Atmospheric chemistry

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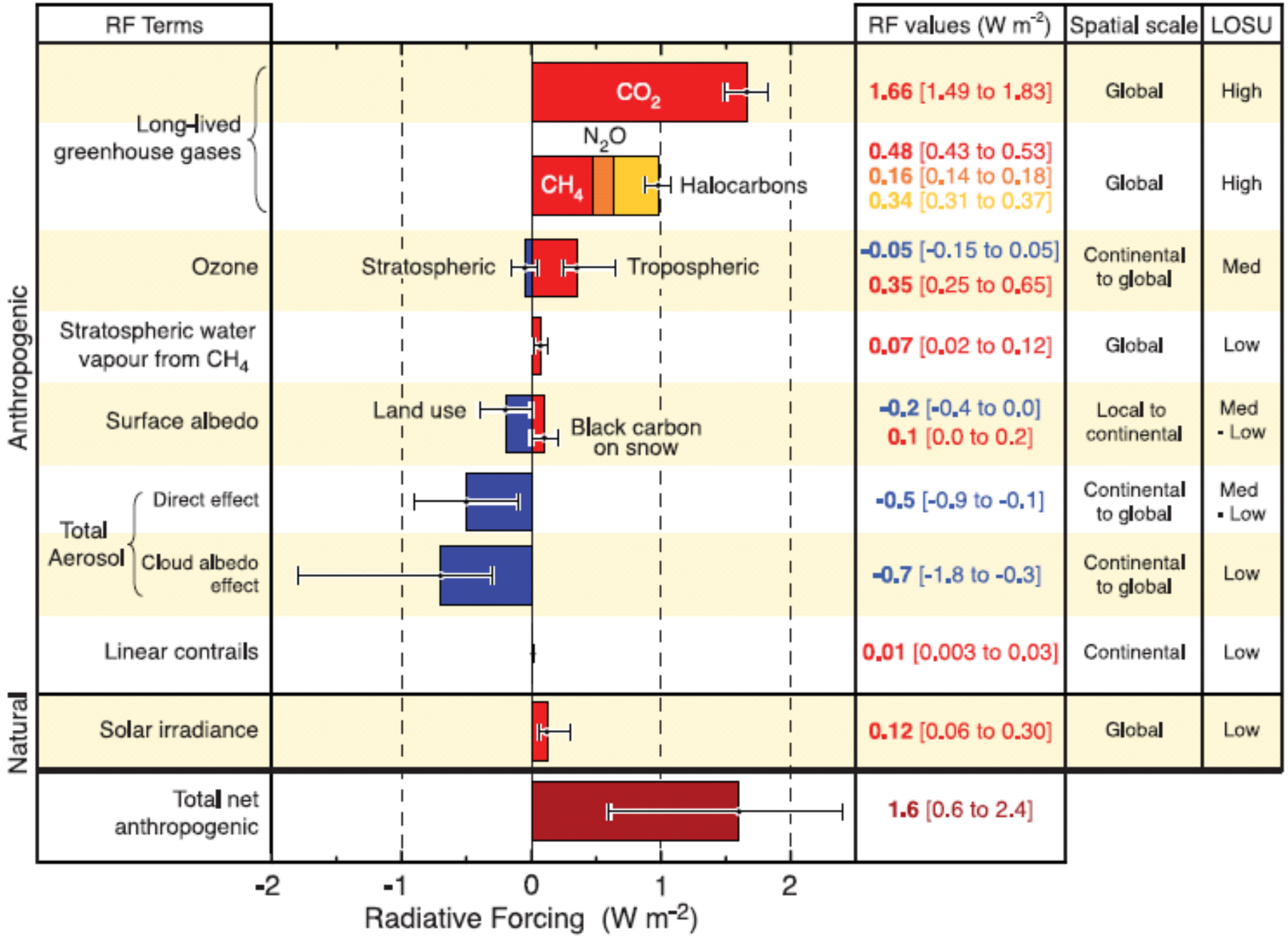
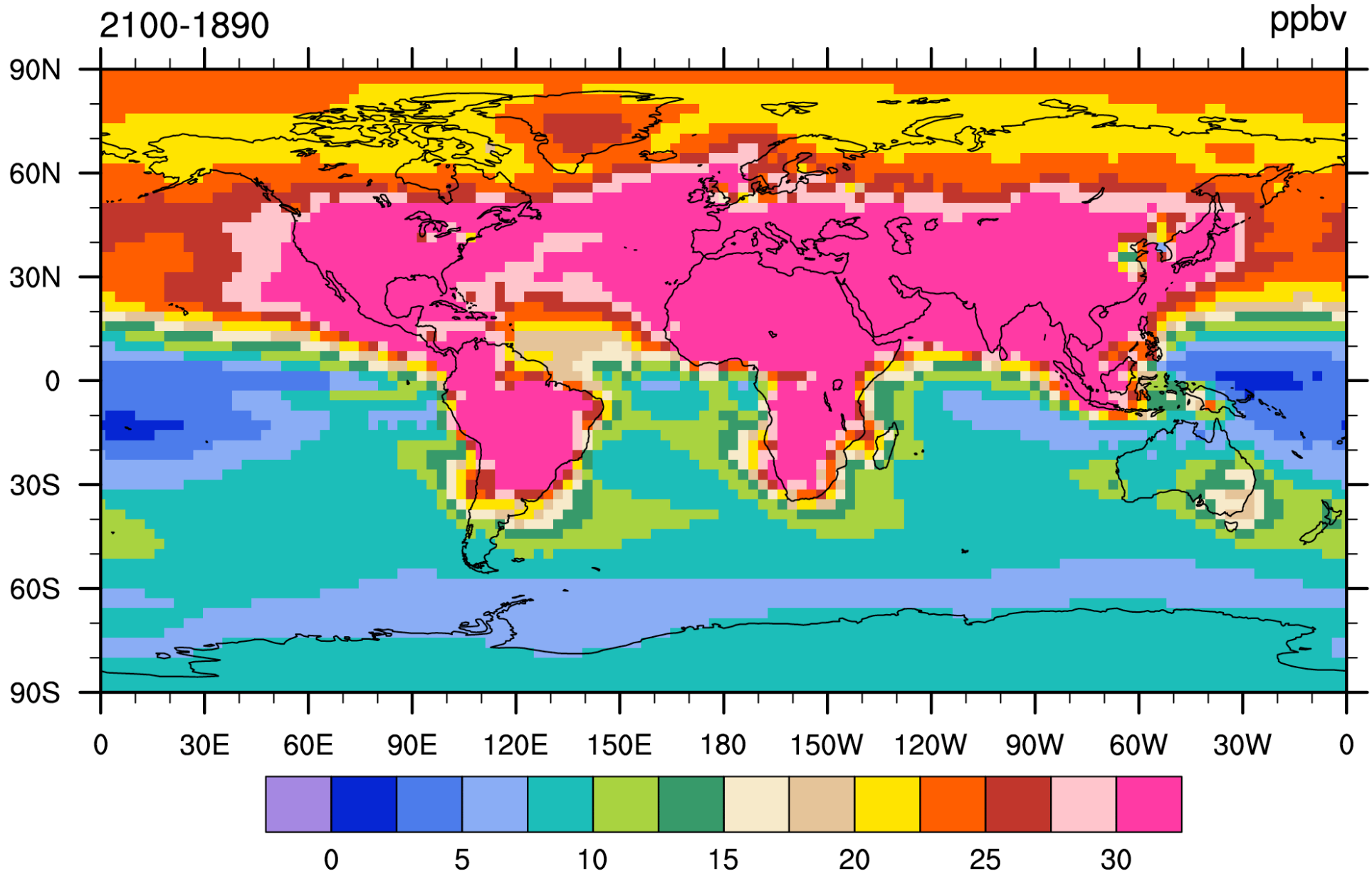
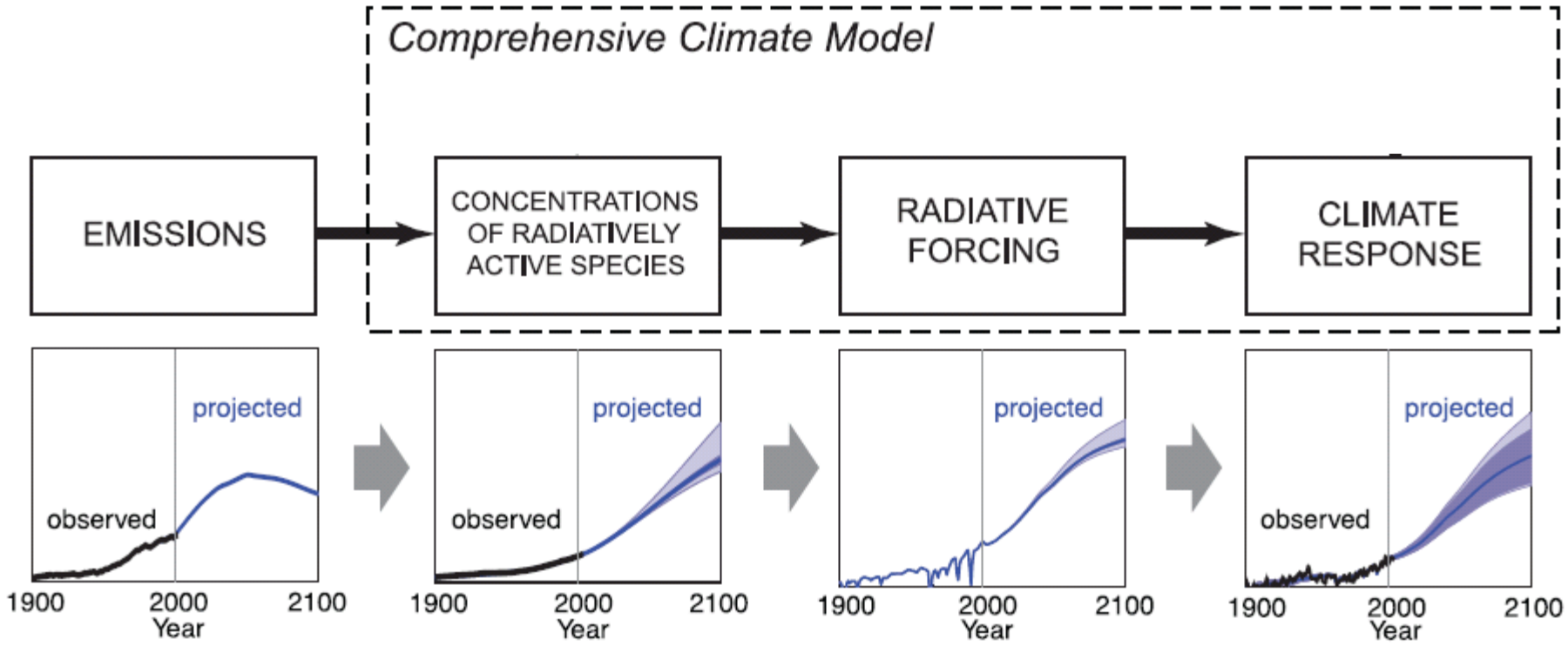
Radiative Forcing Components




