antarctic vortex in spring.

5 5.1. The effect of decreasing vertical resolution in the stratosphere and mesosphere

This section compares CTM simulations using the original FVGCM 55 levels (“Full Vert”) and one with 33 levels wind fields (“Reduced Vert”); both models have the same lid (0.015 hPa) and horizontal resolution. The number of levels is reduced by a process that maps the u and v wind fields to a different set of vertical levels in a way that  
10 conserves the sum of the vertical winds between the original levels. The resolution is very similar from 225–43 hPa, but from 43–1 hPa Full Vert has twice the vertical resolution and above 1 hPa it has three times the resolution.

Figure 2 summarizes the circulation differences. The top panels show annual zonal mean distributions of CH<sub>4</sub> and O<sub>3</sub>, and the mean age in Full Vert after 5 years, while the lower panels show the differences between the experiments. Methane is sensitive to vertical transport in the middle stratosphere and above, yet the differences due to reduced resolution are almost negligible. Ozone differences greater than 2% only occur in the tropical lower stratosphere in the region with large vertical gradients and slight differences in level spacings. Mean age differences are insignificant. (The calculation  
15 of the true mean age would require a 20-year integration. After 5 years, the mean ages are asymptotically approaching their “true” value. The difference between mean ages in the two simulations reaches its asymptotic limit much sooner, thus, the mean age differences after Year 4 are nearly converged.)

Figure 4 examines the process of ascent using the arrival of the age tracer on 57 hPa and 10 hPa surfaces. The age tracer arrives at the tropical tropopause (100 hPa) with the same timing and distributions in both simulations (not shown). Between 57–100 hPa (380–500 K), the levels in Reduced Vert are more closely spaced and the age tracer arrives later (i.e. has slower ascent). But at 43 hPa and above, the levels of Full  
25

---

**Implementation  
issues in chemistry  
and transport models**

S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

---

**Implementation  
issues in chemistry  
and transport models**

---

S. E. Strahan and  
B. C. Polansky

---

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

Vert are more closely spaced and the arrival time at 10 hPa shows that its ascent and meridional spread are slower. The relationship between level spacing and ascent is quite strong in the mesosphere, where Reduced Vert has only 1/3 of the levels of Full Vert. This relationship is expected because the transport spreads the tracer uniformly through the grid box, and the fewer the grid boxes, the faster the diffusion (A. R. Douglass, private comm.). Figure 5 shows that after nearly 2 years of simulation, the Reduced Vert age tracer has filled much more of the lower mesosphere than Full Vert.

Faster ascent and poleward transport lead to stronger exchange between tropical and midlatitude air masses. Figure 6 shows the probability distribution functions (pdfs) for CH<sub>4</sub> between 10° S and 46° N on isentropic surfaces in the lower and middle stratosphere. The shape of a long-lived tracer distribution indicates the distinctness of tropical and midlatitude air (Sparling, 2000) and was used to discriminate between meteorological fields in GMI model evaluation tests (Douglass et al., 1999). All simulations show a minimum between the tropical and midlatitude distributions which indicates a subtropical barrier to mixing; this is seen in winter and summer and at both levels. The tropical peaks at 500 K (~45 hPa) sort themselves by ascent rate, with slower ascent corresponding to higher CH<sub>4</sub> (less exchange with the midlatitudes), consistent with the age tracer comparison shown in Fig. 4. Ascent in Low Lid and Low Res will be discussed later in Sect. 5.

The annual cycle of CH<sub>4</sub> in polar upper stratosphere is a good diagnostic for several processes on seasonal time scales (Strahan and Douglass, 2004). Figure 7 shows a contoured pdf time series of CH<sub>4</sub> at 1200 K (~5 hPa) in the Antarctic for Reduced Vert, with an outline of Full Vert contours overlaying it. From Austral summer to early fall (December–April), CH<sub>4</sub> declines sharply and has little variability. These features are the result of photochemical loss, weak wave activity, and by early fall, descent. As wave activity increases in the fall (April–June), tropical upper stratospheric air with high CH<sub>4</sub> is transported poleward. Wave activity is low in winter but increases again in spring (October–December), resulting in large variability due to transport of higher CH<sub>4</sub> air from lower latitudes. Ultimately the vortex is destroyed and midlatitude air is thoroughly

---

**Implementation  
issues in chemistry  
and transport models**

---

S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

mixed into the polar region. The upper stratospheric CH<sub>4</sub> annual cycle in Reduced Vert has nearly the same distributions as Full Vert and only slightly less variability. The same results are found in the Arctic and at higher levels in the stratosphere. Although Fig. 5 showed that Reduced Vert has rapid mesospheric transport, because mesospheric CH<sub>4</sub> values do not differ much between the simulations, these transport differences do not impact CH<sub>4</sub> in the upper stratosphere. We will see later that it is the presence of a full mesosphere that matters to stratospheric CH<sub>4</sub>.

The behavior of the lower stratospheric Antarctic vortex in spring is examined in Fig. 8. The details and interpretation of this analysis, including a description of the HALOE data set used to derive this test, can be found in Strahan and Douglass (2004). The springtime CH<sub>4</sub> pdfs, one from 60°–80° S (mostly vortex air, blue) and one from 44°–60° S (mostly midlatitude air, red), illustrate vortex isolation and the manner in which it erodes. The September Full Vert vortex has a sharper edge than HALOE, indicated by much greater separation of the pdfs. During November, the model and analyzed pdfs are very similar in shape, separation, and most probable value. This is interpreted as the model forming a strong vortex earlier than observed by HALOE, but having a realistic dynamical evolution during spring. Results for Reduced Vert are not plotted because they are indistinguishable from Full Vert. This behavior demonstrates that reduced vertical resolution in the middle stratosphere and above has no significant impact on the processes that maintain and erode the lower stratospheric Antarctic vortex in spring. Similar behavior is found in HALOE and the models at 600 K.

## 5.2. The effect of lowering the model lid without decreasing stratospheric resolution

This section compares the 33 level simulation having a 0.015 hPa lid, referred to as Reduced Vert in previous section, with a 28 level version having a lower lid (0.4 hPa). The lowest 27 levels of these simulations (surface to 1.33 hPa) are identical, as are their horizontal resolutions. In this section, Reduced Vert will be referred to as “High Lid” and the 28 level model will be called “Low Lid” in order to emphasize their difference.

Figure 9 summarizes the mean circulation differences in the same way as Fig. 2.

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**Implementation  
issues in chemistry  
and transport models**

---

S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

Lowering the lid has a much greater effect than reducing the vertical resolution above 43 hPa. Low Lid has roughly 1% higher CH<sub>4</sub> in the lower stratosphere but 10–30% less CH<sub>4</sub> in the upper stratosphere. This is consistent with the pattern of mean age differences: the air is younger where CH<sub>4</sub> is higher and older where CH<sub>4</sub> is lower. In contrast to CH<sub>4</sub>, O<sub>3</sub> and age are more strongly affected by the lower lid in the southern hemisphere (SH). High Lid has low ozone in the mesosphere that descends to the upper stratosphere during late summer and fall. The absence of a source of low ozone in Low Lid is probably the reason for its higher ozone in the polar upper stratosphere. (Methane has very small vertical gradients in this region and is insensitive to this.) The lack of a full mesosphere has a negligible effect on middle and lower stratospheric ozone in the northern hemisphere (NH) in this particular winter. This is consistent with trajectory analyses of Rosenfield and Schoeberl (2001) that showed that the composition of the Arctic lower stratospheric vortex is often, though not always, composed of air of middle and upper stratospheric origin, while the Antarctic vortex generally contains a significant contribution from mesospheric air.

The age tracer at 31 hPa (not shown) is nearly identical at all latitudes in the two simulations, implying that the mesospheric lid height has little effect on middle and lower stratospheric tropical ascent and meridional transport. This is consistent with the identical tropical-midlatitude separations at 500 K shown in Fig. 6 (green and yellow). Figure 6 shows small differences due to the lid height have appeared at 1000 K (~8 hPa).

