An Upper Boundary Condition for Chemical Species

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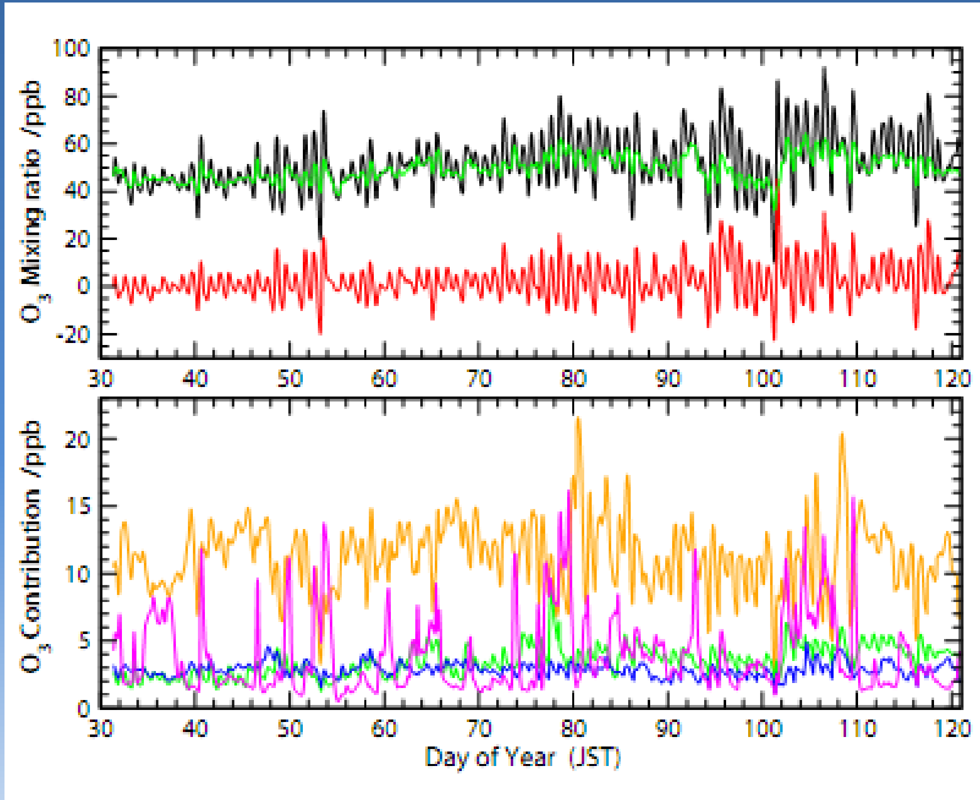
Motivation – Stratosphere affects the troposphere

FRSGC/UCI model-predicted surface O_3 in Tokyo and source attribution for February-April 2001



Total O_3
O_3 from Japanese sources
O_3 from other sources

O_3 from stratosphere
O_3 from China
O_3 from Europe
O_3 form North American sources

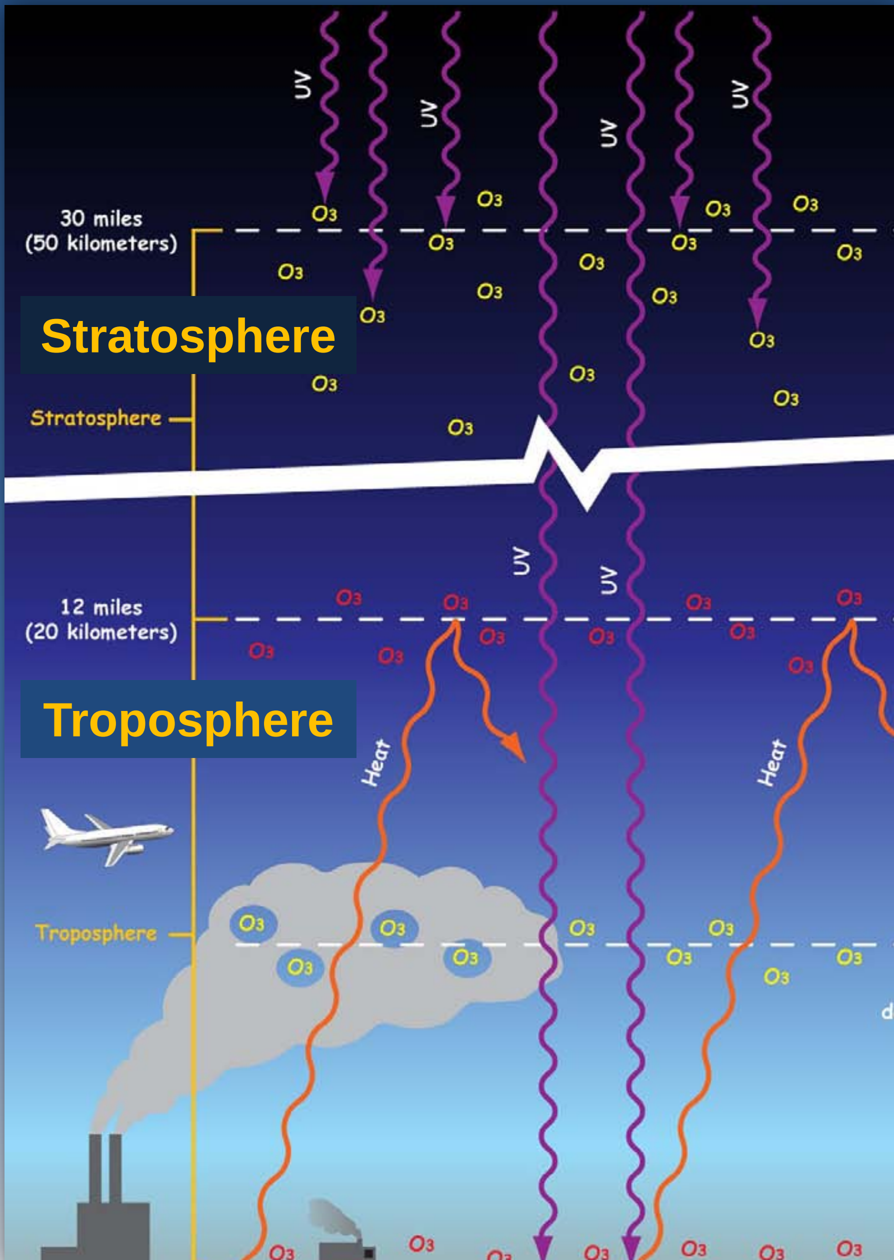
From Yoshitomi et al., ACPD, 2011

Motivation –
Stratosphere affects the troposphere

- For simulations over long time periods (≥ month)
- For chemistry-climate studies
- For studies during active periods of stratosphere-troposphere exchange (much happens in late spring)
- For studies that include evaluation with satellite data