2100-1890
ppbv
90N
60N
30N
0
30S
60S
90S
0
30E
60E
90E
120E
150E
180
150W
120W
90W
60W
30W
0
5
10
15
20
25
30

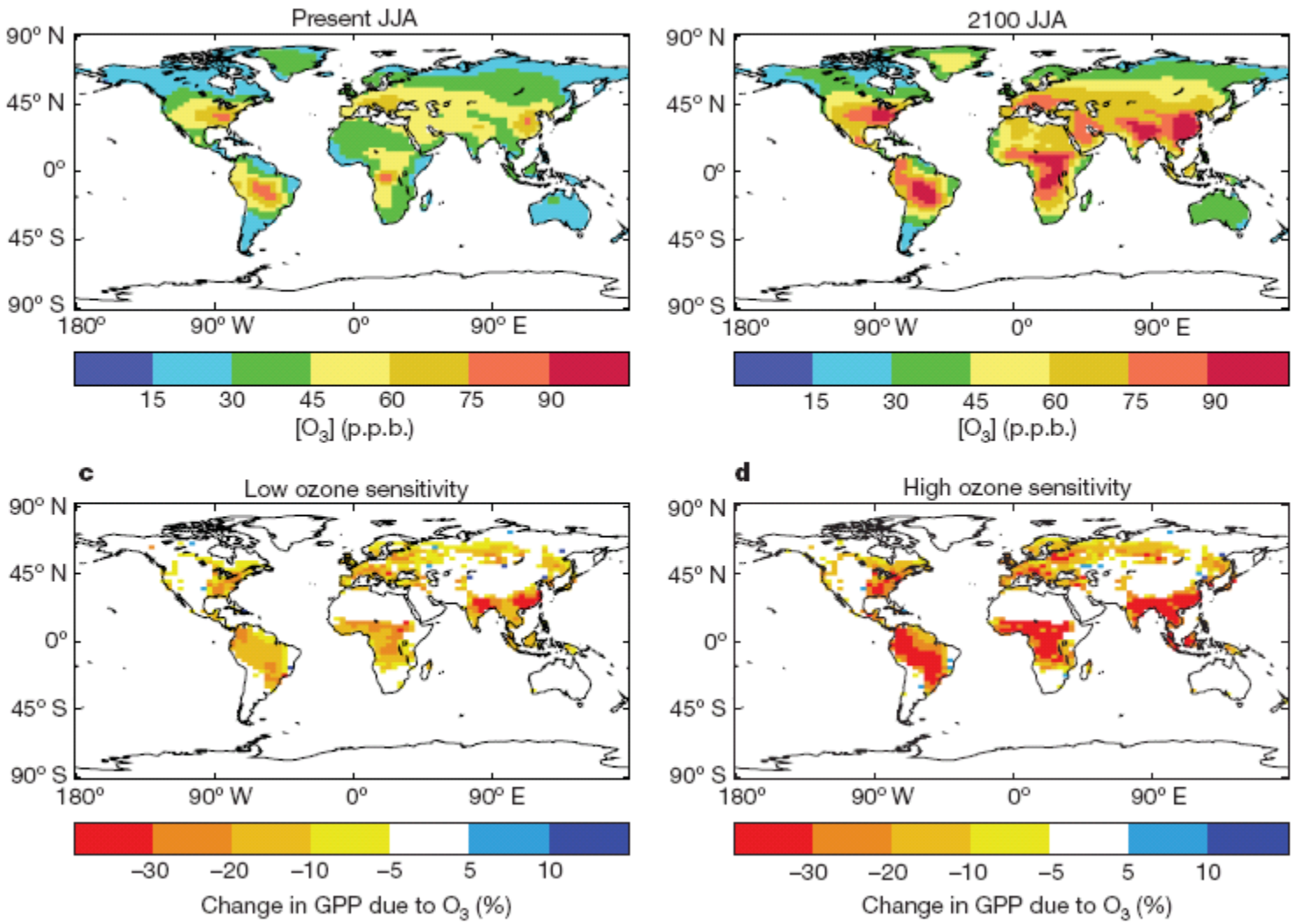
Chemistry to climate



Importance of chemistry

- Climate forcing
  - Direct radiative forcing: ozone and methane, aerosols
  - Aerosol indirect effects
- Impact on vegetation
  - Ozone poisoning
  - Nitrogen deposition
- Air quality
  - Ozone and carbon monoxide
  - PM1, PM2.5

Ozone and vegetation



Sitch et al., 2007

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Air quality during the 2003 heat wave

International Herald Tribune | 5
Wednesday, September 10, 2003

Heat claimed 15,000 in France

Estimate by funeral director exceeds latest by government

From news reports

PARIS: The number of people who died in France because of the August heat wave is 15,000, the country's largest undertaker estimated Tuesday, placing the death toll about 3,500 higher than the official government figure.

Isabelle Dubois-Costes, a spokeswoman for General Funeral Services, said the revised total includes deaths from the second half of August, after record-breaking temperatures had abated.

Late last month, the government issued its official estimate of 11,435, but the Health Surveillance Institute, which calculated the death toll for the government, said Tuesday that the total only counted deaths through the first

died. At the time, the government put the figure at a maximum of 3,000.

The heat wave brought suffocating temperatures of up to 40 degrees Celsius (104 degrees Fahrenheit) in the first two weeks of August in a country where air conditioning is rare. The heat baked many parts of Europe, but nowhere was

The revised total includes deaths from the second half of August.

the toll higher than in France.

While the bulk of the victims — many

families were away on lengthy August vacations. Authorities reportedly had difficulty making contact with survivors who were away on vacation.

A team of medial experts named by the Health Ministry to conduct the first official inquiry into the crisis issued a scathing report Monday that found "an error in anticipation, organization and coordination," and said "the response was not suited" to the situation.

The experts said the "compartmentalization" of services between the health and other ministries and workers in the field prevented a pooling of available information about the scope of the crisis.

French doctors on Tuesday reacted angrily to the government report.