Figure 10 shows latitude-height cross-sections of zonal mean age tracer for High Lid and Low Lid on three dates in the 2nd and 3rd years of the simulations. High Lid produces the two-lobed circulation in the mesosphere (1 April and 10 May), consistent with CH<sub>4</sub> structures seen by HALOE (Ruth et al., 1997) near equinox. This circulation fills the lower mesosphere, and when cooling begins in the Austral fall, poleward and downward transport of air from the lower mesosphere fills the Antarctic upper stratosphere. By 10 May, horizontal transport near 1 hPa has brought the tracer to the Antarctic in High Lid while similar transport is clearly lacking in Low Lid. The bottom panels (5

---

**Implementation  
issues in chemistry  
and transport models**

S. E. Strahan and  
B. C. Polansky

---

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

September) illustrate how the missing mesospheric circulation has a similar effect as the Arctic vortex is forming. Without a mesospheric circulation, the upper stratospheric transport is “short-circuited” in Low Lid and the Arctic upper stratosphere is still completely isolated after more than 2 years. Having a lid near the mesopause ( $\sim 0.01$  hPa) results in more effective constituent transport in the upper stratosphere.

Differences in equator-to-pole transport in these models are also observed in the  $\text{CH}_4$  polar upper stratospheric annual cycle (contoured pdfs) shown in Fig. 11. Red and orange indicate the most probable values for the models. Pdfs of CLAES measurements during 5 southern hemispheric viewing periods ( $\sim 35$  days each) are overlaid on the model results with black contours; the innermost contour indicates the most probable value. Both simulations show large variability associated with the breakdown of the vortex in late spring (October–November). Model mixing ratios fall rapidly throughout the summer (December–April). This is the only season that High Lid does not behave like the observations, which show high  $\text{CH}_4$  maintained in the Antarctic through mid summer. In April, both models and CLAES show a minimum in the annual cycle, but by the end of fall (June), CLAES and High Lid have much higher  $\text{CH}_4$  as a result of strong transport from lower latitudes. Weak upper stratospheric poleward transport in “Low lid” is indicated by persistently low  $\text{CH}_4$  from May–September; this is also shown by the age tracer in Fig. 10 (10 May). Arctic  $\text{CH}_4$  in High Lid is systematically higher in the upper stratosphere than Low Lid, but CLAES  $\text{CH}_4$  is higher still, suggesting that neither model has strong enough horizontal transport in the NH upper stratosphere. In the SH, High Lid compares very closely with CLAES (with the exception of summer), suggesting that the upper mesospheric lid is important for producing realistic transport in the upper stratosphere.

Although Low Lid has too little upper stratospheric  $\text{CH}_4$  in the fall, by late winter in the Antarctic lower stratosphere it has too much, consistent with the pattern of general circulation differences seen in Fig. 9. The differences caused by the lid are greatest in the Antarctic vortex, as seen in Figs. 9 and 12. In Fig. 12, the midlatitude distributions of the two simulations are indistinguishable, but the vortex pdf in Low Lid has much higher

---

**Implementation  
issues in chemistry  
and transport models**

---

S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

CH<sub>4</sub>. Air descending in the Low Lid vortex is subject to stronger horizontal transport in the middle stratosphere and below, resulting in higher CH<sub>4</sub> that descends to the lower stratospheric vortex by the end of winter. Both simulations show vortex and midlatitude distributions that remain isolated from each other in spring, in good agreement with the analysis of HALOE CH<sub>4</sub> behavior in Strahan and Douglass (2004). Vortex isolation is slightly better in High Lid. High Lid vortex pdfs in September and November (solid blue lines) have greater overlap (53%) than Low Lid vortex pdfs (dashed blue lines, 41%). That is, the Low Lid vortex pdfs change more during spring because more midlatitude air is able to mix in. Similar differences in behavior are found in the NH.

### 5.3. The effect of lower horizontal resolution

This section compares two simulations having the same vertical levels and lids (28 levels and 0.4 hPa), but different horizontal resolution: Low Lid (2° × 2.5°) and “Low Res” (4° × 5°). Low Res winds were created by subsampling the 2° × 2.5° wind fields.

The comparison of mean CH<sub>4</sub>, O<sub>3</sub>, and age differences in Fig. 13 shows large effects due to decreased horizontal resolution, much greater than those caused by reducing the vertical resolution or the CTM lid height. In the lower stratosphere, Low Res has lower CH<sub>4</sub> at low latitudes and higher CH<sub>4</sub> at high latitudes, indicating that strong horizontal mixing flattens the meridional gradients. Higher O<sub>3</sub> in the northern lower and middle stratosphere suggests stronger transport out of the tropical production region.

The patterns of age and CH<sub>4</sub> differences are very similar. With young air more likely to circulate poleward than upward, the middle stratosphere and above are “depleted” in young air, increasing the mean age there and decreasing the age in the polar lower stratosphere. The mean age comparisons shown in Figs. 3, 9, and 13 show that lowering the lid or decreasing the horizontal resolution noticeably compromises transport, making it harder for air to get to the upper atmosphere but easier to mix poleward in the lower stratosphere.

These circulation problems are easily traced to several transport processes. Figure 14 shows age spectra in the polar lower stratosphere (57 hPa) and near the trop-

---

**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

ical O<sub>3</sub> maximum (10 hPa) from four CTM simulations. The Low Res age is markedly different from all the 2°×2.5° age spectra, especially in the southern hemisphere. In the polar lower stratosphere, Low Res air arrives much sooner and continuously, rather than having an annual cycle of transport as seen in all other implementations. In the tropical middle stratosphere, it arrives at 10 hPa sooner than the others but there is less of it because more has mixed out of the tropics before arriving there.

These three panels show that 4°×5° resolution allows too much leakage out of the lower stratospheric tropical pipe and explains the structure of the mean age difference in Fig. 13. Low Res allows greater mixing of young and old (midlatitude) air in the lower stratosphere, making the tropics older and the extratropics younger, and results in slightly older air ascending to the middle and upper stratosphere. This effect was also seen in Fig. 6, where the Low Res 500 K tropical and midlatitude peaks are shifted toward each other (more exchange of air) compared to the 2°×2.5° simulations. At 1000 K (above 10 hPa), both peaks are shifted to lower mixing ratios, reflecting the difficulty of getting young air above the tropical lower stratosphere in the 4°×5° model.

The excessive horizontal mixing in Low Res actually compensates for the inadequate upper stratospheric equator-to-pole transport caused by the lower lid (Fig. 11), demonstrating that two wrongs can appear to make a right. Figure 15 shows how meridional gradients of CH<sub>4</sub> in the upper stratosphere are affected by the change in horizontal resolution and lid during Austral winter. In June, the strongest gradients are between 40–60° S and are similar in all 3 simulations shown. By September, the two 2°×2.5° simulations show parallel gradients at the vortex edge while the 4°×5° is weaker. Figure 11 showed that CH<sub>4</sub> in the upper stratospheric vortex at the end of winter was simulated well by High Lid but was too low in Low Lid. Figure 15 shows that Low Res moderates the low vortex values seen in Low Lid; unfortunately, this improvement is caused by the inability of Low Res to maintain a vortex edge gradient and the improved vortex agreement comes at the expense of midlatitude values.

The behavior of the Low Res Antarctic vortex demonstrates a serious consequence of decreased horizontal resolution. Consistent with Fig. 15, Fig. 16 shows that 450 K



---

**Implementation  
issues in chemistry  
and transport models**

---

S. E. Strahan and  
B. C. Polansky

---

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

vortex and midlatitude air masses in September are less separated at  $4^\circ \times 5^\circ$  than at  $2^\circ \times 2.5^\circ$ . In spite of Low Res having too little  $\text{CH}_4$  in the Antarctic upper stratosphere in fall, its excessive horizontal mixing results in too much  $\text{CH}_4$  in the lower stratosphere by spring. By November, the Low Res vortex air mass has significantly increased mixing ratios compared to Low Lid. The overlap between the September and November vortex distributions indicates how much the vortex air has changed. Low Res has only 19% overlap, compared to 41% for Low Lid and 53% for High Lid, indicating considerable incorporation of midlatitude air. In November, Low Res pdfs are overlapped and the vortex peak has increased by  $\sim 200$  ppb since September. This contrasts with the Full Vert vortex peak change of about +50 ppb during spring. The lack of a strong barrier to mixing has important consequences for the maintenance of the high  $\text{Cl}_y$ /low  $\text{NO}_x$  environment required to successfully simulate Antarctic ozone depletion, and for the dispersion of ozone-depleted air into the midlatitudes.

