Satellite Observations and Chemistry Climate Models – A Meandering Path Towards Better Predictions

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Talk Outline

• Introduction
  – Assessment and prediction
    • What will happen to ozone as CFCs decrease?
    • What will happen to ozone as climate changes?
  – Satellite data

• Model evaluation
  – A natural experiment
  – Process evaluation – one step further
  – Upper stratospheric ozone – using the present day ozone response to temperature to explain variance in prediction

• Future Directions and conclusions
Overall agreement of time dependence reflects boundary conditions that prescribe mixing ratios of anthropogenic chlorine containing species.

Total column ozone timeseries 60S – 60N from many Chemistry Climate Models (normalized to 1980) compared with observations (stars)

Merged Ozone Data Set (Stolarski and Frith, 2006) Nimbus 4 BUV (70-72), Nimbus 7 TOMS (79 – 93), Earth Probe TOMS (96-05), OMI (04 – present); 4 SBUV instruments: NOAA 9 (85 – 98) NOAA 11 (89 – 03), NOAA 16 (00 – present), NOAA 17 (02 – present)
Clearly, comparisons with total ozone alone do not discriminate among simulations. For years, justification for satellite programs partially rests on the need for observations to compare with simulated fields in order to identify the physical and photochemical processes that control the ozone distribution. This information should improve the model physical basis and decrease uncertainty in prediction . . . Can’t we do any better than this???
Stratospheric Chemical Processes

- UV Radiation
- Polar Ozone Depletion
- Polar Stratospheric Clouds
- Tropopause Folds
- Tropics
- Mid-latitudes
- Poles
- H₂O, CFC’s, CH₄, N₂O, SO₂
- CFC’s
- Troposphere
- Stratosphere
EOS Aura Satellite

- Orbit: Polar, 705 km, sun-synchronous, 98° inclination, ascending 1:45 PM equator crossing time.
- Six Year Spacecraft Life.
ACE FTS on Sci-Sat
- a high spectral resolution (0.02 cm$^{-1}$) Fourier Transform Spectrometer (FTS)
- an occultation instrument (sunrise and sunset profiles of many constituents)

For many constituents the vertical domain extends into the upper troposphere (O3, H$_2$O, N$_2$O, CH$_4$, HNO$_3$, CFC-11)
Building blocks of an ozone assessment simulation

• Observe atmospheric constituents and meteorological fields
  • Laboratory experiments
    – Develop chemical mechanism
    – Measure reaction rates, cross sections . . .
  • Field experiments
    – Identify transport processes
    – Test photochemical concepts
• Develop a global model that encapsulates present knowledge of the general circulation and the photochemical processes that control ozone
• TEST THAT MODEL!
• Use the model for predictions
Three examples of model validation/evaluation

- A natural experiment (Aura MLS)
- The Chemistry Climate Evaluation (CCMVal) tests of stratospheric transport ($N_2O$ from SciSat ACE and Aura MLS along with mean age values derived from aircraft and balloon measurements of $SF_6$ and $CO_2$)
- Upper stratospheric ozone – using the response of ozone to temperature change in the present atmosphere to explain the differences among predictions
A natural experiment – a blob that refused to die!

• The ‘blob’ is air with high N$_2$O pulled into the Aleutian anticyclone very close to the transition to the summer circulation.
• Hess and Holton (*late 80s*) studied such events as seen in LIMS data, and their simulations showed that anomalies persisted in the summer circulation.
• DATA – Aura MLS N$_2$O
• Simulation: Chemistry and Transport Model (CTM) using GEOS-5 assimilated meteorology

Allen et al., *Modeling the Frozen-In Anticyclone in the 2005 Arctic Summer Stratosphere, submitted, 2011*
Testing the model – a natural experiment

Early in March, a blob of tropical air with high N$_2$O is pulled into the Aleutian Anticyclone. The transition to summer circulation took place shortly after this feature appeared.

The ‘blob’ circled the pole many times and remained discernible until the end of August. This is a ‘natural experiment’ to test the fidelity of assimilated meteorology and numerical transport schemes.
GMI ‘replay’ credibly simulates the blob

- Building blocks of the simulation
  - Photochemical mechanism (principle loss for N$_2$O is photolysis, also reaction with O($^{1}$D))
  - Numerical transport scheme (Lin and Rood, 1996)
  - Meteorological analysis (GEOS-5 system, incremental analysis update)

- Together these blocks make up a ‘chemistry and transport model’ (CTM)
The behavior of a simulated N$_2$O anomaly at 850K closely resembles that observed. Specific points of comparison include:

a) Formation of the blob (mid-March/April)

b) Movement of the blob around the pole with little or no change in shape and magnitude (June/July)

c) Mixing with the background until the blob becomes indistinguishable from the background (mid-August).