Gilles Brucker, director of the Health

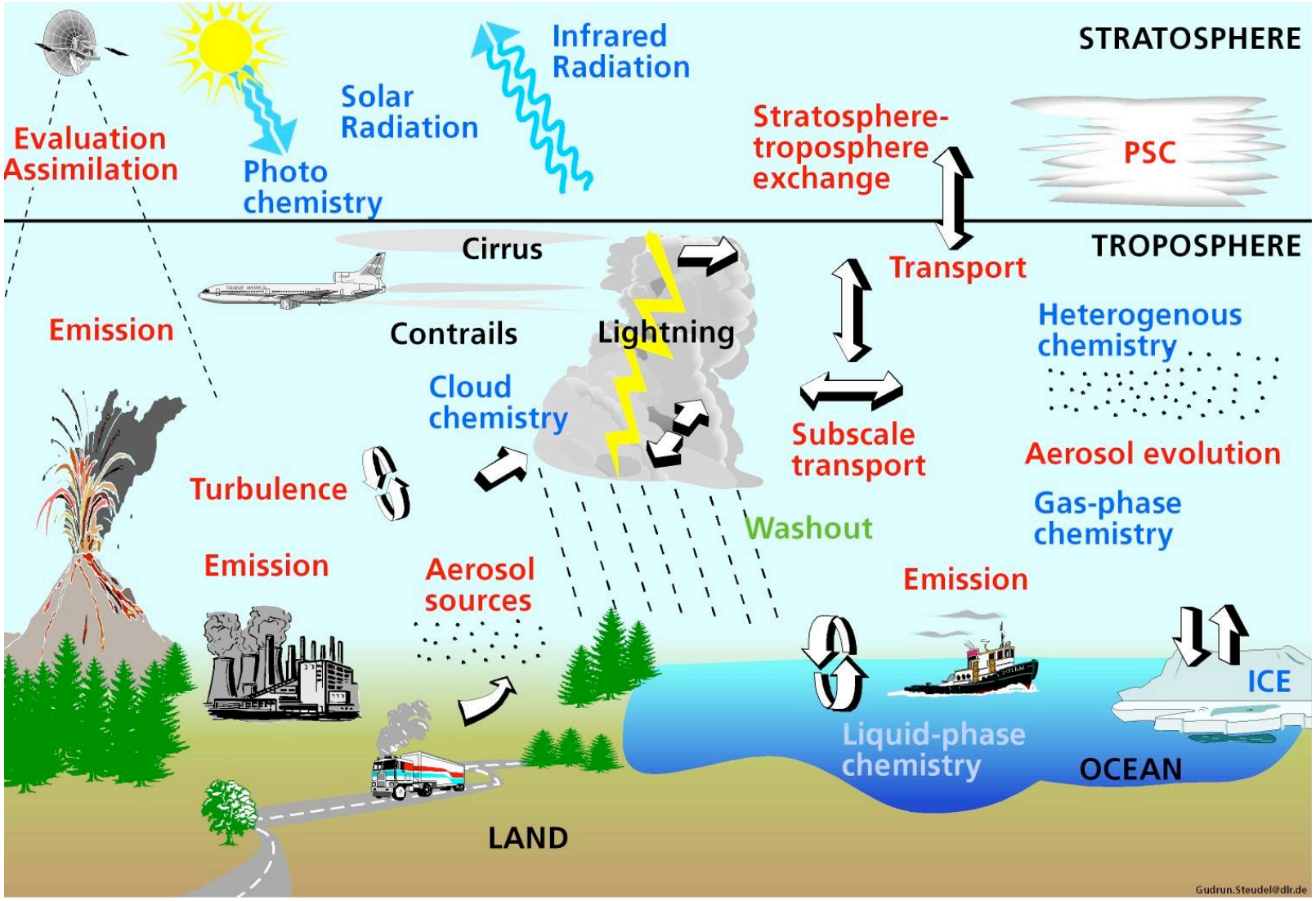
Persistent stagnant conditions
Exceptional drought

⇨

accumulation of pollutant
forest fires

Vautard et al., 2005

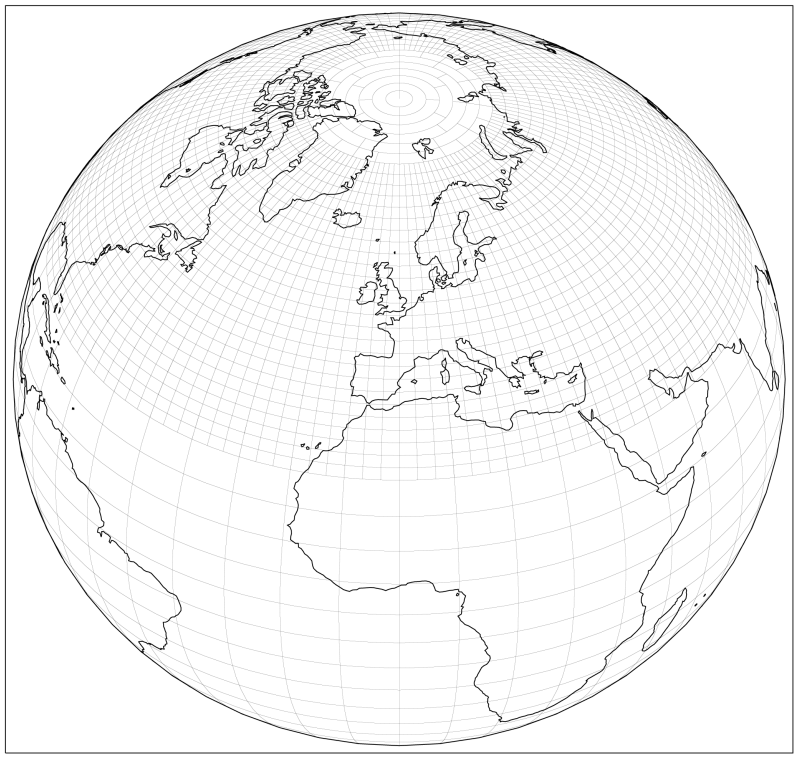
Atmospheric Processes Affecting Chemical Composition



Chemical Composition of the Atmosphere

Concentration of atmospheric trace gas *i*:

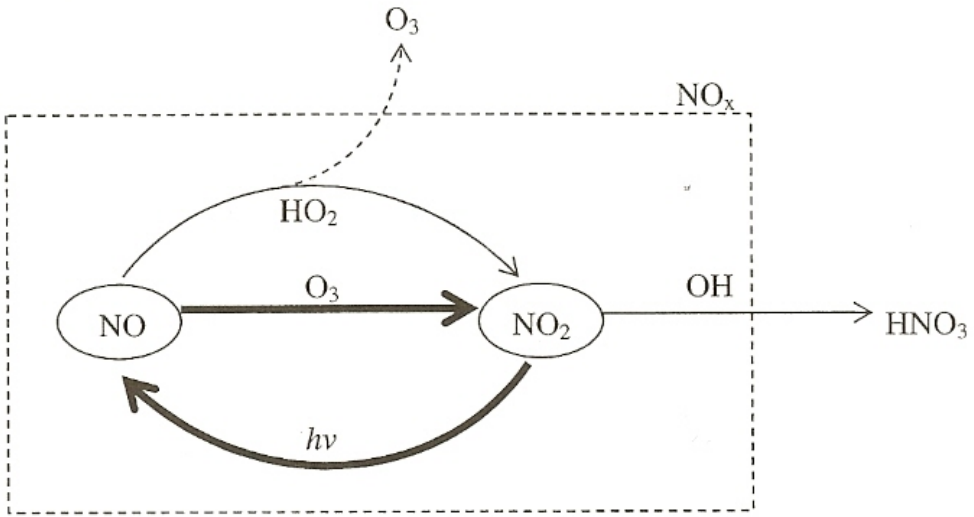
$$\frac{d\rho_i}{dt} = \left(\frac{\partial \rho_i}{\partial t}\right)_{emission} + \left(\frac{\partial \rho_i}{\partial t}\right)_{deposition} + \left(\frac{\partial \rho_i}{\partial t}\right)_{transport} + \left(\frac{\partial \rho_i}{\partial t}\right)_{chemistry}$$