Including a representation of stratospheric chemistry is important

Motivation

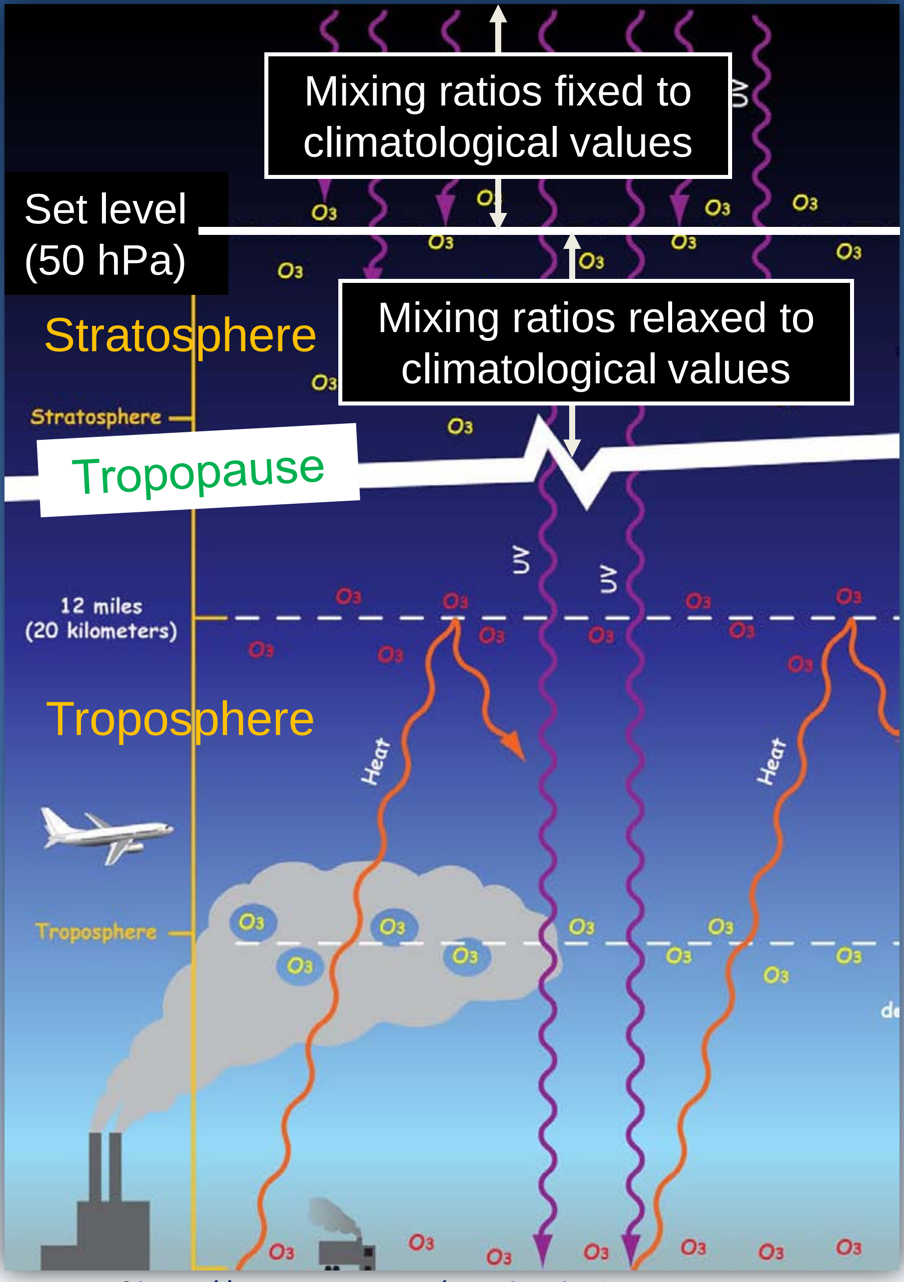


- **WRF-Chem does not include stratospheric chemistry (for any chemistry option)**
- **For long simulations, the stratosphere can influence the upper troposphere**

➢ **Impose an upper boundary condition to keep key species at values representative of the stratosphere**

Courtesy of http://www.aoas.org/article.php?story=20080522125225466

Method



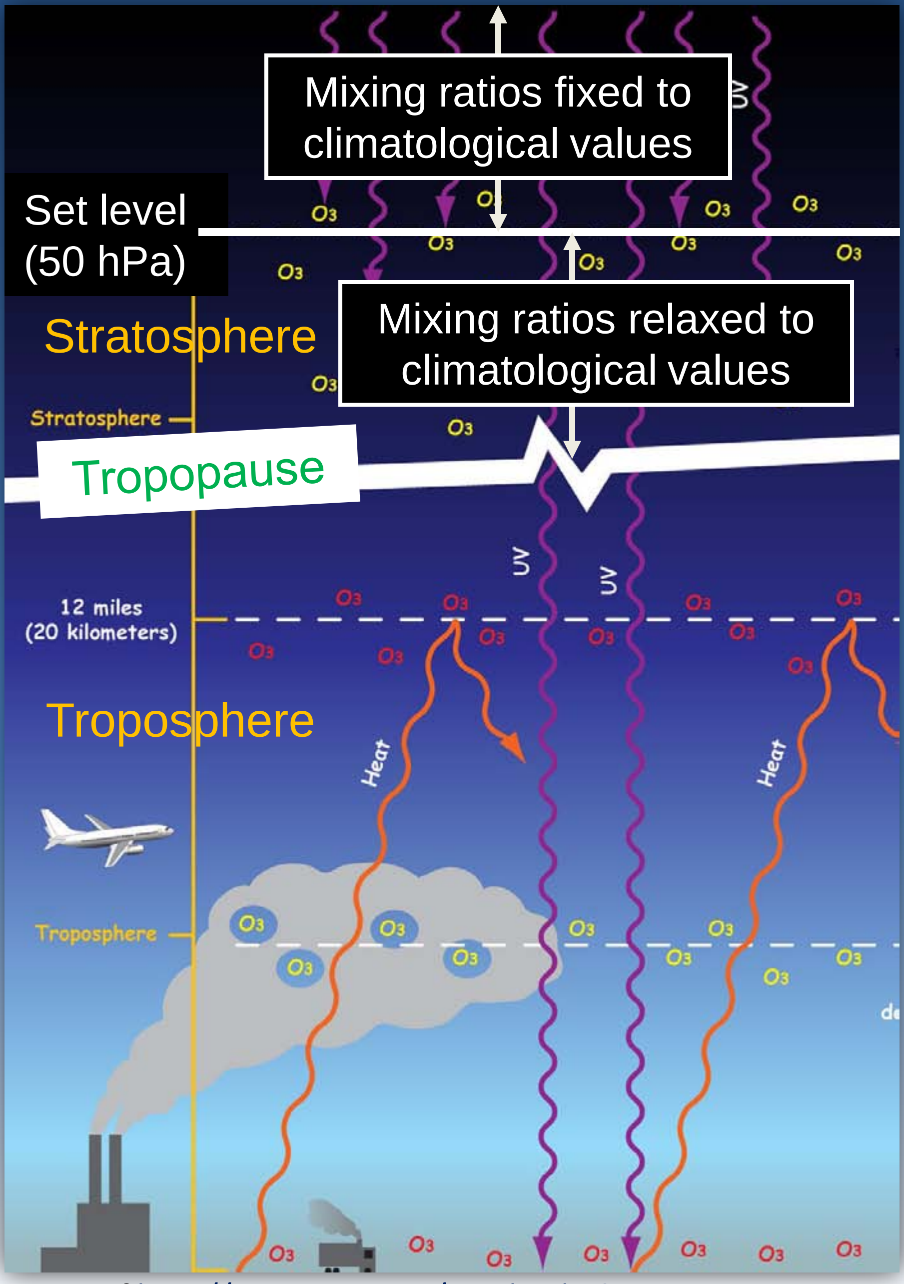
Courtesy of http://www.aoas.org/article.php?story=20080522125225466

- **Above a specified pressure level → species are fixed to climatological values**
- **Between that pressure level and the tropopause → species are relaxed to climatological values**

- **Species:**

  CH_4, CO, O_3, NO, NO_2, HNO_3, N_2O_5, N_2O

Note: Use same algorithm that is in CAM-Chem (global model)



