Air Quality Uncertainties: Choosing among chemical mechanism, meteorology, and model

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CESM Chemistry Climate Working Group Session
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Overview

Research Questions:

What is the impact of the choice of **chemical mechanism**, model, **meteorology**, and resolution on surface chemistry (i.e. O_3 and PM2.5 biases)?

What configuration(s) is (are) the most efficient for human health impact studies? Does this answer depend on region?

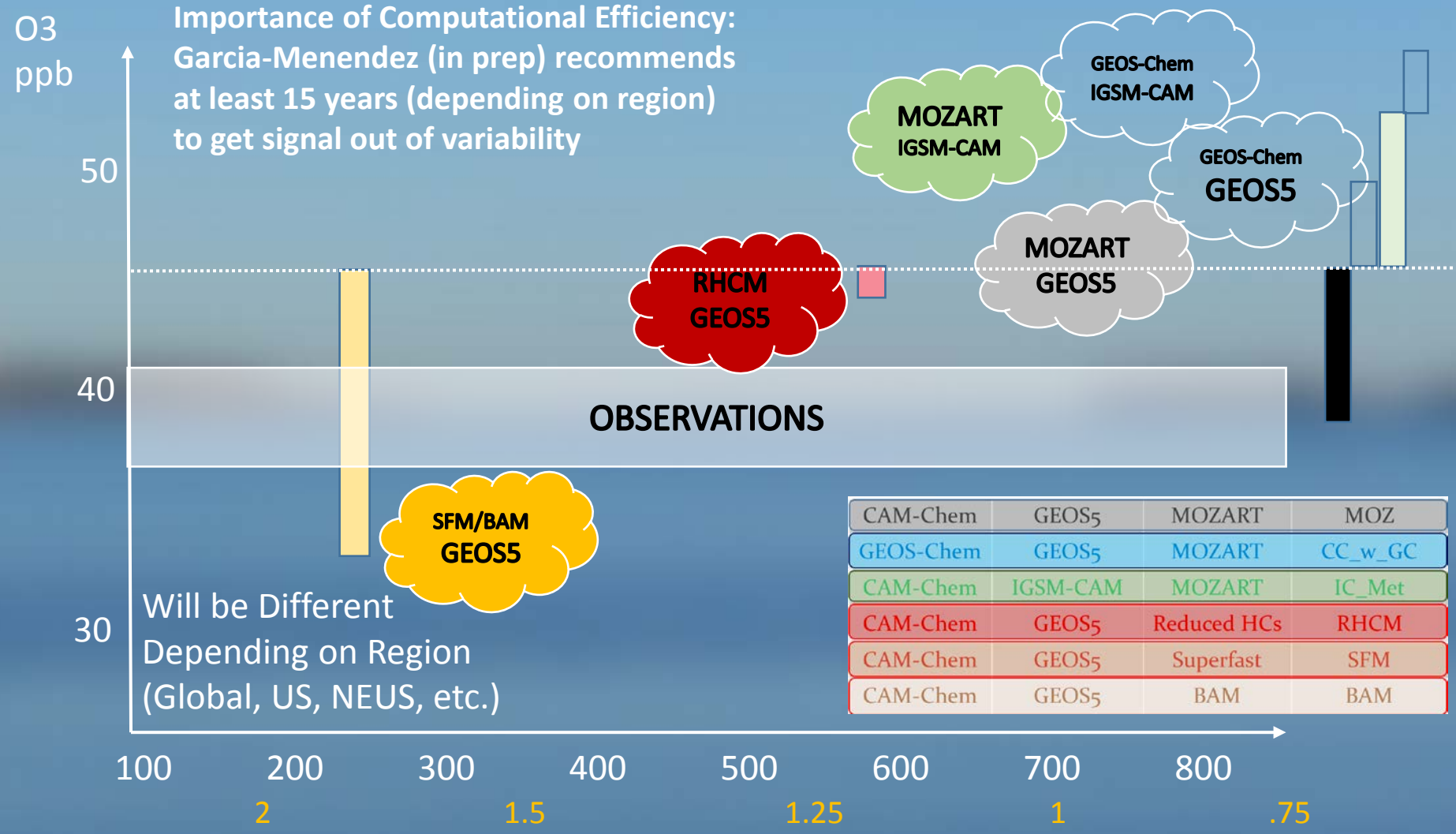
Emissions	Meteorology	Mechanism	Abbreviation
CAM-Chem	GEOS5	MOZART	MOZ
GEOS-Chem	GEOS5	MOZART	CC_w_GC
CAM-Chem	IGSM-CAM	MOZART	IC_Met
CAM-Chem	GEOS5	Reduced HCs	RHCM
CAM-Chem	GEOS5	Superfast	SFM
CAM-Chem	GEOS5	BAM	BAM