#### 5.4. Requirements for producing a realistic vortex edge

Was the leaky vortex behavior of Low Res caused by the  $4^\circ \times 5^\circ$  resolution of the advection calculation? Or, is forcing at scales smaller than  $4^\circ \times 5^\circ$  essential to forming and maintaining the vortex? If it is a resolution effect, do we know that advection at  $2^\circ \times 2.5^\circ$  is adequate? These questions are addressed with two additional experiments. One experiment is run at  $2^\circ \times 2.5^\circ$  resolution, but uses the  $4^\circ \times 5^\circ$  winds that were linearly interpolated back to  $2^\circ \times 2.5^\circ$  and thus contain no wave forcing below the scale of the  $4^\circ \times 5^\circ$  grid (“Smoothed”). The other experiment is run at  $1^\circ \times 1.25^\circ$ . It uses the original  $2^\circ \times 2.5^\circ$  winds linearly interpolated to  $1^\circ \times 1.25^\circ$  (“High Res”) and thus contains no wave forcing below the scale of the  $2^\circ \times 2.5^\circ$  winds (Low Lid). We address the issue of producing a realistic vortex edge by comparing these new experiments with Low Lid and Low Res. These results are specific to the Lin and Rood (1996) advection scheme used in this CTM; Searle et al. (1998) found that the sensitivity to resolution depends on the diffusiveness of the advection scheme.

What makes the Low Lid vortex behavior more realistic than Low Res? The top

---

**Implementation  
issues in chemistry  
and transport models**

---

S. E. Strahan and  
B. C. Polansky

---

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

panels of Fig. 17 compare the state of the November vortex in Low Res (top) and Low Lid (middle) with an intermediate experiment, “Smoothed”, which has  $2^\circ \times 2.5^\circ$  advection but  $4^\circ \times 5^\circ$  information content. All simulations were begun on 1 July from the same initial conditions. The top panel shows that Low Res and Smoothed do not get the same  $\text{CH}_4$  distributions even though the winds have the same scale wave forcings, implying that resolution matters in the formation of the vortex mixing barrier. In the middle panel, the experiments have the same  $2^\circ \times 2.5^\circ$  advection but different information content in the winds. The time evolution of pdfs in these experiments is nearly identical, suggesting that smaller scale waves do not play an important role in vortex behavior. This is consistent with the results of Waugh and Plumb (1994) showing that finescale atmospheric structures could be produced from low resolution wind fields. Realistic vortex behavior is impaired by the  $4^\circ \times 5^\circ$  resolution in this CTM, but not by the lack of small scale wave forcing.

The bottom panel of Fig. 17 compares the  $2^\circ \times 2.5^\circ$  advection of “Low Lid” with an experiment using the same winds as Low Lid interpolated to  $1^\circ \times 1.25^\circ$  (“High Res”). The winds in High Res have the same information content as Low Lid. The differences in the shapes, peaks, and separations of the vortex and midlatitude pdfs are very slight, with High Res having a slightly stronger barrier to mixing (i.e., lower vortex  $\text{CH}_4$ ). The top panel demonstrates a significant improvement in vortex behavior going from  $4^\circ \times 5^\circ$  to  $2^\circ \times 2.5^\circ$ , while the bottom panel shows very little gain in vortex isolation at  $1^\circ \times 1.25^\circ$  resolution. (Since the original resolution of the FVGCM is  $2^\circ \times 2.5^\circ$ , we cannot say whether a higher resolution GCM might produce a better vortex.)

## 6. Summary: implementation effects on transport processes

A chemistry and transport model using stored meteorological fields is a useful tool that can make complex atmospheric studies tractable. It is essential that we understand how our choices in implementation affect the results calculated. To that end, this paper has examined the representation of stratospheric processes using a variety of

implementations in order to identify the consequences of lowering the CTM lid, vertical resolution, and horizontal resolution.

Realistic tropical ascent in models is important to simulating the propagation of an annually varying cycle into the stratosphere, for example, the “tape recorder” in water (Mote et al., 1996). The rate of ascent was affected by level spacing, with more closely spaced levels leading to slower ascent. Mesospheric lid height had no impact on ascent rate below the middle stratosphere, but a low lid slowed ascent slightly in the upper stratosphere. Horizontal resolution affected ascent, with the Low Res ( $4^\circ \times 5^\circ$  model) simulation having faster ascent than all the  $2^\circ \times 2.5^\circ$  simulations (Fig. 14).

The strength of the subtropical mixing barrier is relevant to the impact of lower stratospheric midlatitude aircraft emissions on tropical ozone (Douglass et al., 1999). All CTM versions produced some barrier to tropical-midlatitude exchange in the middle and lower stratosphere, but the barrier was noticeably weaker at  $4^\circ \times 5^\circ$  resolution. The simulation with the slowest ascent also had the strongest barrier to mixing with the mid-latitudes. Surprisingly, the simulation with faster ascent also had older mean age in the upper stratosphere because of the concomitant strong tropical-midlatitude exchange that ages tropical air.

Douglass et al. (2004) demonstrated that transport is important for the simulation of upper stratospheric ozone because the distribution of  $\text{NO}_y$  and  $\text{ClO}_x$  families, which provide the primary losses for  $\text{O}_3$ , are controlled by transport. Polar upper stratospheric transport was not significantly affected by a reduction in vertical levels above the middle stratosphere. However, moving the lid from 0.01 hPa to 0.4 hPa did have a significant effect. The lack of a full mesosphere in Low Lid inhibited transport of air from low to high latitudes, leading to a more isolated polar upper stratosphere. With a low lid and  $4^\circ \times 5^\circ$  resolution, the CTM compensated for weak transport in the polar upper stratosphere by enhanced horizontal mixing. Stronger horizontal mixing flattened the high latitude gradients, “correcting” the low  $\text{CH}_4$  in the polar region. This correction was cosmetic only and did not improve the physical representation.

The behavior of the Antarctic vortex is clearly very important to simulations of the

---

**Implementation  
issues in chemistry  
and transport models**

S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

---

**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

---

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

ozone hole, including those that predict its future disappearance. The reduction of vertical resolution above the lower stratosphere had a negligible effect on the behavior of the Antarctic vortex during spring, but lowering the lid increased poleward horizontal transport and mixing in the middle stratosphere. Low Lid allowed slightly greater mixing between the vortex and midlatitudes. Lowering the horizontal resolution to  $4^\circ \times 5^\circ$  produced a weak barrier, with significant mixing between vortex and midlatitude air masses throughout spring. The results of an experiment run at  $2^\circ \times 2.5^\circ$  with small scale wind structure removed determined that the poor vortex edge behavior was caused by the  $4^\circ \times 5^\circ$  resolution of the advection and not by a lack of small scale winds. A further experiment at  $1^\circ \times 1.25^\circ$  resolution showed only a small increase in vortex isolation. Realistic containment of perturbed chemistry inside the vortex is possible in this CTM integrated at  $2^\circ \times 2.5^\circ$ , but not at lower resolution.

The sensitivity to lid height was not the same in the Arctic and Antarctic lower stratosphere. The age spectra of all the  $2^\circ \times 2.5^\circ$  simulations were nearly identical in the Arctic, while in the Antarctic, the low lid model differed from both high lid models and indicated a greater influence from young air. This shows the need for a full mesosphere to well represent the Antarctic, not just because the mesosphere is a source of old air, but because the vortex mixing barrier is slightly better represented with a high lid. The simulation of Arctic lower stratospheric phenomena requires  $2^\circ \times 2.5^\circ$ , but many Arctic winters could be well represented without a full mesosphere or high vertical resolution above 50 hPa.