Allen et al., Modeling the Frozen-In Anticyclone in the 2005 Arctic Summer Stratosphere, submitted to ACP 2010
The natural experiment - conclusions

• GEOS-5 meteorology is enough like the atmosphere to make a simulation possible;
• The Lin and Rood (1996) numerical transport algorithm (upwind biased, monotonic*, shock-capturing) is good enough
• PROVIDED that the horizontal grid used in the CTM is smaller than the ‘blob’

*scheme does not create new maxima or minima
Transition from Chemistry Transport Model to Chemistry Climate Model

**Why do we need to do this?**

- The ozone mixing ratio at any point depends on some combination of local photochemical processes and transport
- If transport is important, then non-local photochemical processes matter
- Ozone photochemical loss is temperature dependent (more loss at warmer temperature)
- Temperature depends on heating due to absorption of UV by $O_2$ (leading to ozone formation) and $O_3$
- The winds that transport ozone also depend on the temperature

**In a CCM, winds, temperature and ozone are computed self-consistently.**
Transition from Chemistry Transport Model to Chemistry Climate Model

• Building blocks
  – A general circulation model (these are developed using an ozone climatology and include a radiation code)
  – CTM components
    • A photochemical mechanism and solver (~50 photolysis reactions and more than 130 two- and three-body reactions involving radicals (very short lived reactive species), reservoirs (medium lived species that tie up radicals and keep them from doing other things) and source gases (long lived gases of tropospheric origin from which radicals form).
    • A numerical transport scheme

• These blocks must work together realistically (and in a computationally tractable manner)

• How do we test the model?*

*The individual pieces might work separately but not together
Process Evaluation

• CCMs produce fields of constituents (and meteorology) that can only be compared to observations in a statistical sense

• CCMVal Strategy has two elements:
  – (one) Exploit interannual variability to identify fundamental relationships
  – (two) Identify ‘state’ quantities that are important and do not vary year-to-year
Example one: relationship between winter high latitude ozone buildup to the winter heat flux

Heat Flux is calculated using fields from a meteorological analysis.

Ozone columns measured by GOME are used to calculate the spring and fall high latitude averages.

Mar/Oct NH
Oct/Mar SH

This is an example of a robust relationship that is derived from interannual variability of observations and should be reproduced by any CCM.
Example 2 - Mean Age for stratospheric air

- Mean age for a stratospheric parcel is the time since it crossed the tropical tropopause.
- Mean age is generally derived from measurements of something that is increasing in the troposphere like SF$_6$ or CO$_2$.
- Age is typically measured in years – so each ‘parcel’ can be thought of as being made of many elements that have followed different trajectories since crossing the tropopause and thus have different ‘element ages’ – this is the ‘AGE SPECTRUM’
What does an age spectrum look like?

Back trajectory calculations for hundreds of elements are initiated very close to a single point. Keep track of each element until it crosses the tropical tropopause. This is the ‘age’ of the element.

We can easily calculate the age spectrum. We cannot measure it, but we can get information as will be explained later.
What does the mean age look like?

- Air ascends slowly in the tropics with little mixing; it takes close to 3 years for air to reach the upper stratosphere after crossing the tropical tropopause.

- Middle latitude air is older than tropical air at all latitudes.

- There is a sharp transition in age between the tropics and middle latitudes.

Strahan et al., ACPD, Using transport diagnostics.
Do CCMs (or CTMs or 2D models) have realistic mean age?

In 2002, almost universally ‘no’!

Hall et al., 1999 ‘Evaluation of transport in stratospheric models, JGR

In 2006, almost universally ‘yes’!
How can we obtain global information about mean age of air?

Trajectory calculations show that older elements have been to higher altitude.

Loss for all source gases of tropospheric origin increases with altitude; altitude where local lifetime decreases from many years to weeks or days varies with species.
Measured $N_2O$ depends on the history of the elements

RESULT: $N_2O$ (measured by MLS and ACE) is nearly linearly related to mean age in the lower stratosphere.

These elements will have near zero $N_2O$ because they have spent time in the upper atmosphere where $N_2O$ loss is rapid.

These elements will have $N_2O$ close to their tropopause value.
Relationship between ACE climatology for $\text{N}_2\text{O}$ and mean age measurements.

Relationship breaks down for old age because, if mean age is this old, time in the upper stratosphere is great for most elements.
CCMVal used this relationship to evaluate CCMs.

‘bad’ is important – poor agreement indicates problems with the simulated circulation but also implies issues with the balance of terms in the ozone tendency equation (e.g., ‘fast’ circulation so that transport dominates photochemistry over too large a range).
Going back to the original slide - CCMs that best reproduced the relationship between MEAN AGE and N₂O and other important features of stratospheric transport (red lines) predict narrow range for ozone ‘recovery’.
Diagnostics reveal whether or not particular models faithfully represent atmospheric processes. The models that succeed predict similar response for O$_3$ to changes in composition (CFC decrease and CO$_2$ increase) and climate – so this is a *successful diagnostic*. The step not taken – these diagnostics do not provide a framework to explain the differences among predictions.
Upper stratospheric ozone

- Upper stratospheric ozone is important because
  - Largest unambiguous signature of ozone loss due to chlorine increase
  - First place to see the ozone loss had leveled off as chlorine leveled off (Newchurch et al., JGR, 2003)
  - This is where we expect to see evidence of ozone increase as chlorine decreases - BUT
Chlorine is decreasing much more slowly than it increased.