Chemical reactions: Tropospheric ozone production

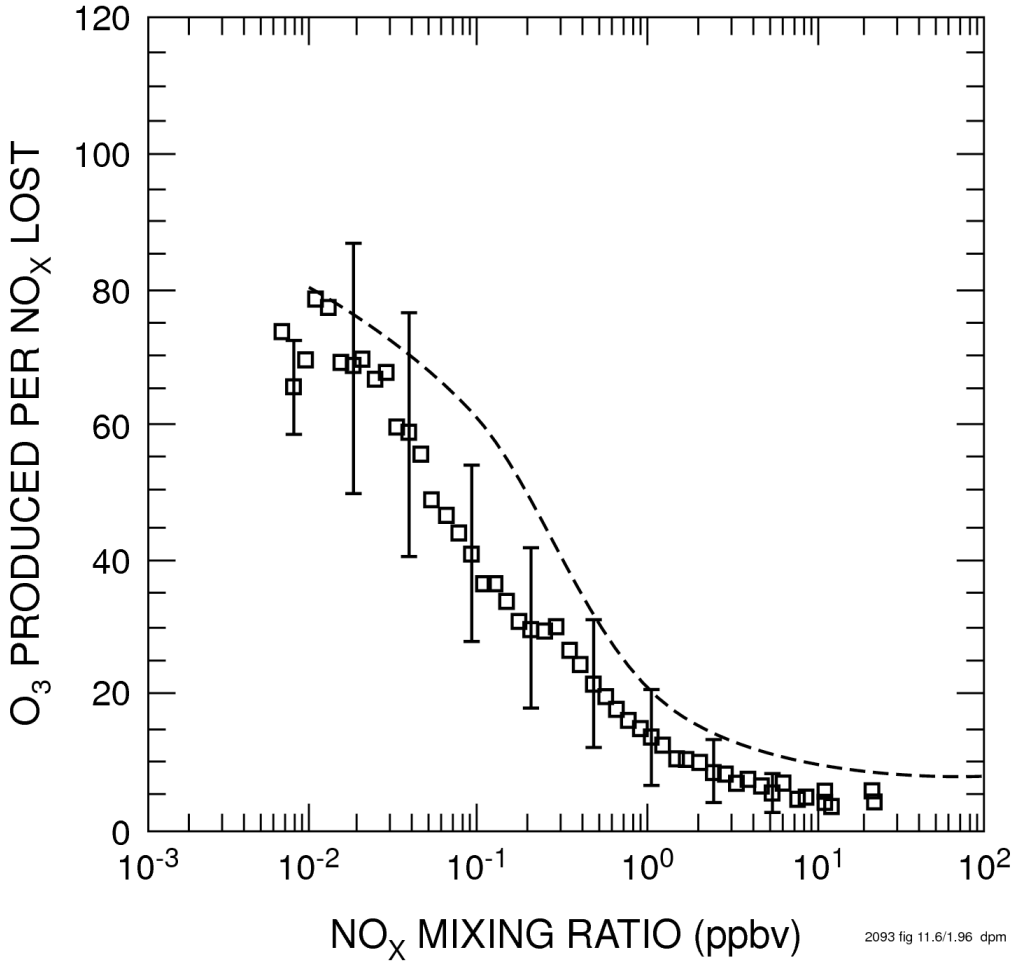
$$\mathrm{CO} + \mathrm{OH} \xrightarrow{\mathrm{O_2}} \mathrm{CO_2} + \mathrm{HO_2}$$
$$\mathrm{HO_2} + \mathrm{NO} \longrightarrow \mathrm{NO_2} + \mathrm{OH}$$
$$\mathrm{NO_2} + h\nu \xrightarrow{\mathrm{O_2}} \mathrm{NO} + \mathrm{O_3}$$

Net: $\mathrm{CO} + 2\mathrm{O_2} + h\nu \longrightarrow \mathrm{CO_2} + \mathrm{O_3}$