Low horizontal resolution compromises the model's ability to confine chemically perturbed air (e.g., high  $\text{Cl}_y$  and low  $\text{NO}_x$ ), which is especially important in the Antarctic vortex in September when ozone loss is rapid. This conclusion applies to the Lin and Rood advection scheme used here. Searle et al. (1998) saw no sensitivity of polar ozone loss to horizontal resolution that ranged from  $1.4^\circ \times 1.4^\circ$  to  $5.6^\circ \times 5.6^\circ$  in their CTM using a second order moments advection scheme (Prather, 1986), which is less diffusive because it carries more information about the constituent distribution within each gridbox; they did find less ozone loss as resolution decreased in a more diffusive

---

**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

advection scheme (Williamson and Rasch, 1989). Our CTM implementation results are consistent with the analyses of two  $4^\circ \times 5^\circ$  simulations with the GMI CTM (Conside et al., 2004). In the Antarctic, they found that high  $\text{Cl}_y$  was not maintained long enough and ozone loss was not fast enough to sufficiently deplete ozone in simulations integrated at  $4^\circ \times 5^\circ$ . Improvement in the containment of perturbed chemistry in the GSFC CTM integrated at  $2^\circ \times 2.5^\circ$  resolution has been seen in a recent 50-year CTM simulation of ozone recovery (Stolarski et al., 2005).

The experiments presented here show that a faithful representation of stratospheric transport in this CTM using Lin and Rood advection is possible with relatively low vertical resolution ( $>4$  km spacing) in the middle stratosphere and above, but lowering the lid from the upper to lower mesosphere has consequences for the realism of upper stratosphere. This ultimately has an effect on the polar lower stratosphere, but more so for the Antarctic than the Arctic. The fidelity of lower stratospheric transport is strongly dependent on the presence of realistic mixing barriers in both the subtropics and high latitudes, and thus requires  $2^\circ \times 2.5^\circ$  resolution. The ability of CTMs to quickly perform sensitivity studies such as these makes them a valuable tool for climate and chemistry assessments and in the development of thoroughly evaluated, credible chemistry-climate models.

*Acknowledgements.* We thank S. Pawson of the Goddard Modeling and Assimilation Office for providing FVGCN model output for the CTM integrations. This work was funded by the NASA Modeling, Analysis, and Prediction Program.

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---

**Implementation  
issues in chemistry  
and transport models**

---

S. E. Strahan and  
B. C. Polansky

---

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

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---

**Implementation  
issues in chemistry  
and transport models**

---

S. E. Strahan and  
B. C. Polansky

---

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

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---

**Implementation  
issues in chemistry  
and transport models**

S. E. Strahan and  
B. C. Polansky

---

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Print Version

[Interactive Discussion](#)



## Implementation issues in chemistry and transport models

S. E. Strahan and  
B. C. Polansky

**Table 1.** FVGCM online simulation and six CTM sensitivity experiments.

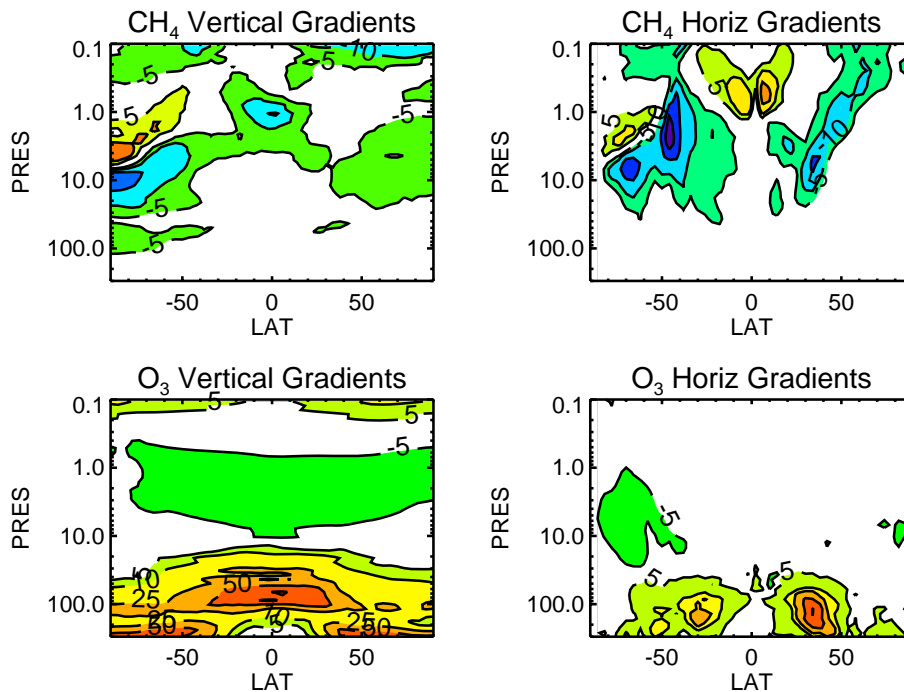
Name	Description	Levels	Model Lid (hPa)	Horizontal Resolution	Spatial Information (if different from resolution)
“Online”	Online Chemistry in a GCM	55	0.015	2°×2.5°	
“Full Vert”	Full resolution CTM	55	0.015	2°×2.5°	
“Reduced Vert” or “High Lid”	Reduced vertical resolution CTM	33	0.015	2°×2.5°	
“Low Lid”	Reduced vertical resolution and low lid CTM	28	0.4	2°×2.5°	
“Low Res”	Reduced vertical and horizontal resolution, low lid CTM	28	0.4	4°×5°	
“Smoothed”	Reduced vertical resolution, low lid, and smoothed winds CTM	28	0.4	2°×2.5°	4°×5°
“High Res”	Higher horizontal resolution with no added spatial information CTM	28	0.4	1°×1.25°	2°×2.5°

[Title Page](#)
[Abstract](#)
[Introduction](#)
[Conclusions](#)
[References](#)
[Tables](#)
[Figures](#)
[⏪](#)
[⏩](#)
[◀](#)
[▶](#)
[Back](#)
[Close](#)
[Full Screen / Esc](#)
[Print Version](#)
[Interactive Discussion](#)

---

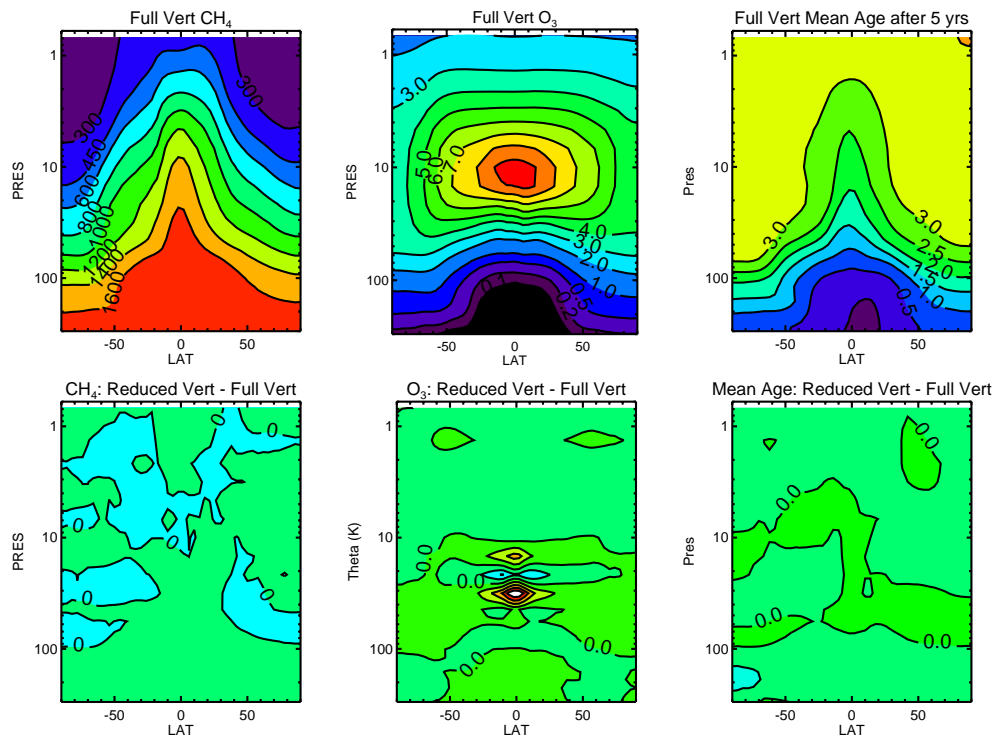
**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