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Needs

1) **Climatology of key species in stratosphere**

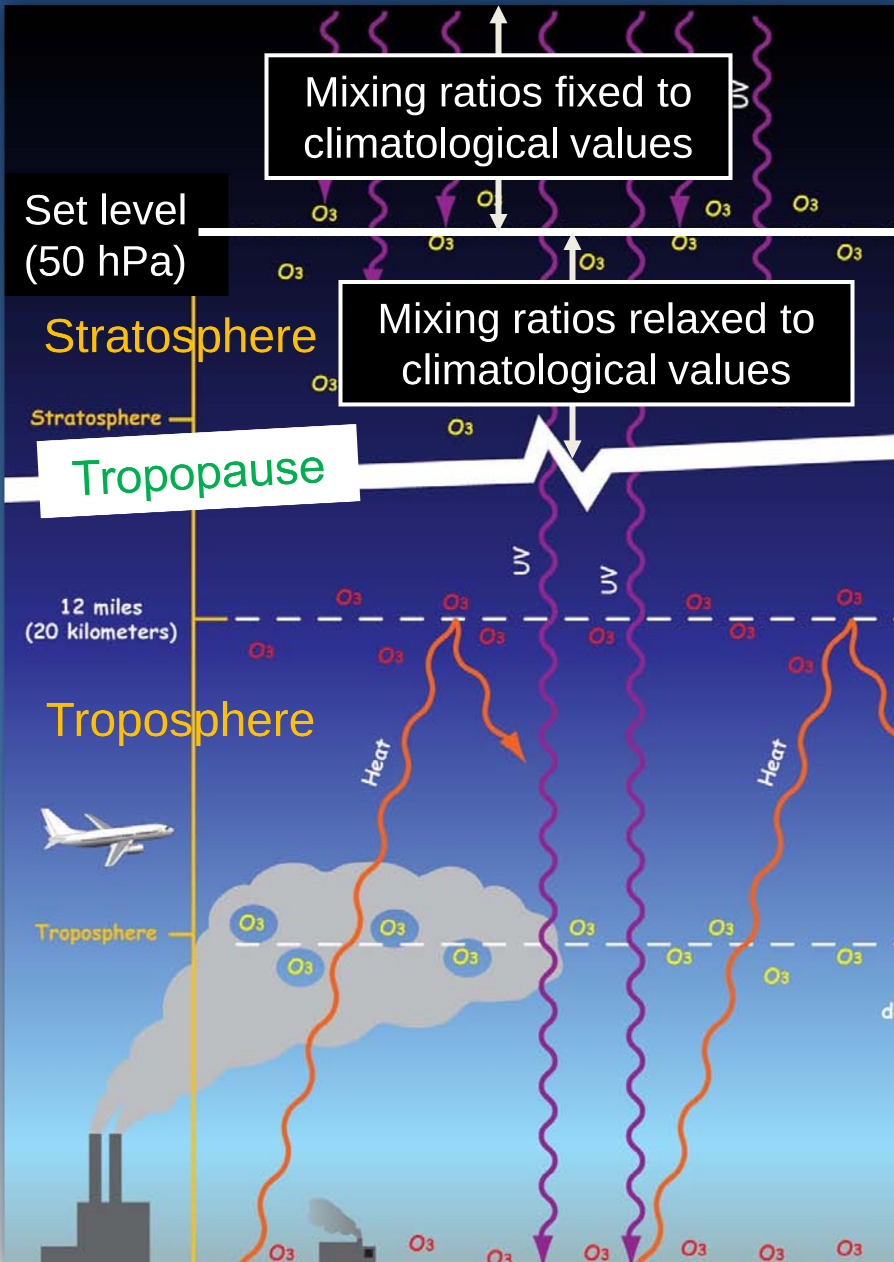
   → Global chemistry transport model results e.g.

   1) **MOZART 3 = troposphere and stratosphere chemistry global chemistry transport model**
   2) **WACCM = whole atmosphere model**

   These are 2-d zonal averages

2) **Location of tropopause**

Needs



Courtesy of http://www.aoas.org/article.php?story=20080522125225466

Calculation of tropopause in WRF

WMO definition:

Lowest level at which the lapse rate decreases to 2°C/km or less, provided that the average lapse rate between this level and 2 km above this level does not exceed 2°C/km.

If cannot find tropopause:

Use climatology model output

→ 2 input files needed

Namelist and Output

Namelist

&chem section:

have_bcs_upper = .true., .true.

fixed_upper_bc = 50., 50.

← Pressure level (hPa) above which values are fixed

Additional Output (2-D arrays)

TROPO_P = Tropopause Pressure

TROPO_Z = Tropopause Height

TROPO_LEV = Model Levels of Tropopause

Tests

1) 1-domain : North America; Eastern Asia
2) 2-domains: Chicago, California
3) Restart simulations
4) 13 days on the North American Monsoon simulation