From Seinfeld and Pandis, 2007

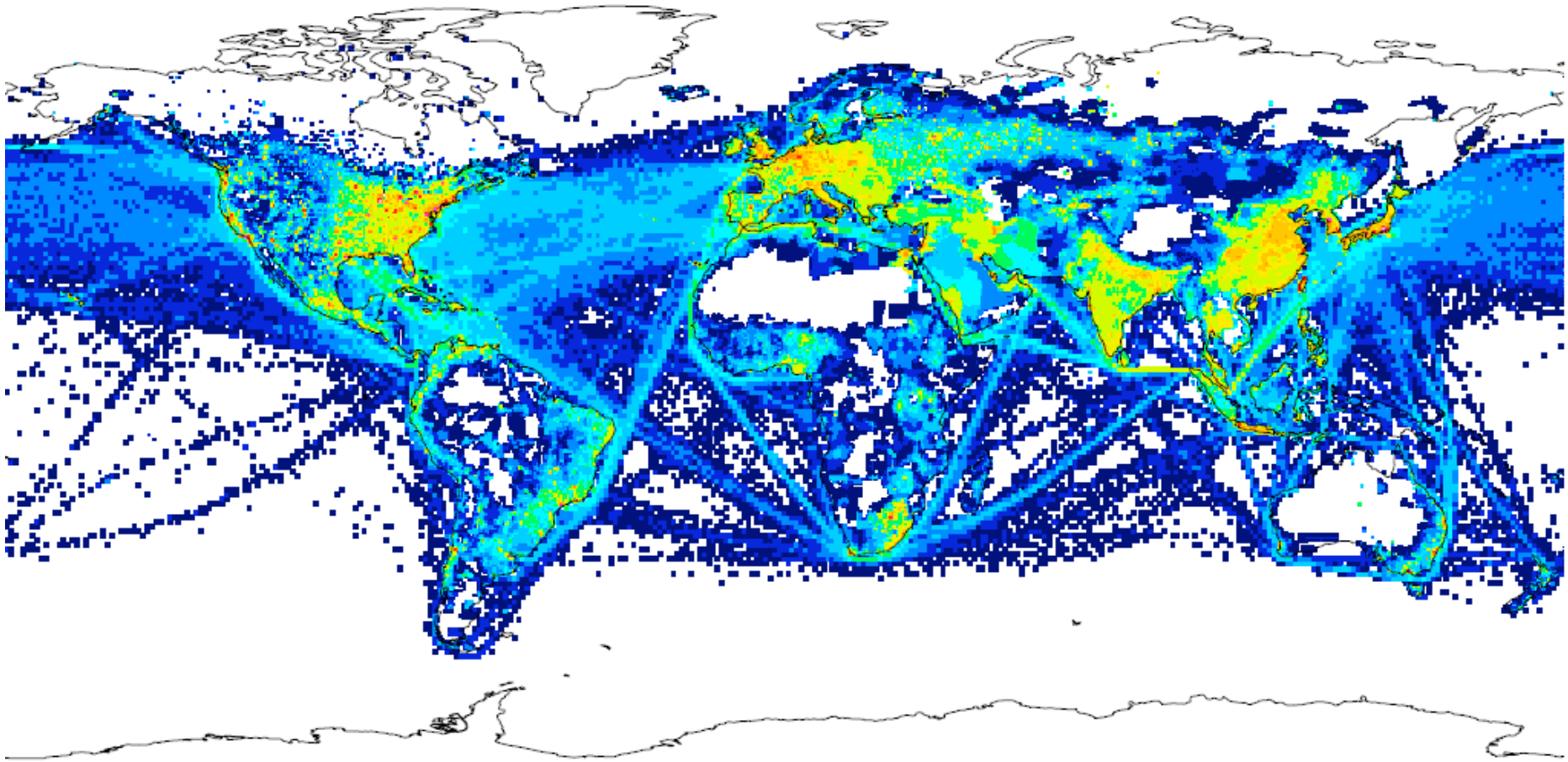
Ozone, NOx and VOCs



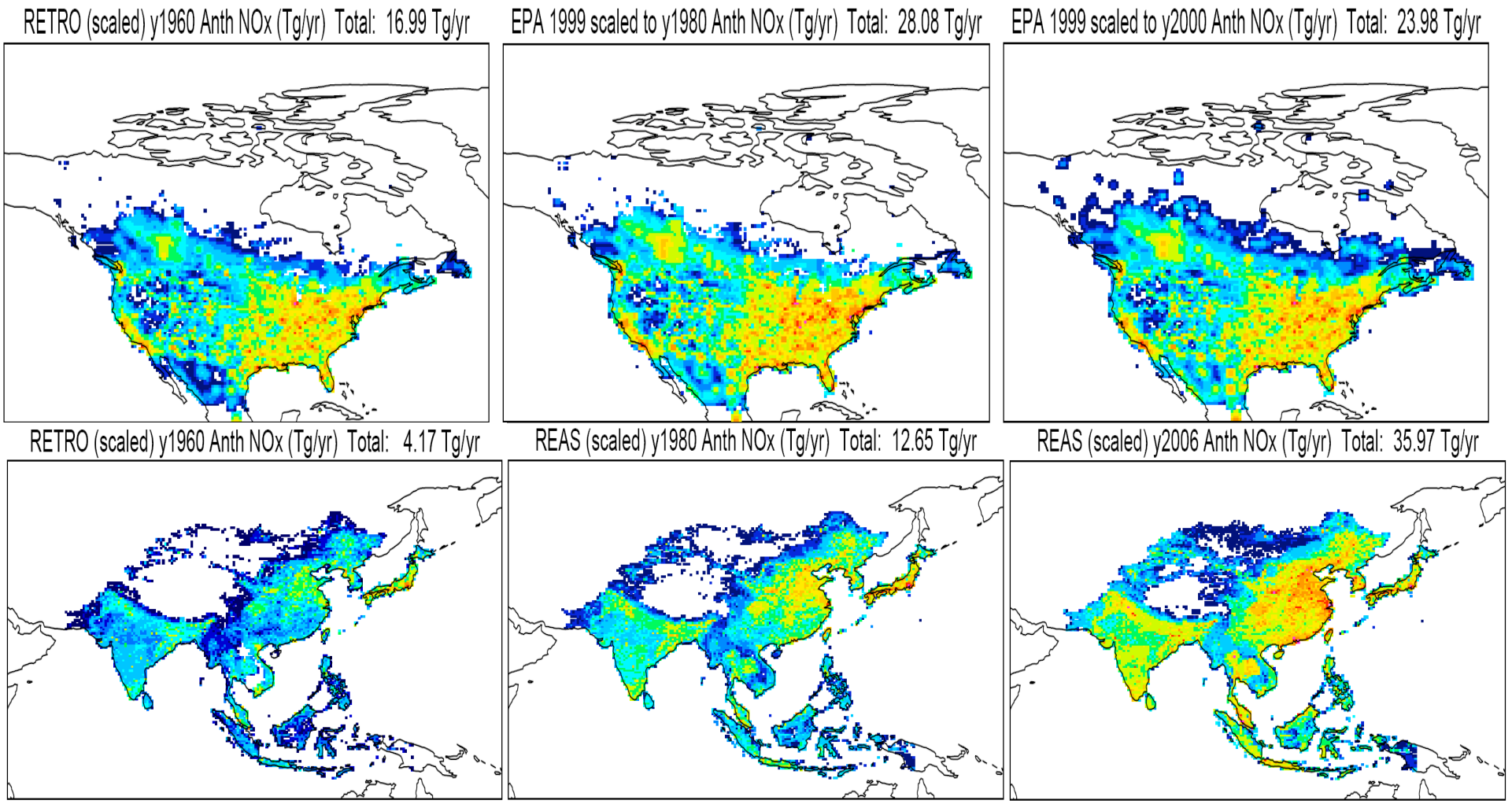
Emissions

- Biogenic: some included in CLM (isoprene, terpene)
- Natural: lightning is climate-dependent
- Anthropogenic: specified by user-specified netcdf files
- Ocean: specified by user-specified netcdf files

RETRO y2000 Anth NOx (Tg/yr) Total: 90.02 Tg/yr

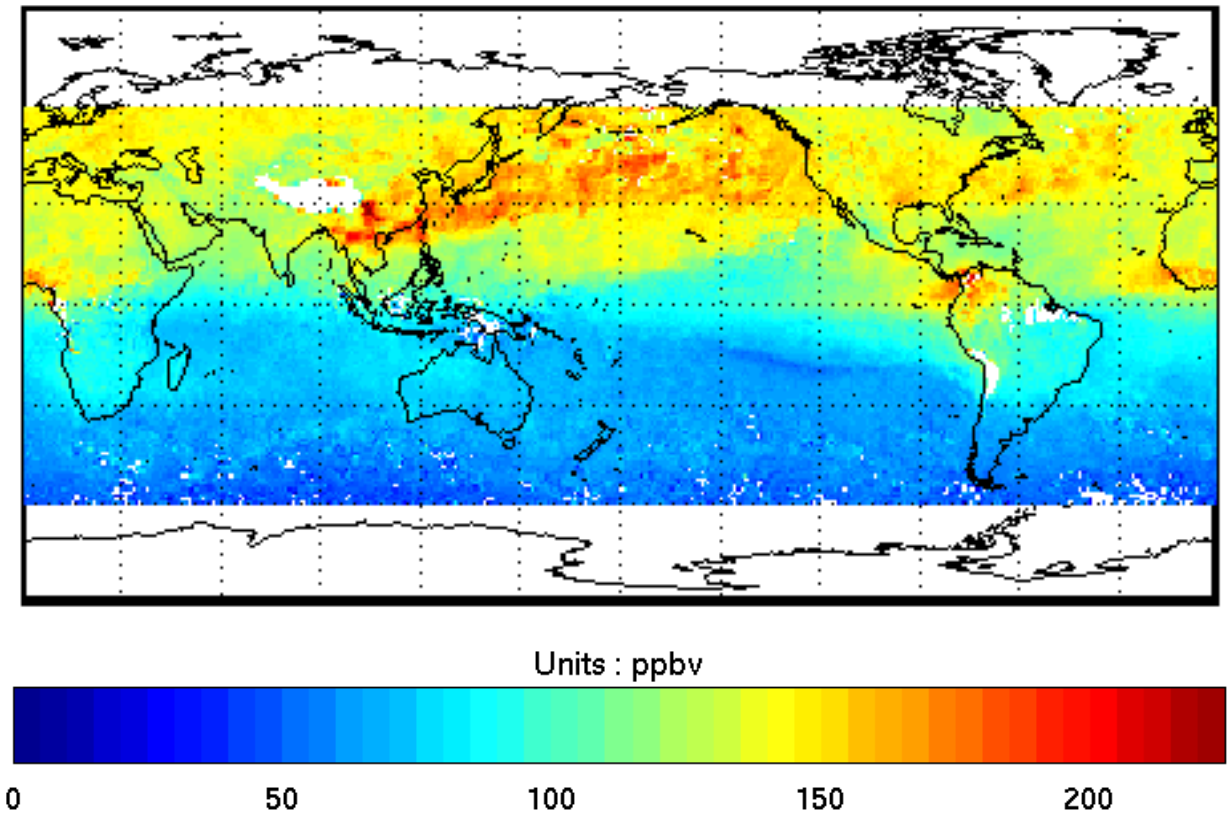


Nox emissions 1960-2006



1960 **1980** **2006 = INTEX-B**

Carbon monoxide from satellite



Deposition processes

- Dry deposition: uptake of chemical constituents by plants and soil (handled by CLM), water
- Wet deposition: uptake of chemical constituents in rain or ice (linked to precipitation, both large-scale and convective)

Doing chemistry in CAM

- Must be done in FV dynamical core (tracer conservation)
- Requires to build CAM with specific option
- Requires use of pre-defined chemistry or user-specified

Code generation flow

Example of preprocessor input file

mechanism file:

```
SPECIES

      Solution
        CO
      End Solution

      Fixed
        OH
      End Fixed

 END SPECIES

 CHEMISTRY

     Reactions
[usr8]  CO + OH -> CO2 + HO2
     End Reactions

     Ext Forcing
        CO<-dataset
     End Ext Forcing

 END CHEMISTRY
```

Example of build configuration

Predefined chemistry packages:

```
-chem trop_mozart | trop_ghg | trop_bam | trop_mam3 |
      trop_mam7 | waccm_mozart | waccm_ghg |
      super_fast_llnl | none
```

Predefined bulk aerosol/GHG packages:

```
 -prog_species  SO4 | DST | SSLT | OC | BC | GHG |
CARBON16
```