---



**Fig. 1.** Gradients of CH<sub>4</sub> and O<sub>3</sub> calculated from April zonal monthly means from the GSFC CTM with 2°×2.5° resolution and 55 vertical levels. The vertical coordinate is pressure (hPa). Vertical gradients (left column) have units of percentage change/km (calculated for mixing ratios (upper box-lower box)×100/lower box) with negative values indicate decreasing tracer with height. Horizontal gradients (right column) have units of percentage change/4° latitude (calculated for mixing ratios (poleward-equatorward)×100/equatorward), with positive values indicating a poleward increase. No values are calculated across the equator. White areas represent gradients of less than 5%. Methane is most sensitive to vertical motions in the polar regions during seasons of descent (fall/winter) while ozone sensitivity is similar in all months.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

Implementation  
issues in chemistry  
and transport modelsS. E. Strahan and  
B. C. Polansky

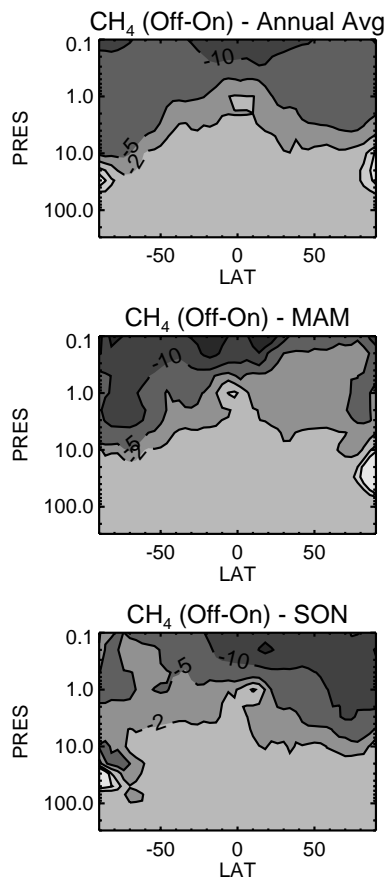
**Fig. 2.** Top panels: Zonal annual mean CH<sub>4</sub> (ppb) and O<sub>3</sub> (ppm), and mean age (years) in the GSFC CTM with full vertical resolution. Bottom panels: Differences in CH<sub>4</sub>, O<sub>3</sub>, and mean age between a reduced resolution CTM and the full resolution CTM (Reduced Vert – Full Vert). The vertical coordinate is pressure (hPa). The intervals in the difference plots are 50 ppb CH<sub>4</sub>, 0.2 ppm O<sub>3</sub>, and 0.1 year. Methane and mean age show very small differences with no particular pattern. Ozone is sensitive to the slightly different spacing of levels in these models near its large tropical gradient.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

---

**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

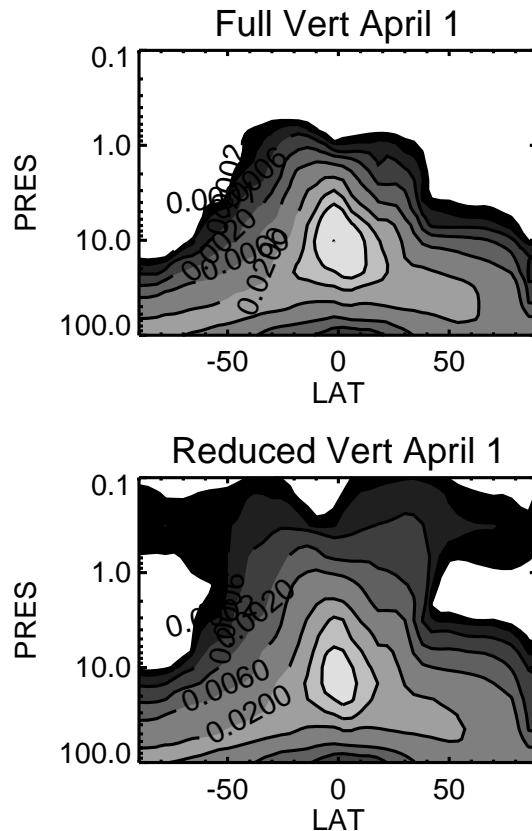
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**Fig. 3.** Percentage difference in CH<sub>4</sub> distributions between the offline CTM calculation and an online chemical calculation in a GCM ( $(\text{offline-online})/\text{online} \times 100\%$ ). Top to bottom: annual average, March-April-May mean, and September-October-November mean. The vertical coordinate is pressure (hPa).

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)



**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

**Fig. 5.** Comparison of Full Vert (top) and Reduced Vert (bottom) age tracer distributions near the end of the 2nd year of simulation. Reduced Vert transports the tracer into the lower mesosphere much more quickly than Full Vert. The vertical coordinate is pressure (hPa).

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

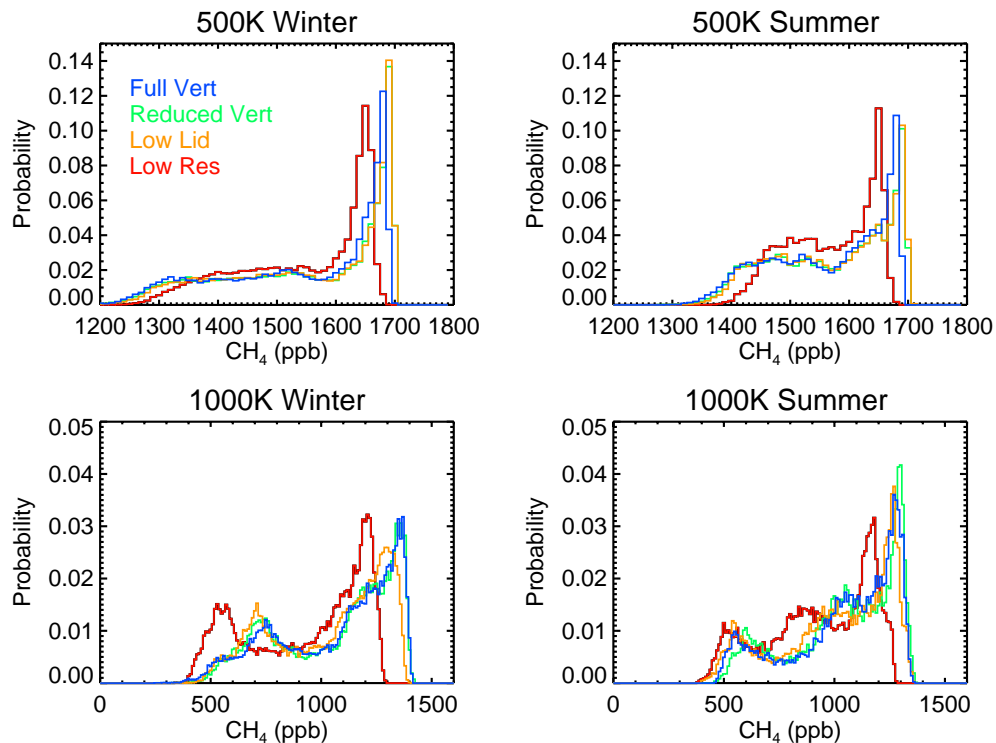
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**Implementation  
issues in chemistry  
and transport models**