→ Show results from this simulation

North American Monsoon Simulation

Simulation dates: July 10 – August 6, 2006

Comparison Study: July 25 – August 3

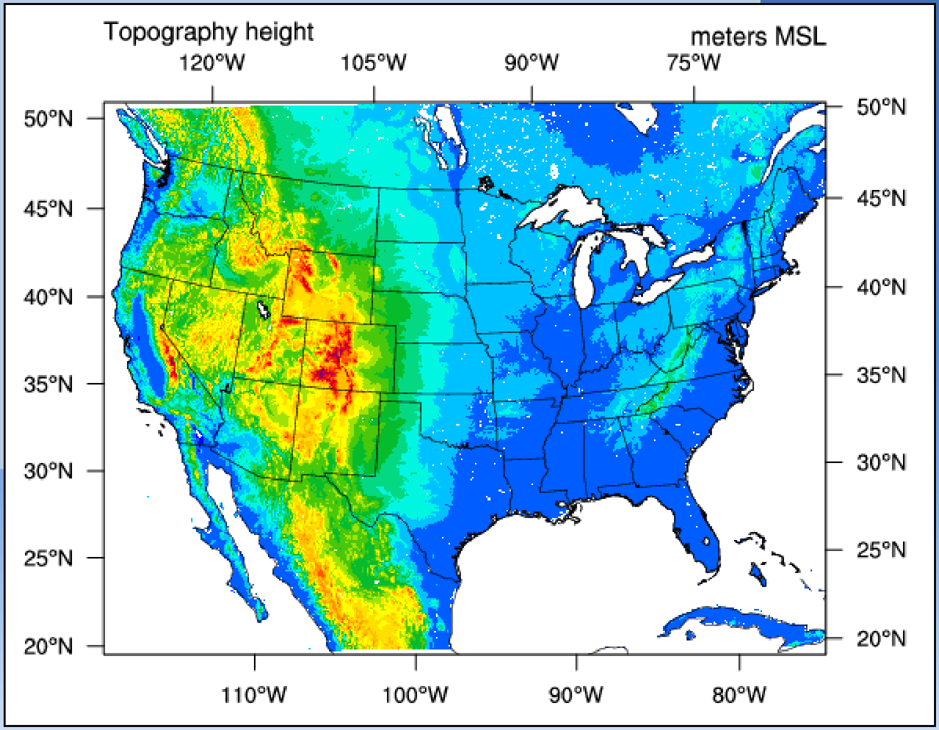
Δt = 20 s; output every 1 hour

1200 x 900 x 51 grid points

p_top = 10 hPa

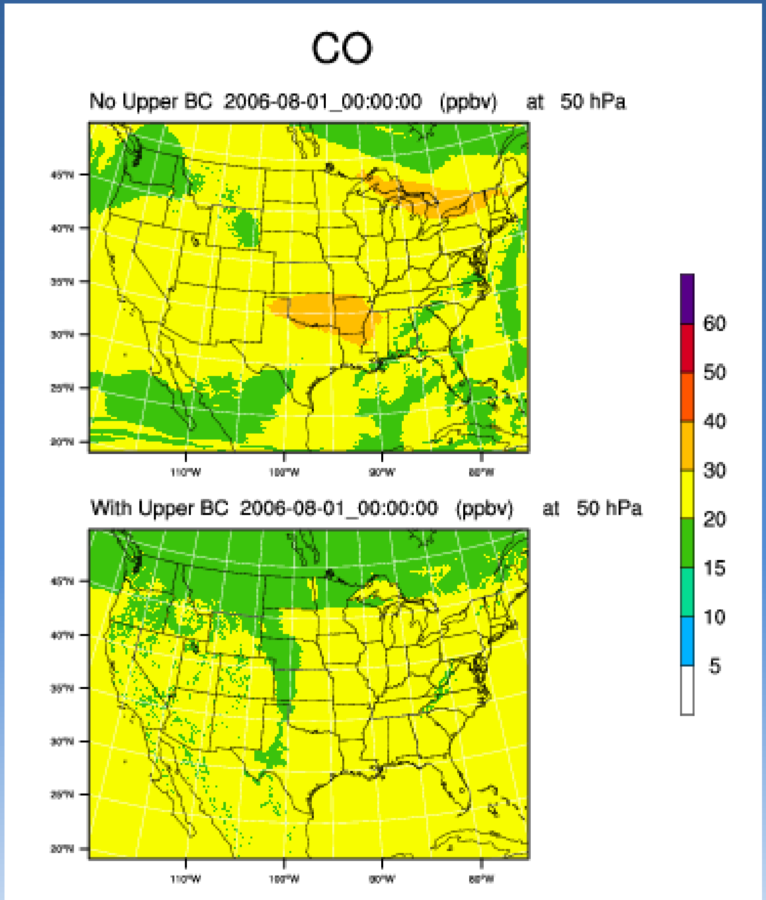
MOZART3 Climatology

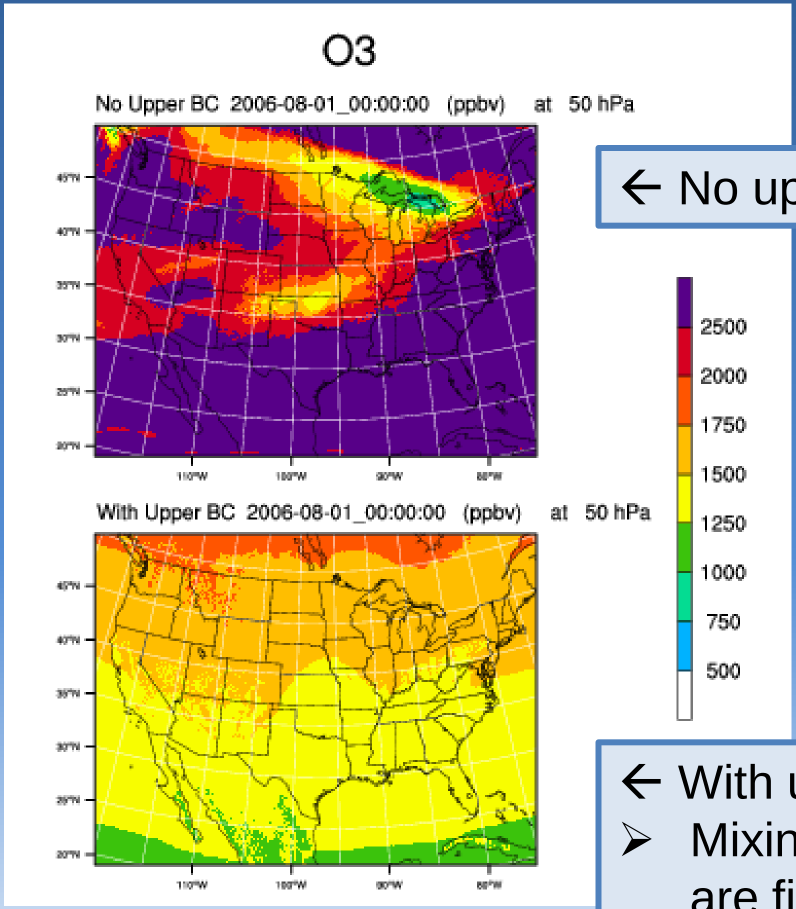
Level to fix values = 50 hPa



Simulations were conducted on the NCAR bluefire supercomputer with support from NCAR/CISL and on the NASA/High End Computing Pleiades computer.

Comparison of CO, O_3 at p=50 hPa (21 km) after 7 days integration with and without the upper BC