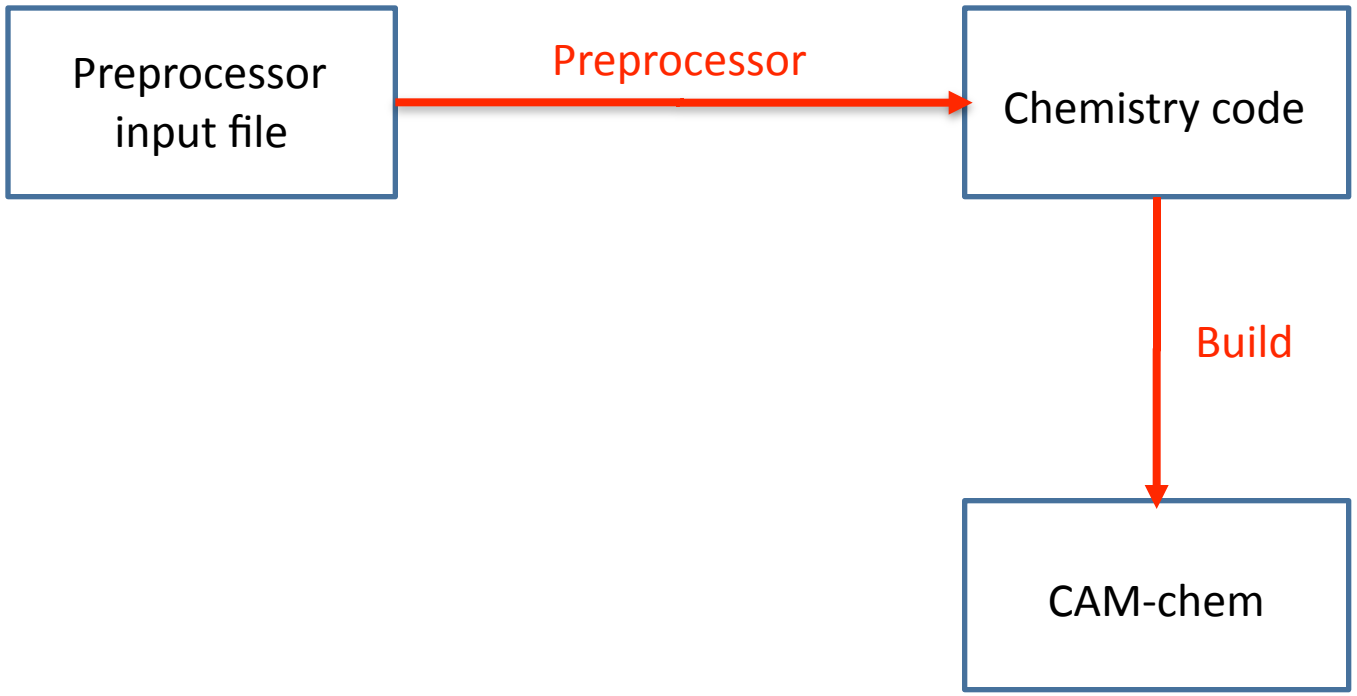
Configure will generate a preprocessor input file for any combination of these predefined prognostic aerosol and GHG packages.

User-specified mechanism

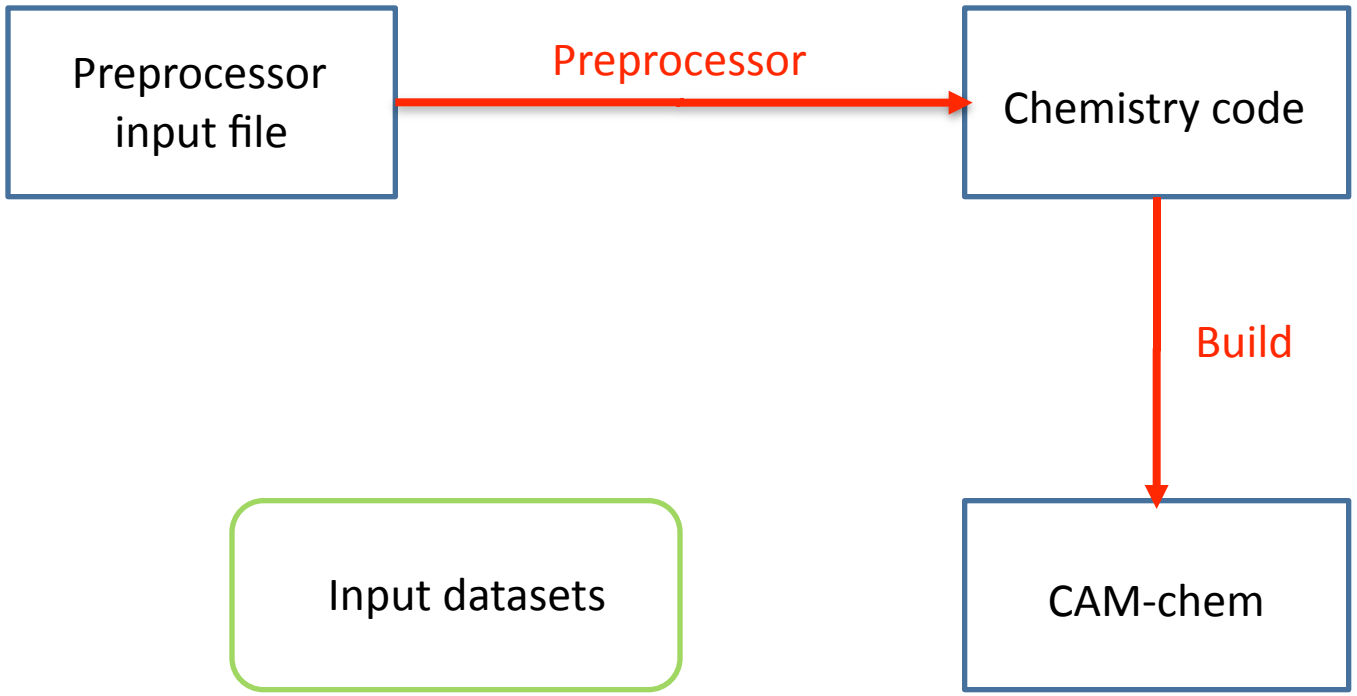
`-usr_mech_infile $mechanism_file`

- Allow user to specify a customized preprocessor input file
- Determines the number of advected tracers

Code generation flow



Code generation flow



Namelist control parameters

- Photolysis rates: LUT or inline
- Surface emissions/Other sources
- Species affected by dry deposition
- Species affected by wet deposition
- Lightning strength
- Lower boundary conditions
- Stratosphere overwriting

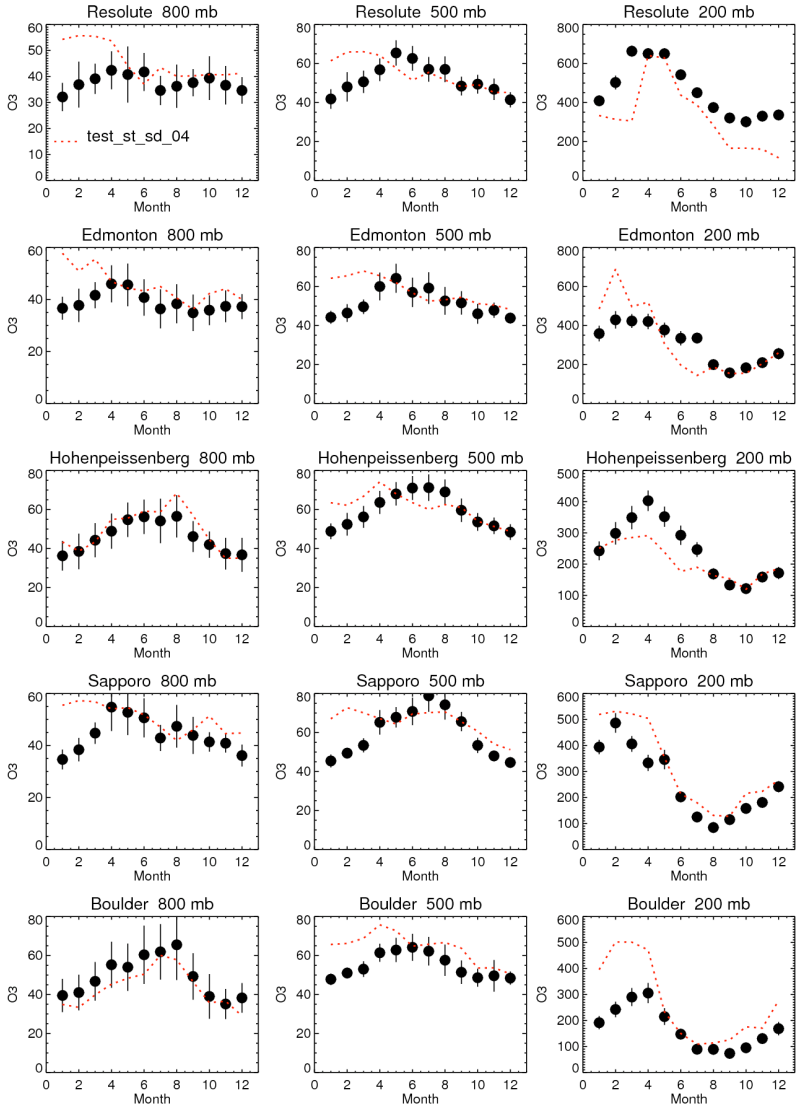
Possibility of using observed meteorology (campaign)