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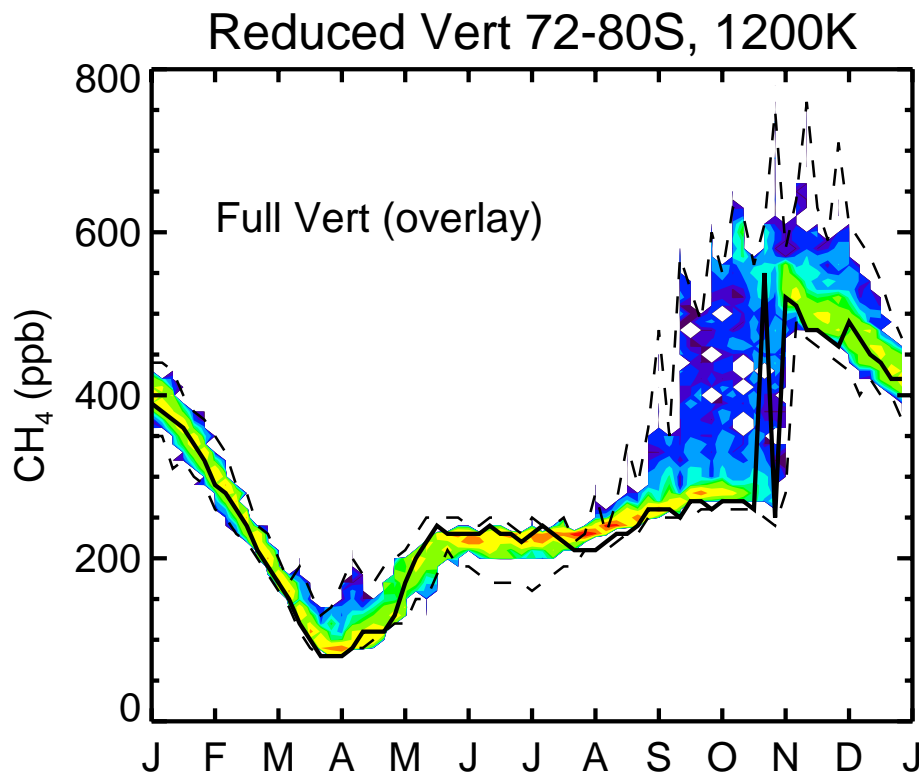
S. E. Strahan and  
B. C. Polansky

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**Fig. 6.** Probability distribution functions (pdfs) of CH<sub>4</sub> at 500 K (top panels) and 1000 K (bottom panels) in winter (left) and summer (right) for 4 CTM simulations. Full Vert (blue), Reduced Vert (green), and Low Lid (orange) all have 2°×2.5° resolution and nearly the same tropical-midlatitude separation. Low Res (red) produces a subtropical mixing barrier, but peak separation differs from the higher resolution models.

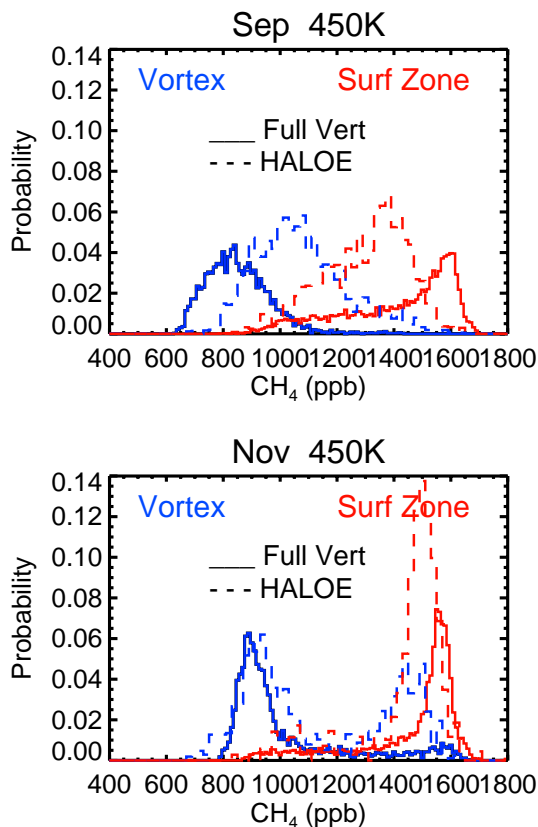
[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

**Fig. 7.** The annual cycle of model CH<sub>4</sub> 72–80° S on the 1200 K surface using contoured pdfs. Yellow and red are high values of the most probable mixing ratio, and purple and blue indicate low probability, or infrequently observed mixing ratios. Reduced Vert is shown in color and the outline of the mean (solid) and range (dashed) for Full Vert is overlaid.

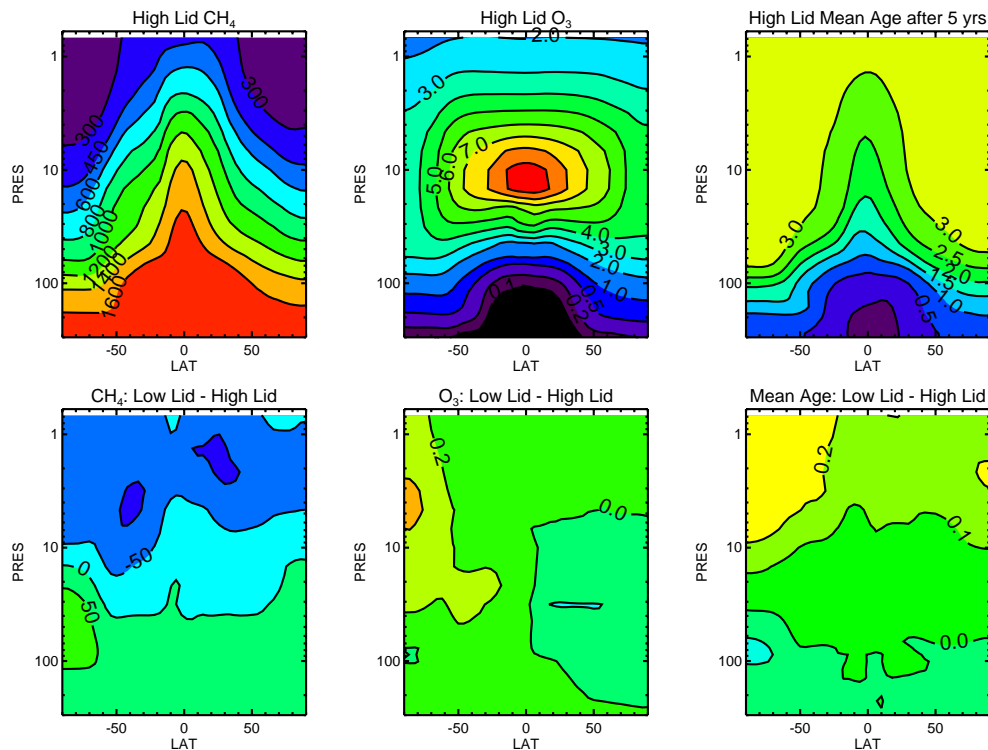
[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)



**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

**Fig. 8.** Comparison of the separation of vortex (60–80° S, blue) and midlatitude (44–60° S, red) air masses in Full Vert (solid) and HALOE (dashed) CH<sub>4</sub> in September and November. Full Vert has a sharper vortex edge in September than seen by HALOE, but by November, model and observed vortex and midlatitude air masses distributions are very similar. Pdfs from Reduced Vert (not shown) are indistinguishable from Full Vert.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

Implementation  
issues in chemistry  
and transport modelsS. E. Strahan and  
B. C. Polansky

**Fig. 9.** Top panels: Zonal annual mean CH<sub>4</sub> and O<sub>3</sub>, and mean age in High Lid (Reduced Vert). Bottom panels: Differences in CH<sub>4</sub>, O<sub>3</sub>, and mean age between Low Lid and High Lid (Low Lid – High Lid). The vertical coordinate is pressure (hPa). Methane and mean age show an altitude dependent pattern of differences. As a percentage, CH<sub>4</sub> differences are largest in the upper stratosphere. Both O<sub>3</sub> and age lack hemispheric symmetry in their differences, possibly related to the influence of mesospheric air on the upper stratosphere.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