model*

met

mechanism

Motivation: **Bias/Error versus Speed**



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GEOS-Chem	GEOS5	MOZART	CC_w_GC
CAM-Chem	IGSM-CAM	MOZART	IC_Met
CAM-Chem	GEOS5	Reduced HCs	RHCM
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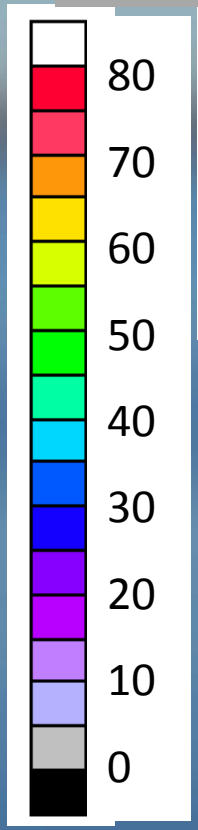
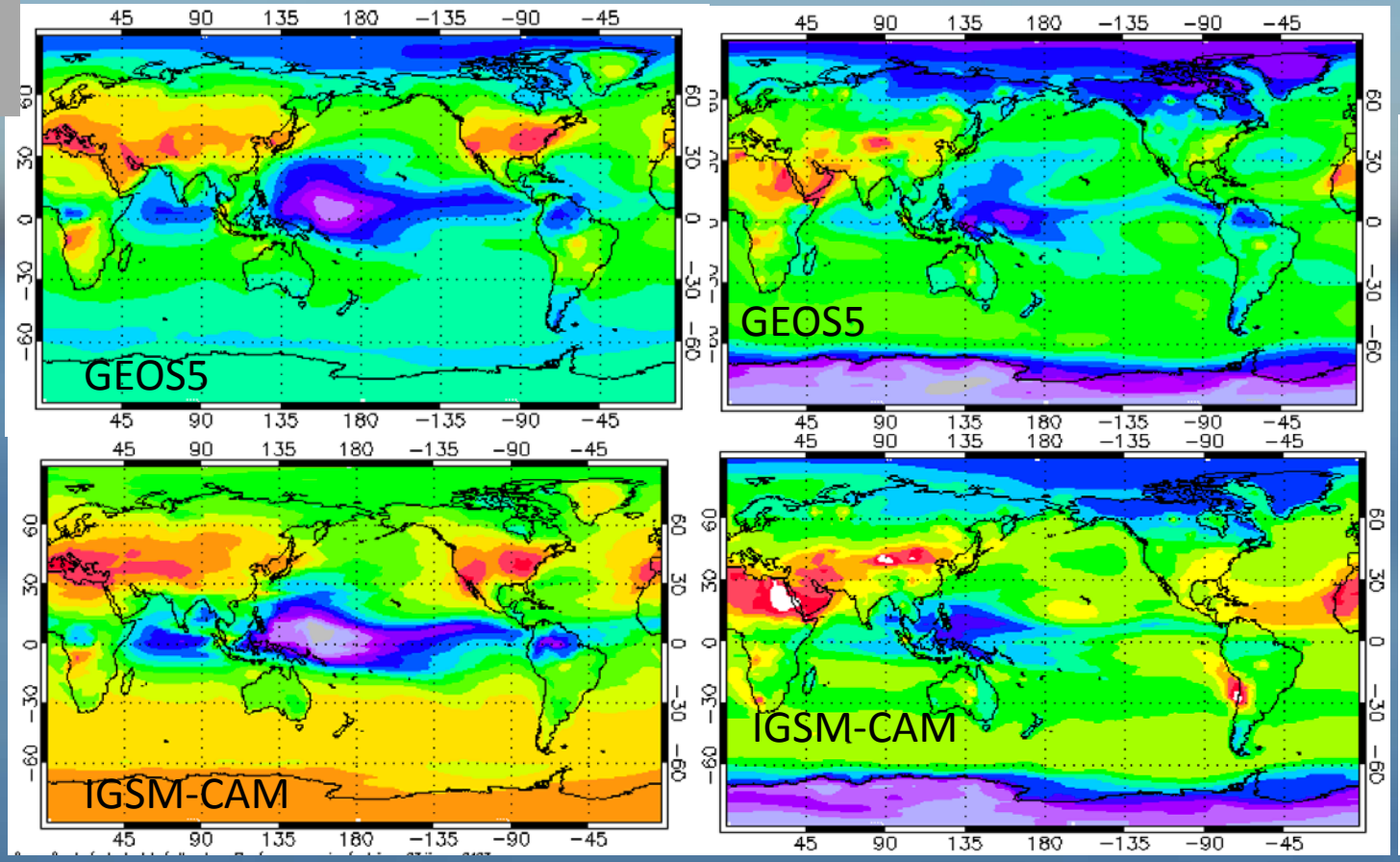
CAM-Chem	GEOS5	MOZART	MOZ
CAM-Chem	IGSM-CAM	MOZART	IC_Met