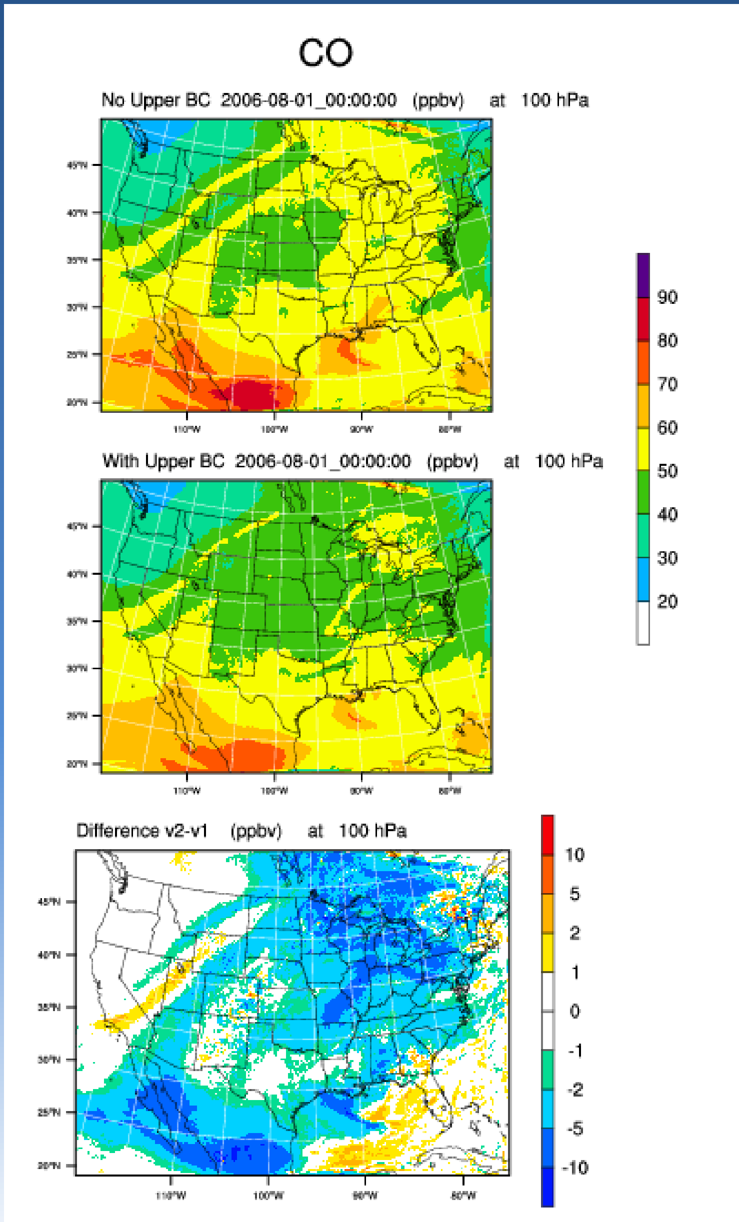


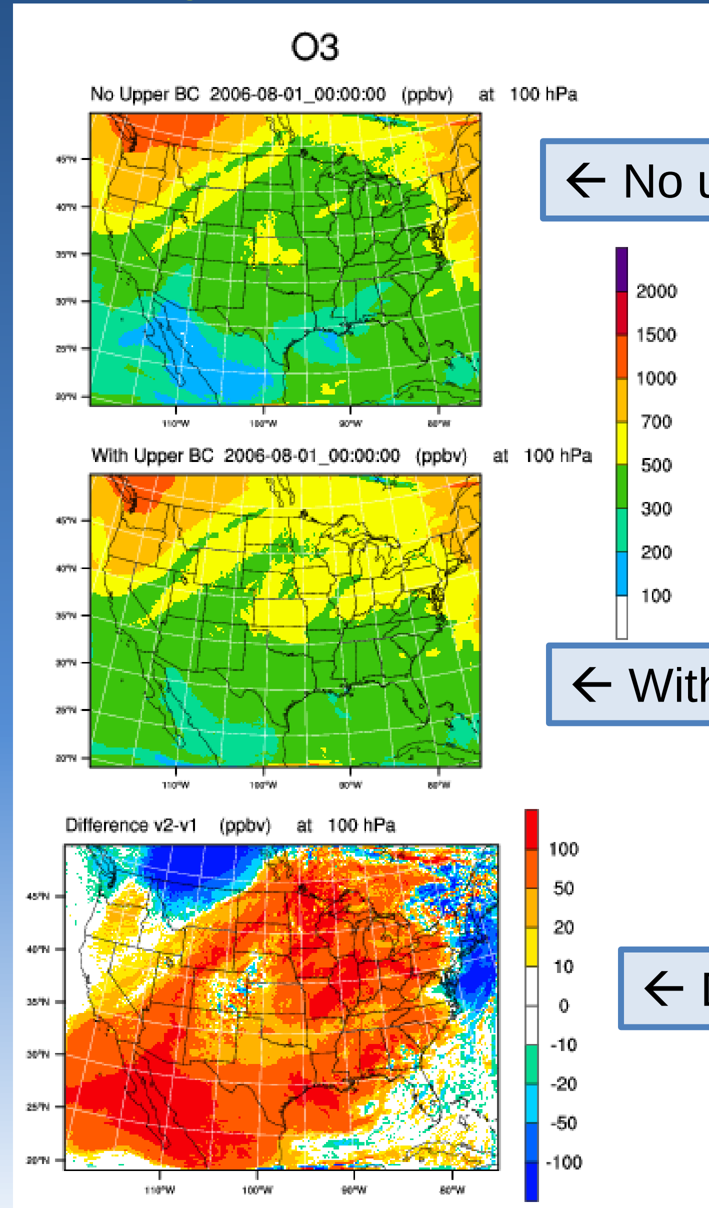
← No upper BC

← With upper BC

➢ Mixing ratios are fixed to these values

Comparison of CO, O_3 at p=100 hPa (16 km)



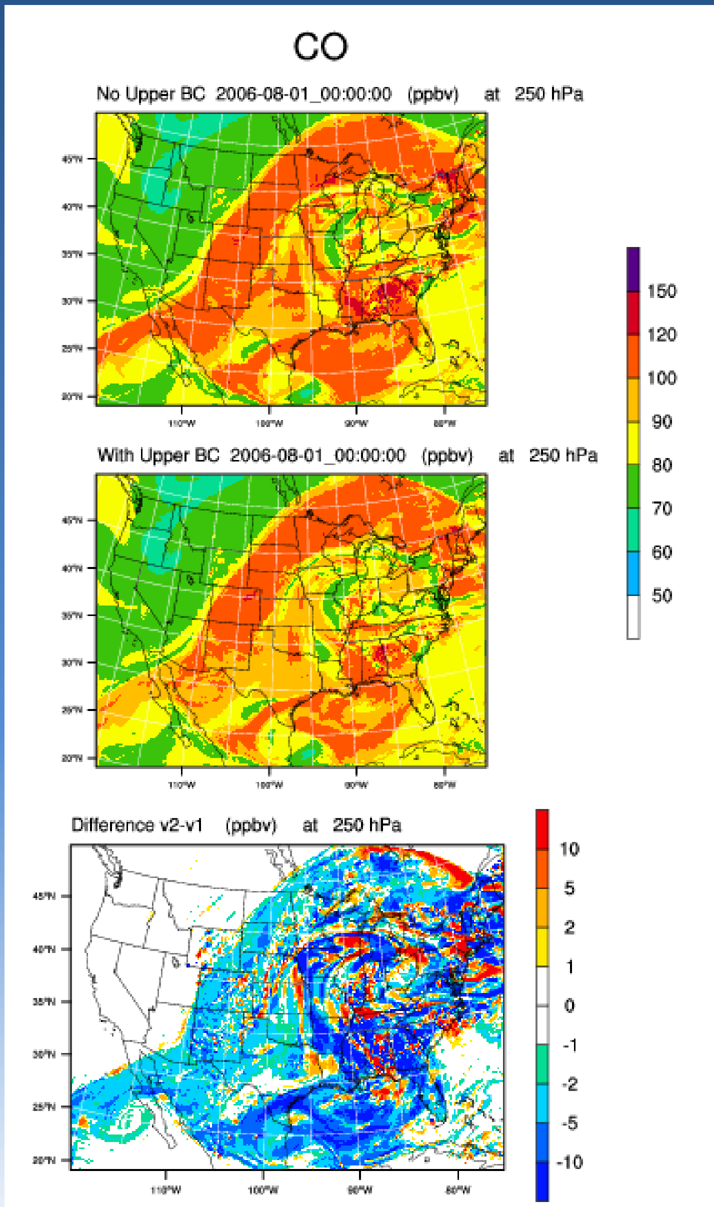


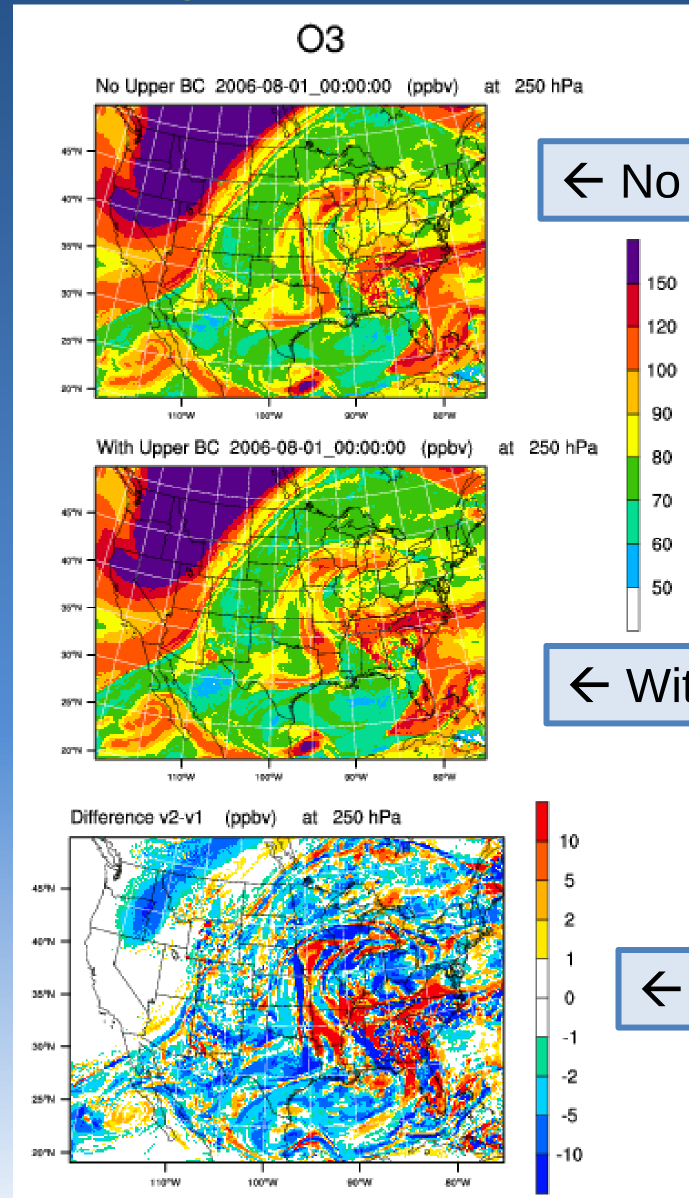
← No upper BC

← With upper BC

← Difference

Comparison of CO, O_3 at p=250 hPa (11 km)