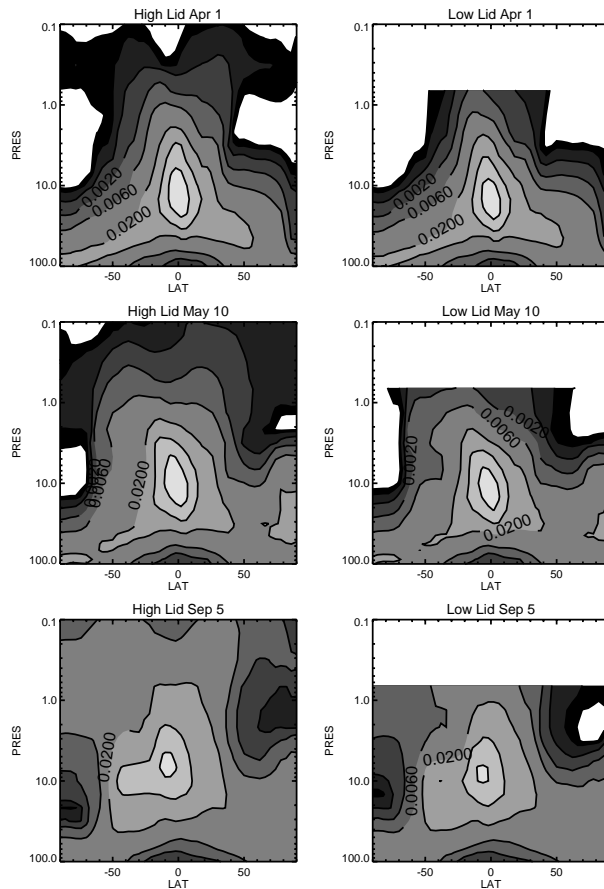
Print Version

Interactive Discussion

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**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

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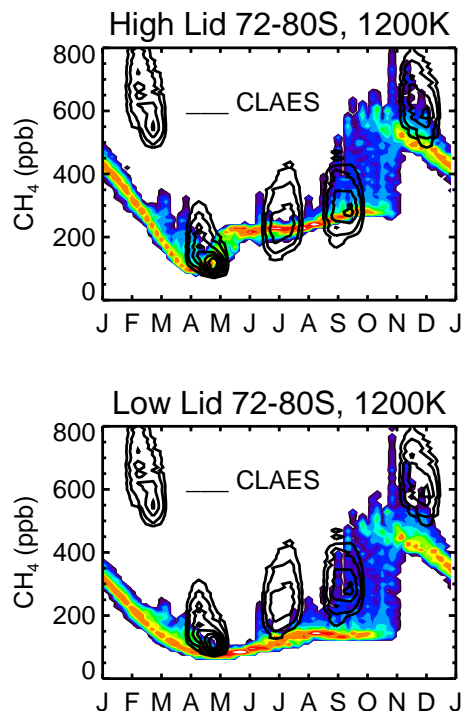
**Fig. 10.** Zonal mean age tracer distributions for High Lid (left panels) and Low Lid (right panels) for 1 April (day 641), 10 May (day 680), and 5 September (day 797). The vertical coordinate is pressure (hPa). High Lid is able to transport the tracer through the lower mesosphere and back down into the polar upper stratosphere. Lacking this pathway, Low Lid transports air to this region much more slowly.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

---

**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

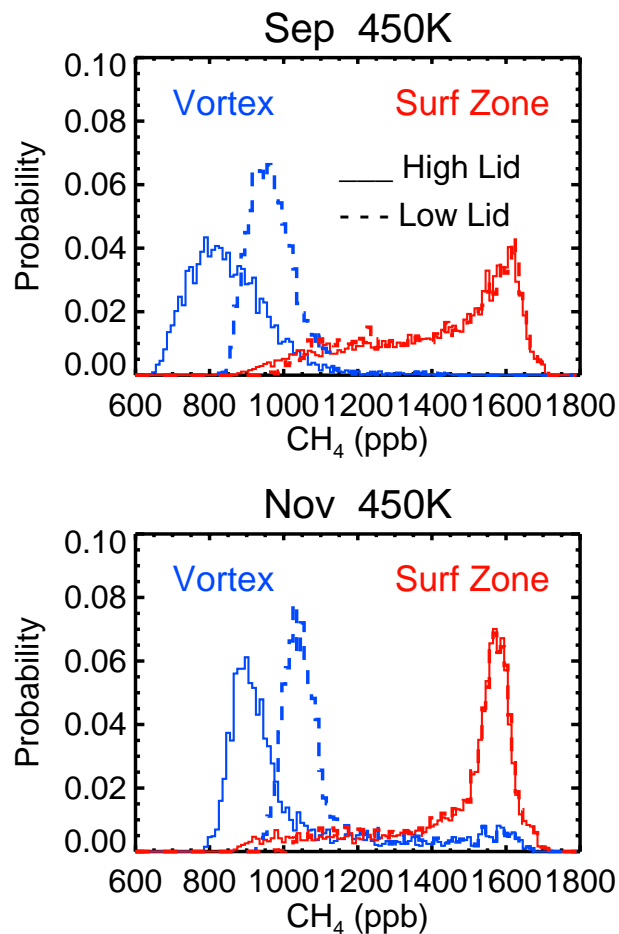
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**Fig. 11.** The annual cycle of CLAES and model  $\text{CH}_4$  72–80° S on the 1200K surface using contoured pdfs. Yellow and red are high values of the most probable mixing ratio, and purple and blue indicate low probability, or infrequently observed values. CLAES pdfs from 5 southern hemisphere viewing periods are overlaid on the High Lid (top) and Low Lid (bottom) annual cycles. The innermost contours of the CLAES pdfs are the most probable values.

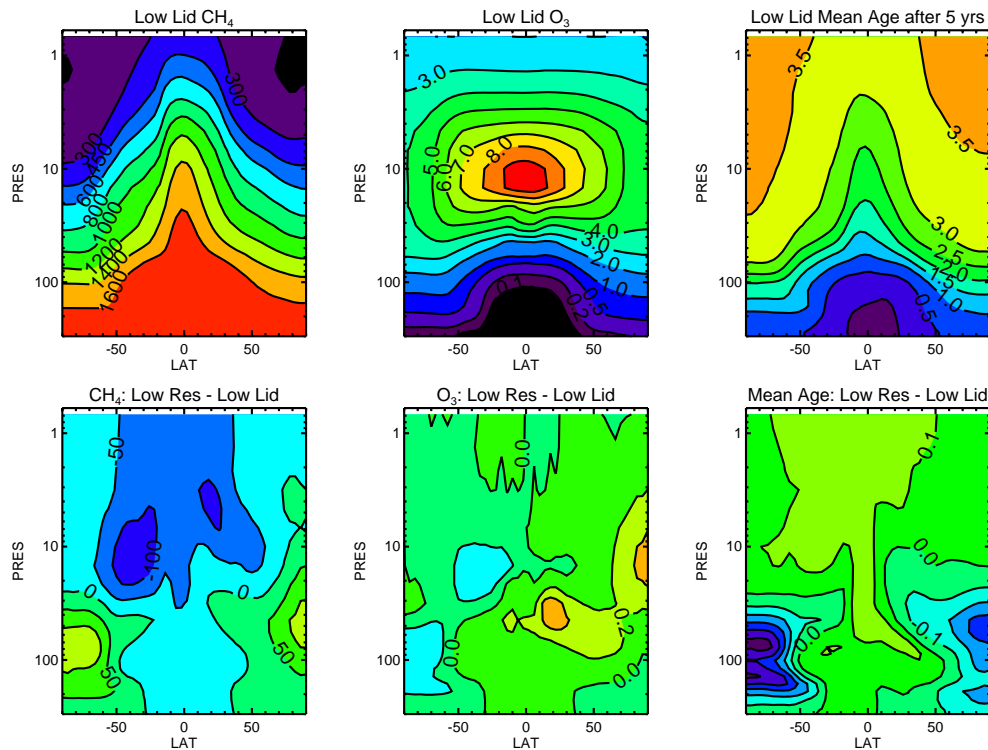
[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

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**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

**Fig. 12.** Comparison of the separation of vortex (60–80° S, blue) and midlatitude (44–60° S, red) air masses in High Lid (solid) and Low Lid (dashed) in September and November. The lid height does not affect the midlatitude distributions, but the High Lid vortex maintains lower CH<sub>4</sub>.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