- Goal: use meteorological fields as close as possible to observed conditions
- Method

    1) CAM: processing of meteorological fields through dynamical core
    2) WACCM: relaxation

Comparison with obs. (IDL package)

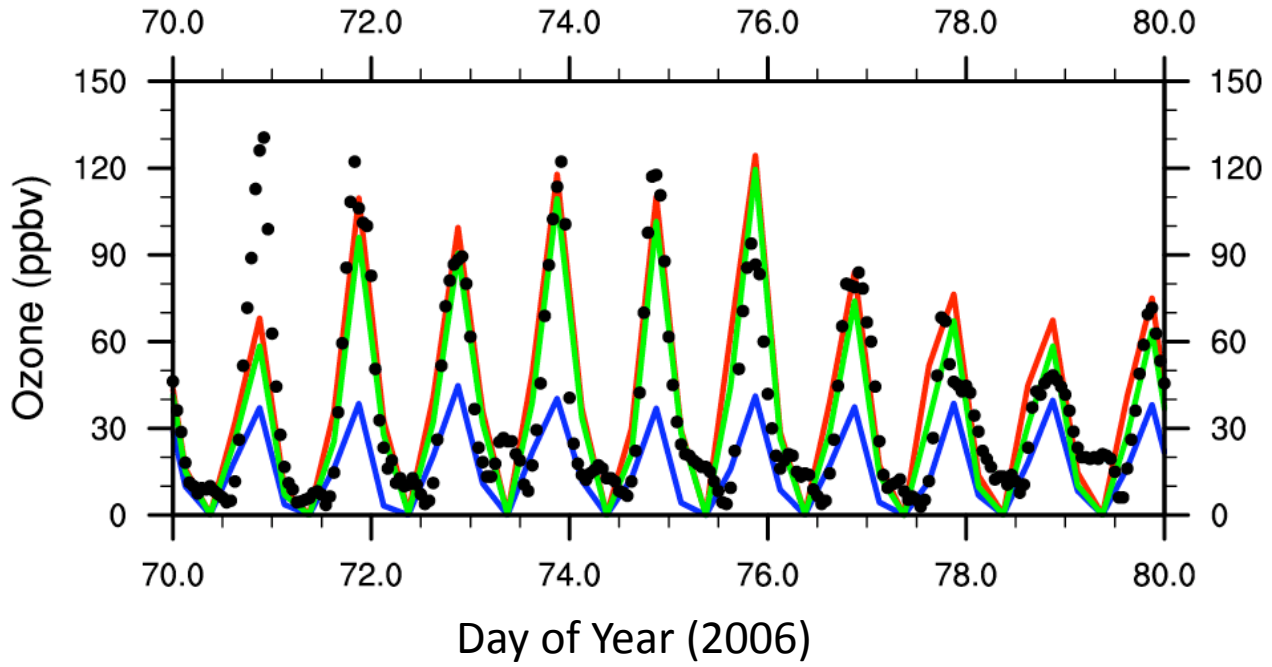
Ozone sondes



Applications

- Mexico City pollution: 0.5-degree with observed meteorology
- Long-term trends

Air quality: Comparison with Mexico City surface observations



Red: Full mechanism

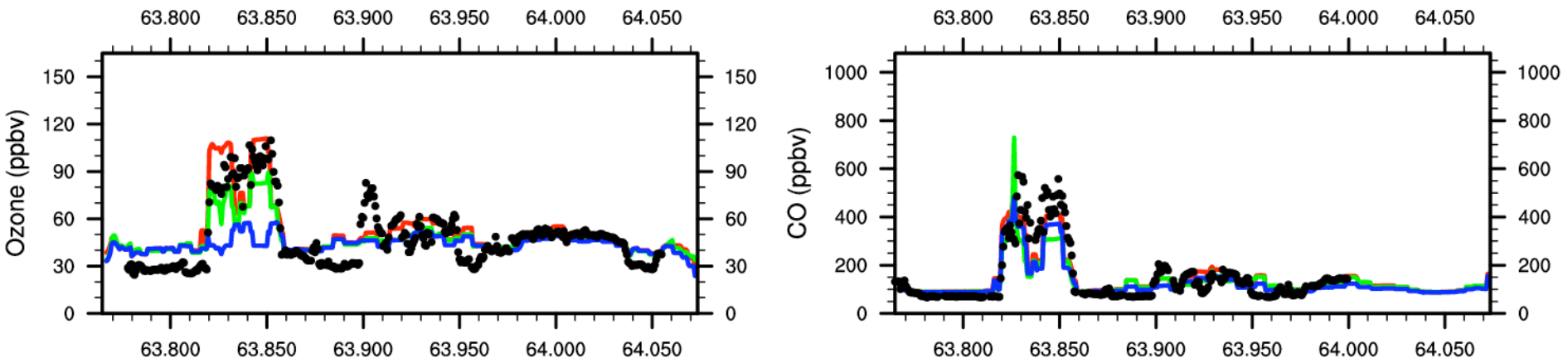
Green: Intermediate mechanism

Blue: Fast mechanism

Dots: observations

On most days, full and intermediate capture well the diurnal cycle and amplitude; the fast mechanism is much lower

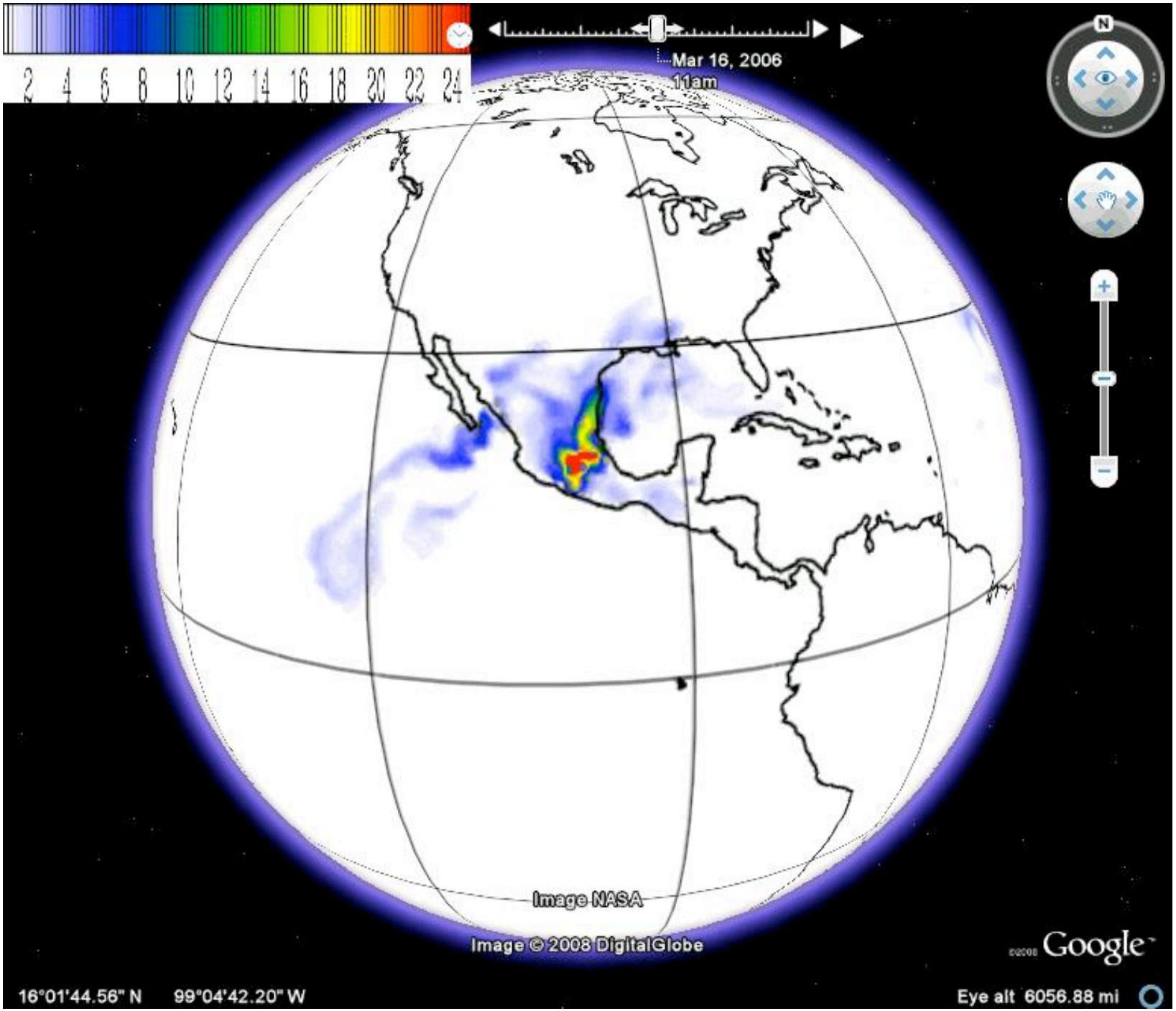
Air quality: Comparison with aircraft observations



Day of Year (2006)

Red: Full mechanism
Green: Intermediate mechanism
Blue: Fast mechanism
Dots: observations

1. On most days, full and intermediate capture well the background and plume ozone; the fast mechanism captures well the background.
2. CO is well captured by all.