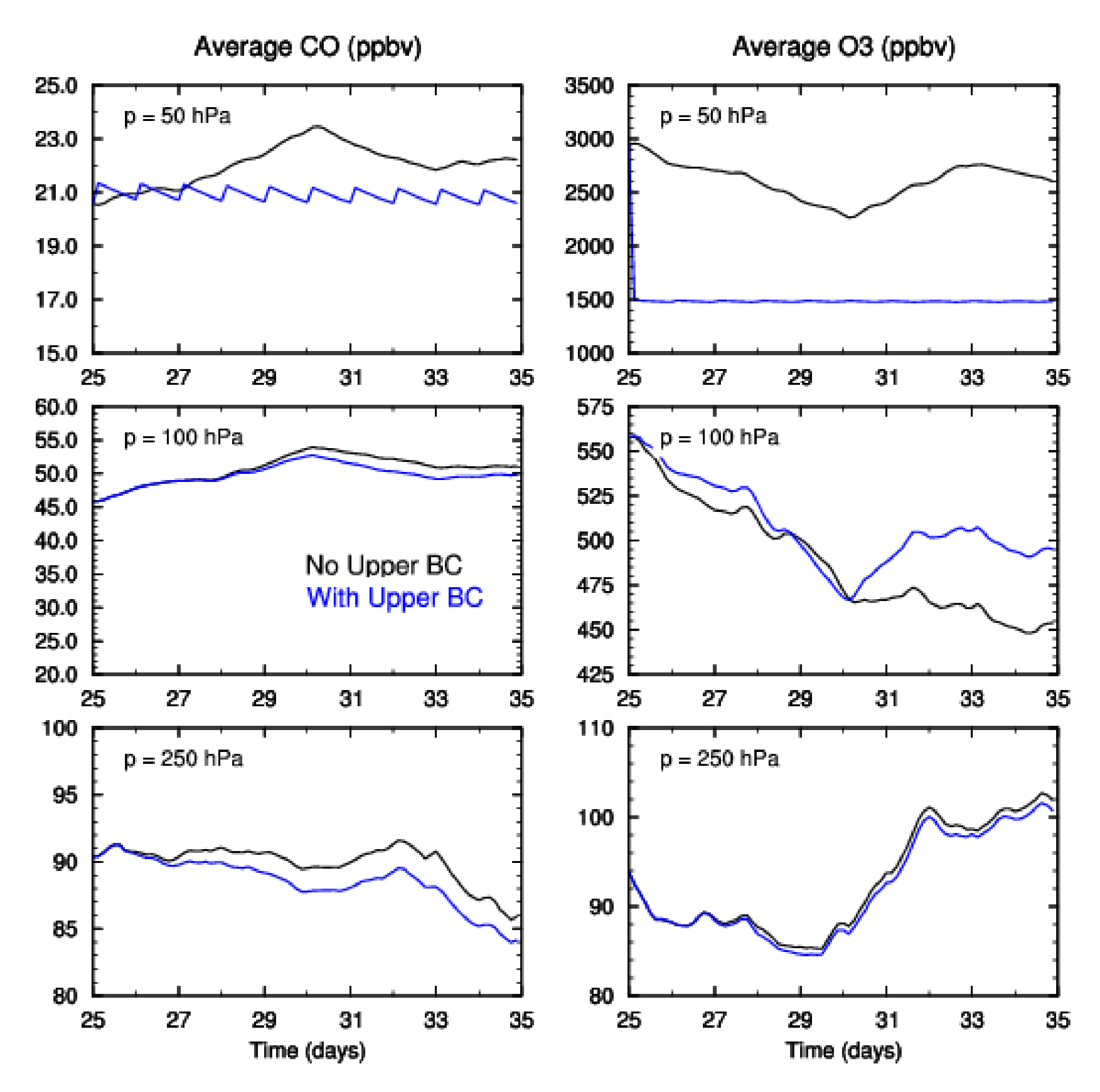


← No upper BC

← With upper BC

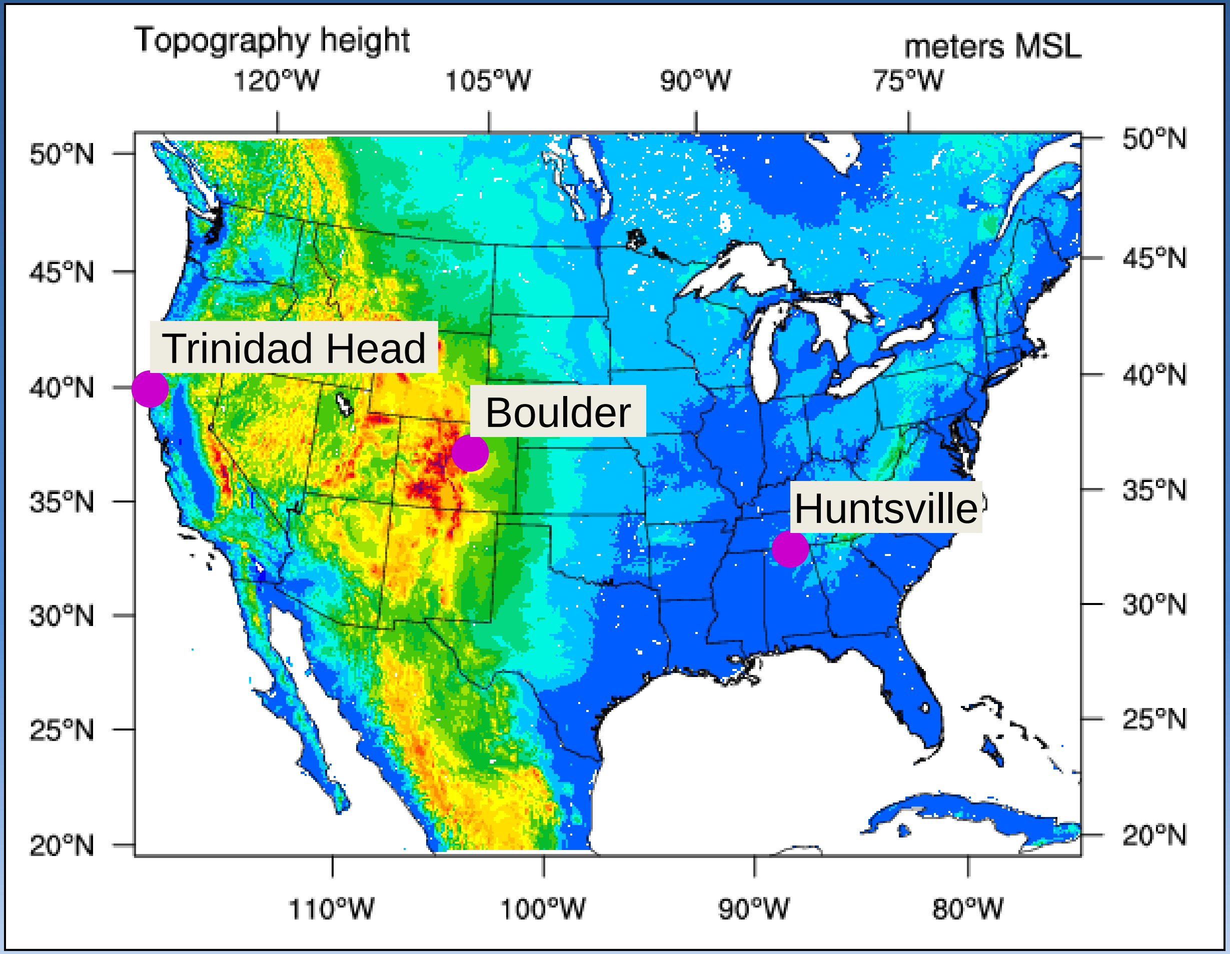
← Difference

Comparison of CO, O_3 averaged over model domain



In relaxation zone and below → model prediction tends to diverge with time

Comparison with Ozonesonde Data



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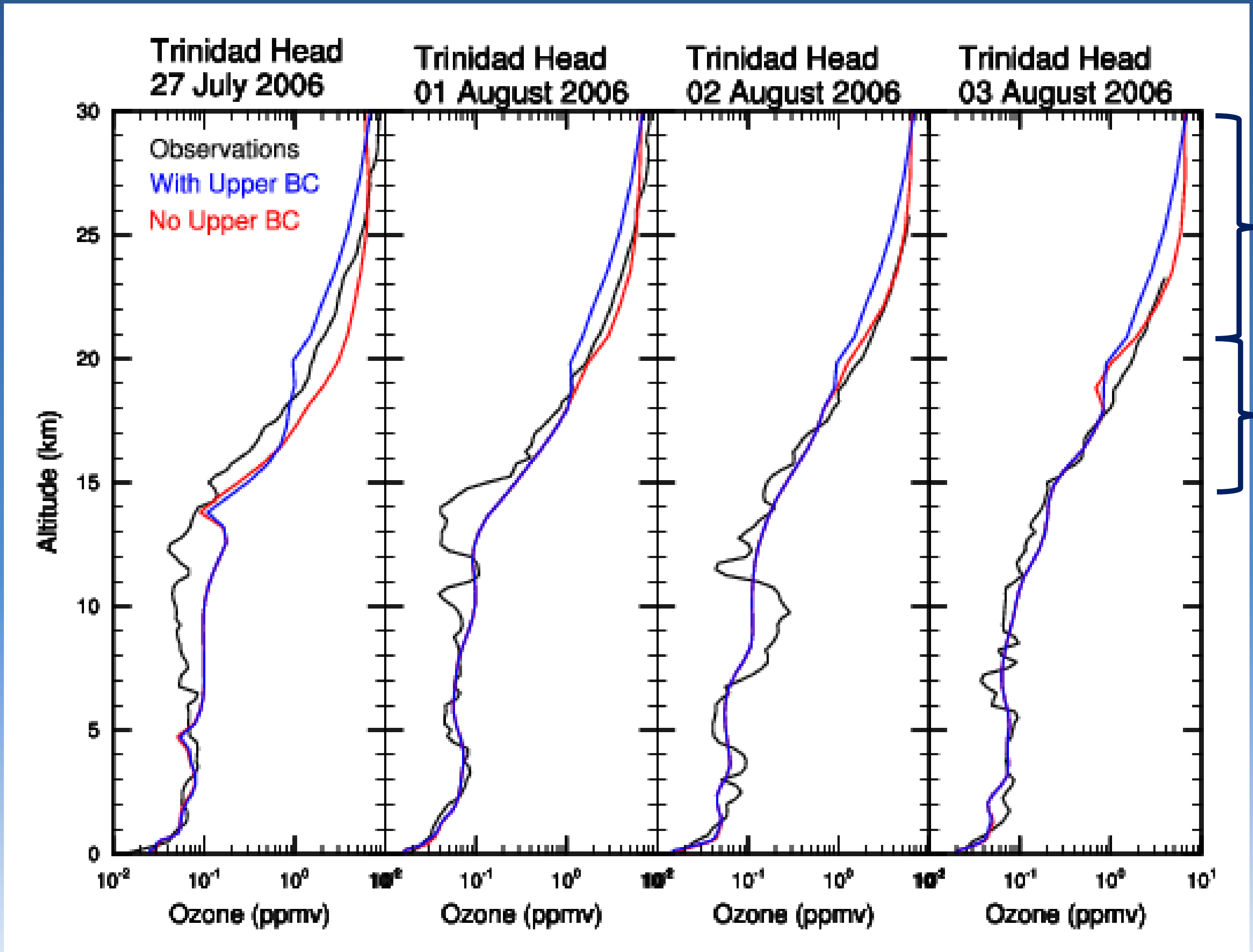
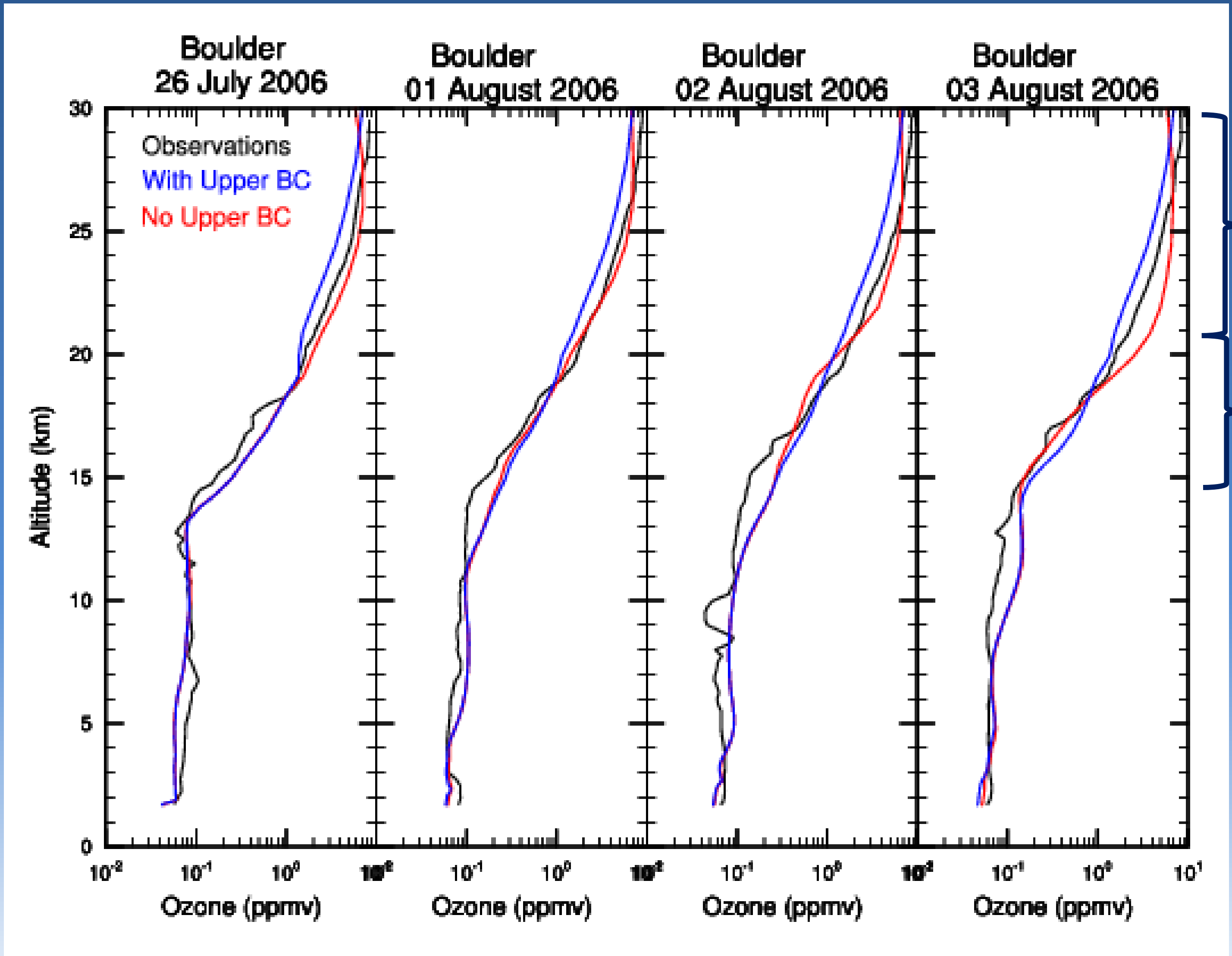