Implementation  
issues in chemistry  
and transport modelsS. E. Strahan and  
B. C. Polansky

**Fig. 13.** Top panels: Zonal annual mean CH<sub>4</sub> and O<sub>3</sub>, and mean age in the GSFC CTM with reduced vertical resolution and low lid (Low Lid). Bottom panels: Differences in CH<sub>4</sub>, O<sub>3</sub>, and mean age between a 4°×5° resolution CTM (Low Res) and the 2°×2.5° resolution Low Lid. The vertical coordinate is pressure (hPa). Lowering the horizontal resolution has the largest effect of any of the implementation changes. The tropical pipe is not as isolated and poleward transport is much stronger in the lower stratosphere.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Print Version

Interactive Discussion

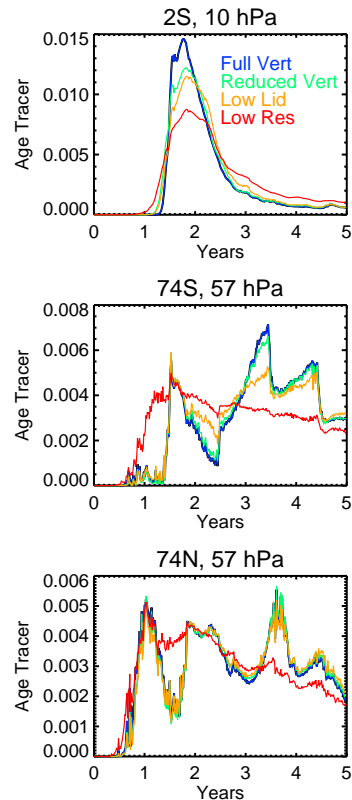
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**Implementation  
issues in chemistry  
and transport models**

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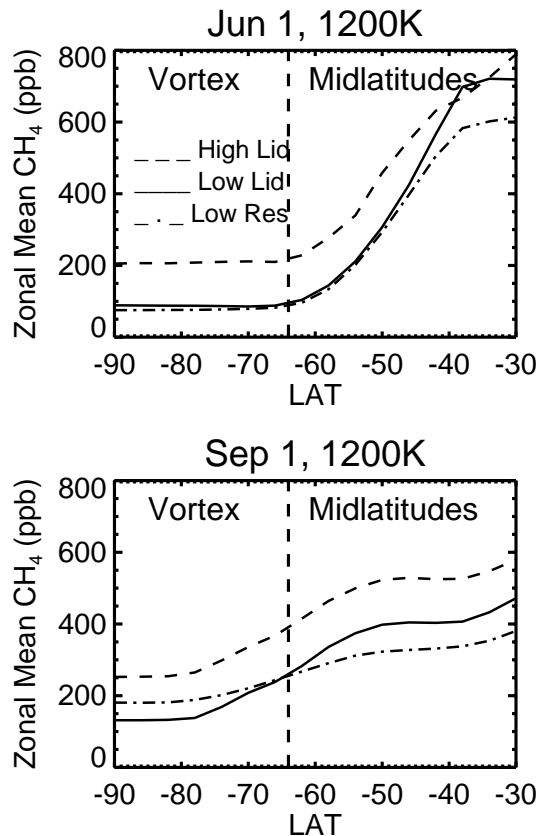
S. E. Strahan and  
B. C. Polansky

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**Fig. 14.** Five-year age spectra in the tropical middle stratosphere (top), and Antarctic (middle) and Arctic (bottom) lower stratosphere from 4 simulations. In the middle stratosphere, the simulation with the highest (lowest) spatial resolution (Full Vert, blue and Low Res, red) has the slowest (fastest) tropical ascent with the greatest (least) tropical isolation. Low Lid shows transport differences from the high lid simulations in the Antarctic but not in the Arctic.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

**Fig. 15.** Methane meridional gradients in the SH for High Lid (dashed), Low Lid (solid), and Low Res (dot-dash). The gradients of the three simulations are similar in late fall (top), but by the end of winter (bottom), the Low Res gradient between the midlatitudes and the vortex is much flatter than the two  $2^\circ \times 2.5^\circ$  simulations.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

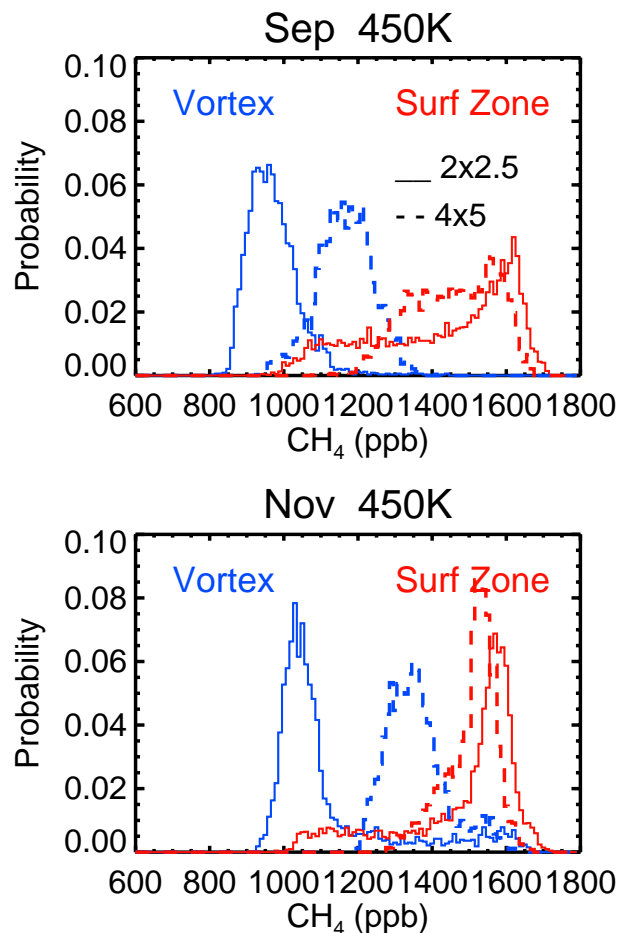
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Full Screen / Esc

Print Version

Interactive Discussion



**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

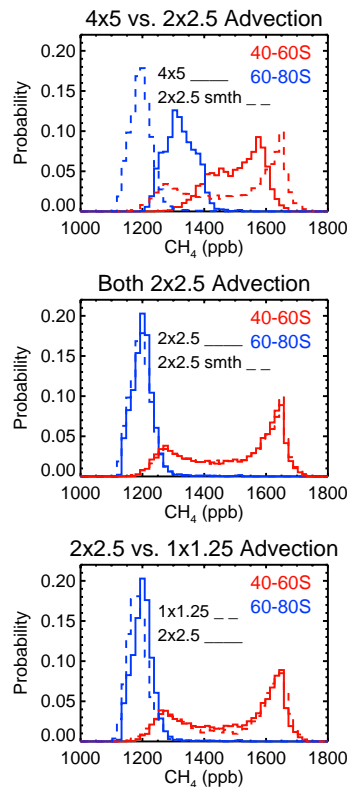
**Fig. 16.** Comparison of the separation of vortex (60–80° S, blue) and midlatitude (44–60° S, red) air masses in Low Lid (solid) and Low Res (dashed) in September and November. The large shift in Low Res vortex mixing ratios indicates vortex isolation is compromised by low horizontal resolution.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)

---

**Implementation  
issues in chemistry  
and transport models**S. E. Strahan and  
B. C. Polansky

---



**Fig. 17.** The effects of advection resolution and small scale winds on vortex behavior, demonstrated with the evolution of vortex and midlatitude  $\text{CH}_4$  pdfs. All simulations began with the same initial conditions on 1 July. Top: simulations with different horizontal resolution but same scale forcing in the wind fields ( $4^\circ \times 5^\circ$ ). Middle: simulations with the same resolution ( $2^\circ \times 2.5^\circ$ ) but different scale forcing in the wind fields. Bottom: simulations with different horizontal resolution but same scale forcing in the wind fields ( $2^\circ \times 2.5^\circ$ ).

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)