Rate of decrease
- 0.027 ppb/year
Froidevaux et al., GRL, 2006 (Aura MLS)

Compared to
Rate of increase
+ 0.110 ppb/year
Anderson et al., JGR 2000 (UARS HALOE)
High altitude station data are noisy; chlorine decrease since 2000 is small; solar effects confuse the record; AND

Temperature trend during the whole period (decrease) leads to less efficient ozone destruction (i.e., ozone increase) throughout the entire period.

Shaded region on figure is ‘model range’ – exactly what do we mean by that?

Data are five month running average; simulations are 24 month running average (remove QBO and annual mean)
The ‘shaded’ range on the previous slide is a range of model results that reveal different sensitivities to chlorine change, temperature change and solar cycle.
The CCMVal simulations show a wide range of values for ozone mixing ratio and temperature.

GOAL: analyze the base state (i.e., simulation in the year 2000) and use observations to understand what causes the differences and similarities among the projections.
Clear relationship between the ozone mixing ratio and its sensitivity to temperature as revealed by the seasonal cycle.
Upper atmospheric ozone loss

- Chapman Chemistry
  - $O + O_3 \rightarrow 2 O_2$

- Chlorine catalytic cycle
  - $ClO + O \rightarrow Cl + O_2$
  - $Cl + O_3 \rightarrow ClO + O_2$  \[\text{NET} \quad O + O_3 \rightarrow 2 O_2\]

- Similar cycles involving nitrogen radicals ($NO, NO_2$) and hydrogen radicals ($OH, HO_2, H$)
The temperature dependence of each loss process is unique

- $O + O_3$ – most temperature dependent
- $ClO + O$ – least temperature dependent
- $O_3$ Sensitivity to T will likely match that derived from observations if the mix of loss processes is correct
- If mean T is high biased, then simulated ozone will be low (and vice versa)
What about those ‘outliers’?

- The outliers are from a model that is missing ClO + OH → HCl + O₂;
- ClO + O is more important without this competing process.
- Chlorine loss process is too important and O₃ is less sensitive to temperature.
Does data tell if sensitivity is realistic?

Sensitivity derived from Aura MLS 2005 - 2008

Annual Mean Ozone from MLS (simulations are too low – but simulated T is also 5-10 degrees too warm
Chlorine increased when CFCs were in use and is now decreasing due to the Montreal Protocol and amendments.

- $O + O_3$ – most temperature dependent
- $ClO + O$ – least temperature dependent

So – as chlorine increases, temperature sensitivity decreases; as chlorine returns to background values, temperature sensitivity increases.
Ozone sensitivity to temperature increases as chlorine decreases in all simulations

All models conform to the general idea that as the mix of loss processes changes the sensitivity of ozone to temperature can change.
One step further – sensitivity of ozone to temperature, mix of loss processes is related to predicted ozone change
Upper Stratospheric Ozone Conclusions

• In all simulations, ozone becomes more sensitive to temperature as chlorine decreases.
• Ozone sensitivity to temperature change varies among models, showing that the mix of upper stratospheric loss processes is not the same across models.
• If simulated ozone is more sensitive to temperature change for present conditions, future simulated ozone increase is greater.
Summary (1)

• Natural Experiment
  – Numerical transport and assimilated fields reproduce an event that led to a large persistent anomaly; Simulation anomaly tracked observed with fidelity for 5 months

• CCMVal transport evaluation
  – Simulations that reproduce important aspects of stratospheric transport predict similar future behavior for stratospheric ozone
Summary (2)

• Upper Stratospheric Ozone
  – Sensitivity to temperature tells about the mix of loss processes that control ozone
  – Sensitivity varies among simulations; predictions of future ozone change vary according to present-day sensitivity (i.e., variance in prediction is explainable using observations and follows from basic understanding of photochemistry)

• Challenge: Can we develop approaches based on other diagnostics that focus more on the response to a perturbation rather than on the state?
  – E.g., Newman et al. show that the Antarctic ozone hole variability is explained by interannual variations in temperature and the slow change in total chlorine. Do models produce this relationship?
Grand Conclusions

• Global observations are a necessary building block for the foundation and evaluation of global models.
• We have work to do to take the next step to reduce uncertainty in prediction
  – Continue in the use of process oriented diagnostics because this is a path towards both an improved conceptual model and its more realistic implementation
  – Identify performance metrics (and groups of metrics) that explain why different models respond differently to the same perturbation
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