2 4 6 8 10 12 14 16 18 20 22 24
Mar 16, 2006
11am
N
Image NASA
Image © 2008 DigitalGlobe
©2008 Google
16°01'44.56" N 99°04'42.20" W
Eye alt 6056.88 mi

Applications

- Mexico City pollution: 0.5-degree with observed meteorology
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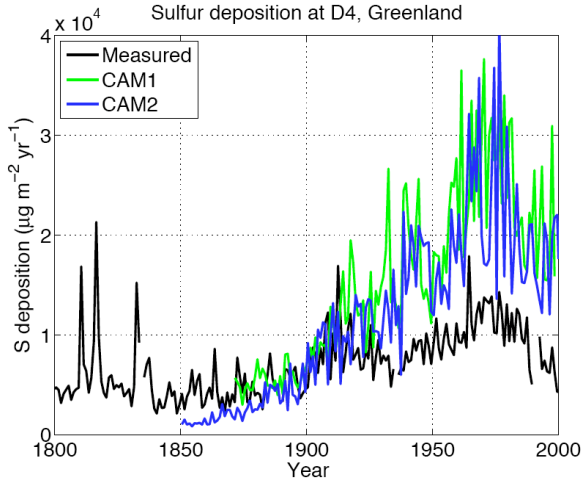
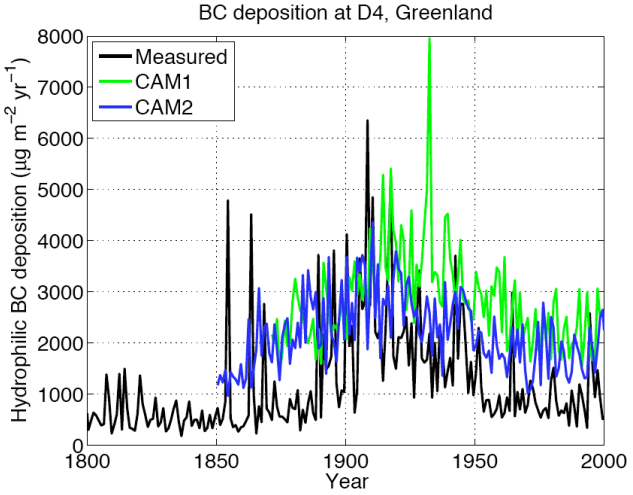
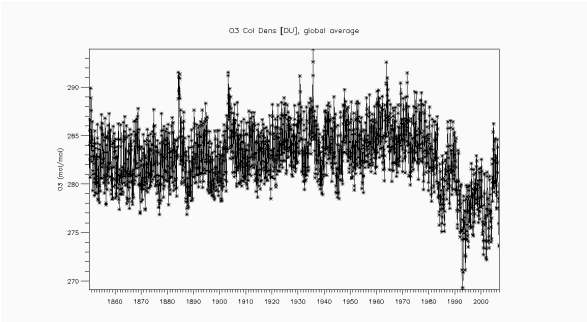
20th century simulation

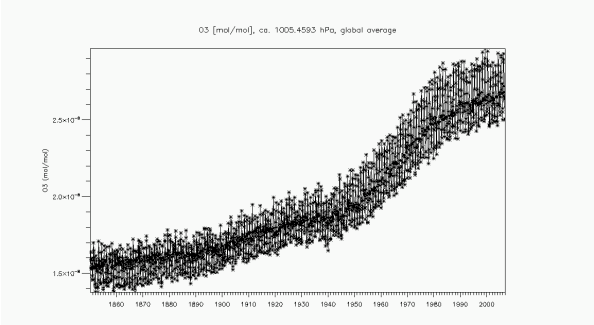




Courtesy of M. Flanner

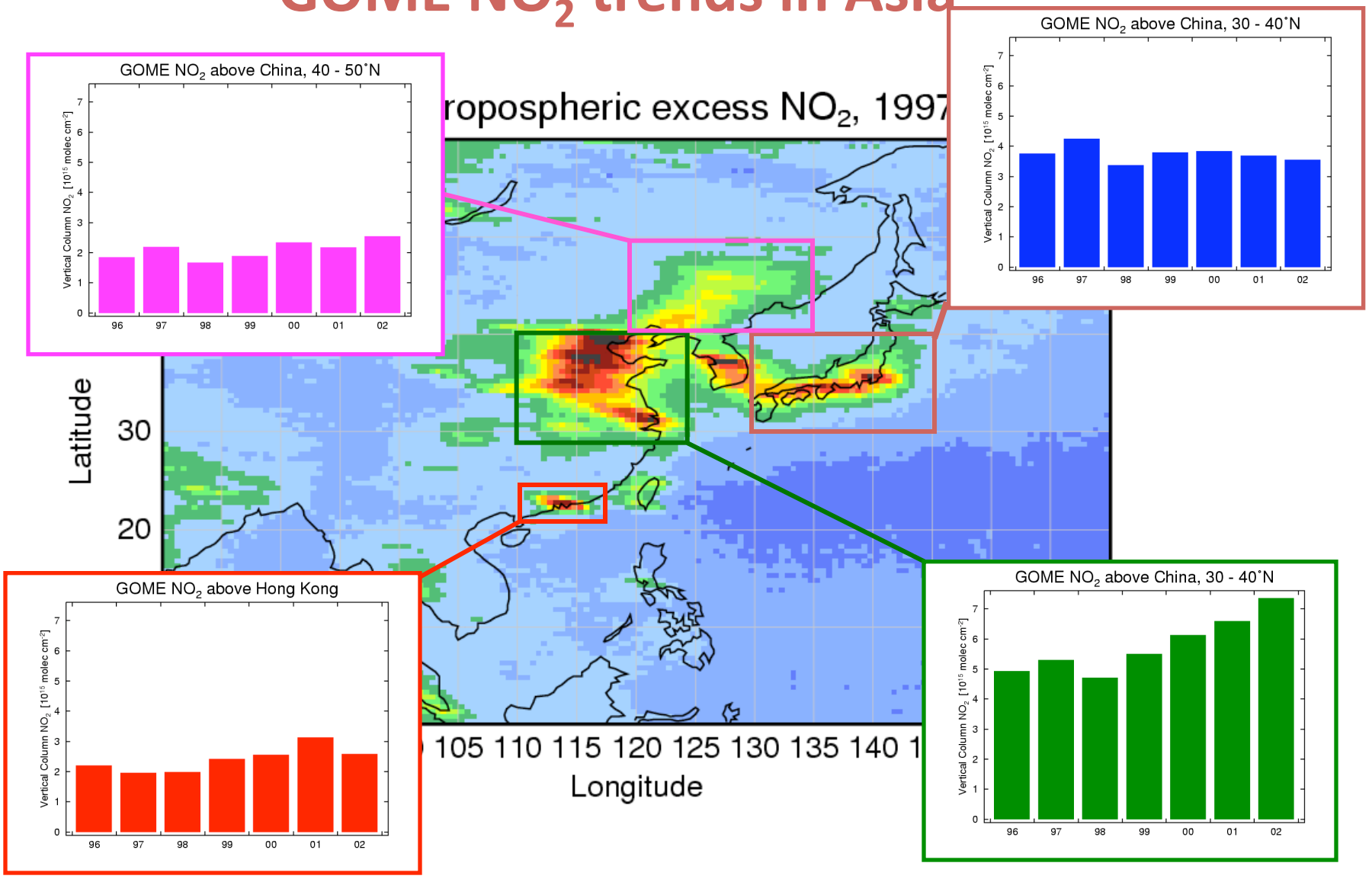


Total ozone column



Surface ozone

GOME NO_2 trends in Asia



From A. Richter, Uni Bremen

Atmospheric Chemistry in the Earth System

Based on P. Cox, 2004