Mixing ratios fixed to climatology

Relaxation zone

Comparison with Ozonesonde Data



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Relaxation zone

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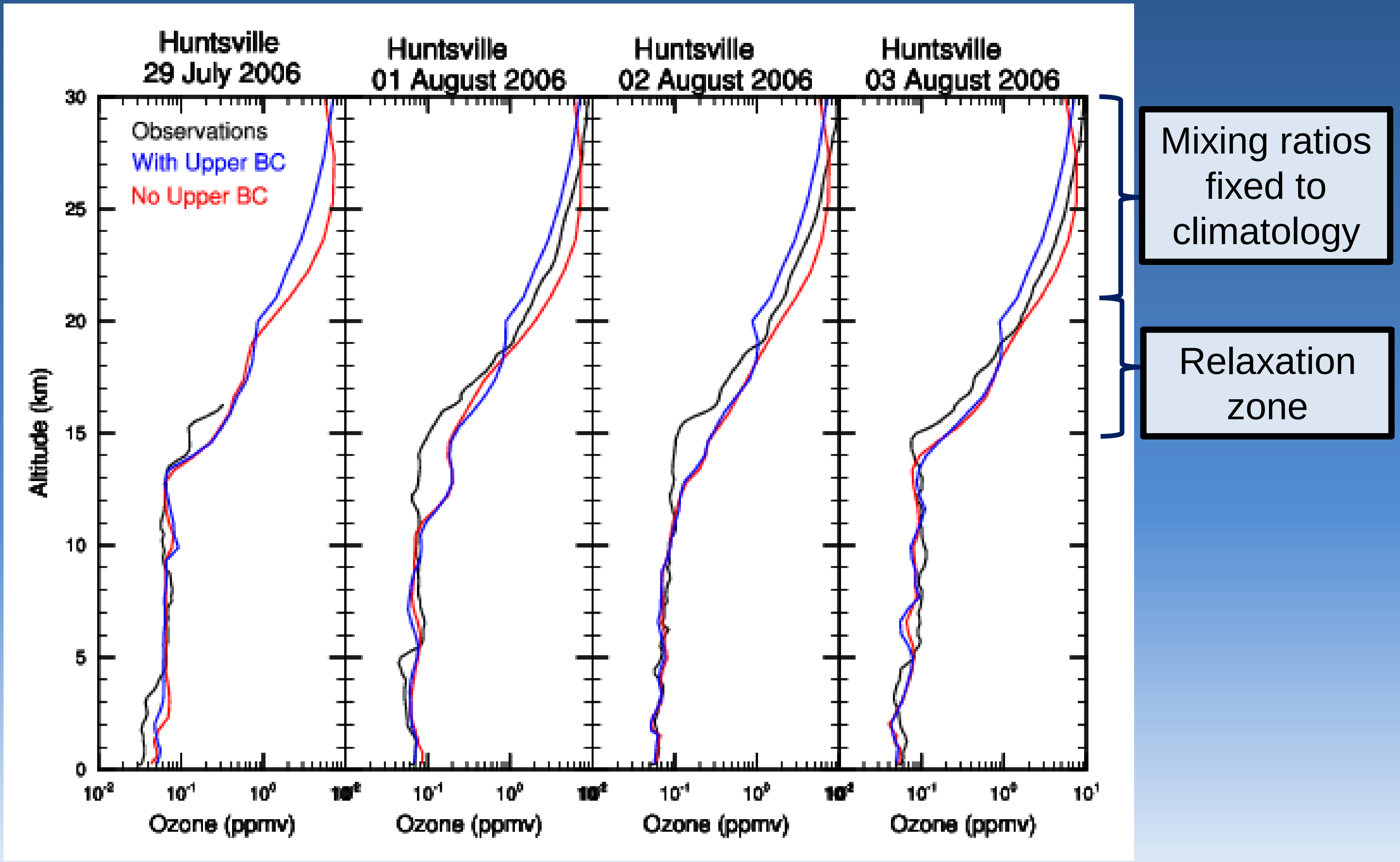
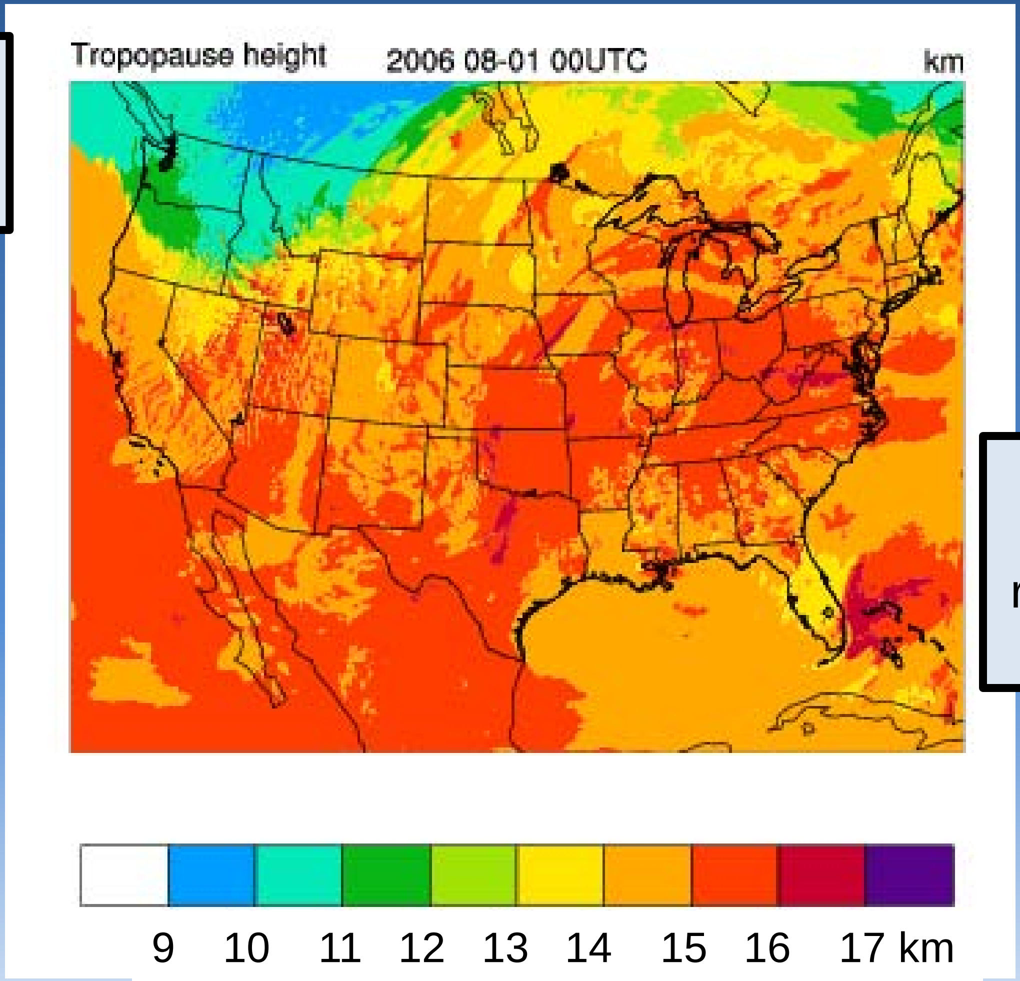


Diagnosed Tropopause Height

Lower tropopause with stratosphere air



Should be able to evaluate these results with analysis data

Summary

- Stratosphere affects the troposphere
  - For simulations over long time periods (≥ month)
  - For chemistry-climate studies
  - For studies during active periods of stratosphere-troposphere exchange (much happens in late spring)
  - For studies that include evaluation with satellite data
- Upper boundary condition for chemical species
  - Currently being implemented in V3.3
  - WACCM climatology

Other WRF-Chem Developments at NCAR/ACD

- Chemical Species Tendency Diagnostics [J. Wong; U. Colorado]
  - Total change due to chemistry, to vertical advection, to horizontal advection, to convective transport, to dry deposition/vertical mixing
  - List of species can be modified with changes to Registry
- Wet Scavenging Scheme for gases – G. Pfister's talk

  Reduced Chemistry

  Aircraft Tracking Tool

  Fire Emissions Preprocessor "Fire_Emis"
- Simplified framework for modeling secondary organic aerosols – A. Hodzic's poster