Comparing Meteorologies

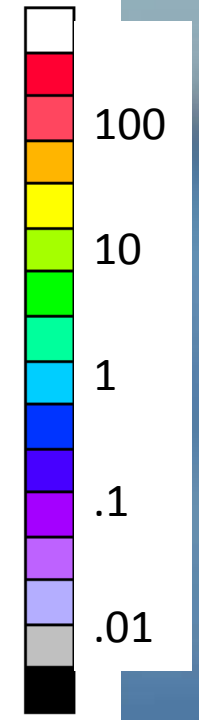
Summertime (JJA) Daily Surface Average, 2004 - 2007

O3 ppb





PM2.5 ug/kg



CAM-Chem	GEOS5	MOZART	MOZ
CAM-Chem	IGSM-CAM	MOZART	IC_Met

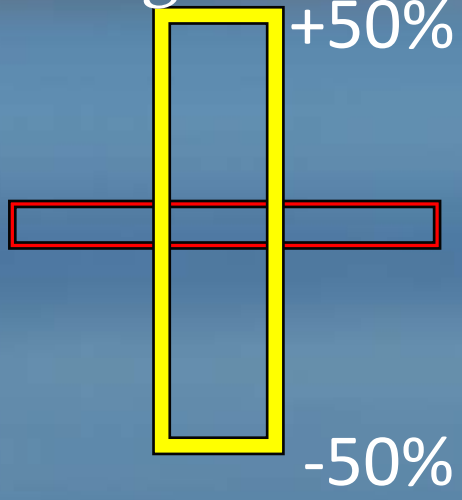
Comparing Meteorologies

Relative Difference:

IGSM-CAM Meteorology

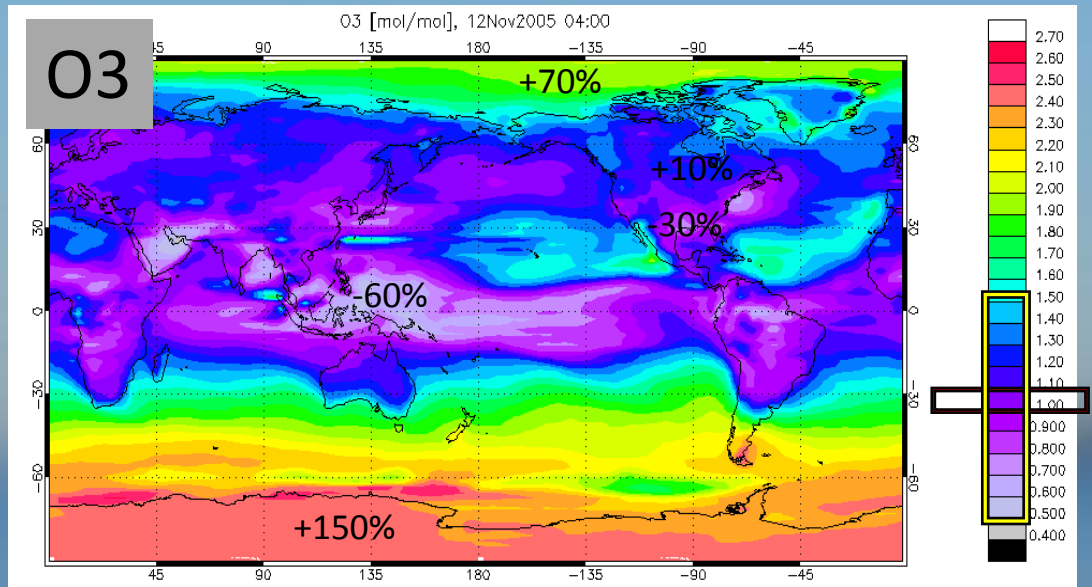
GEOS-5 Meteorology

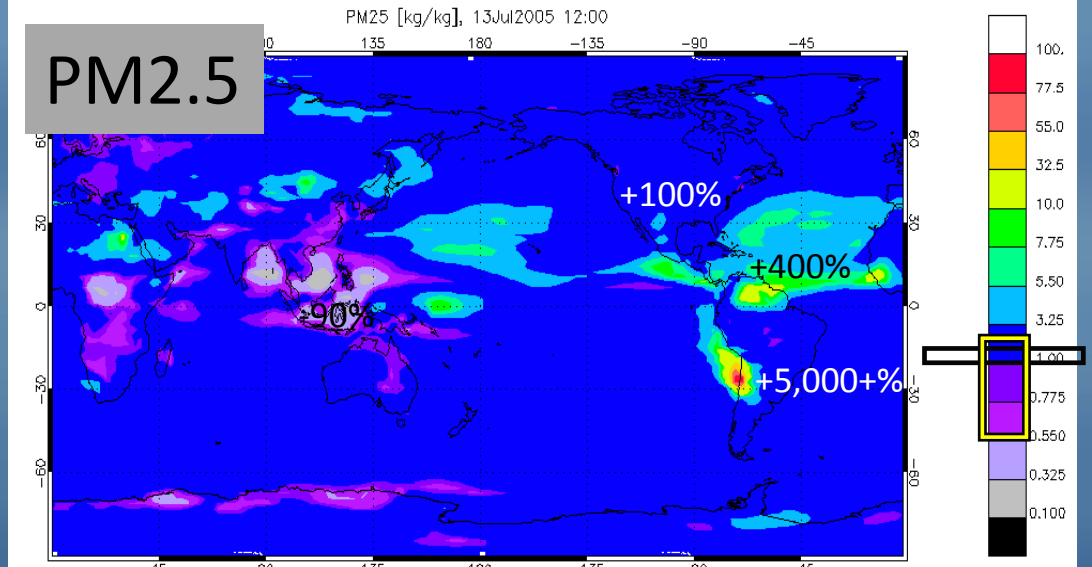
Widget:



JJA Surface O3

JJA Surface PM2.5



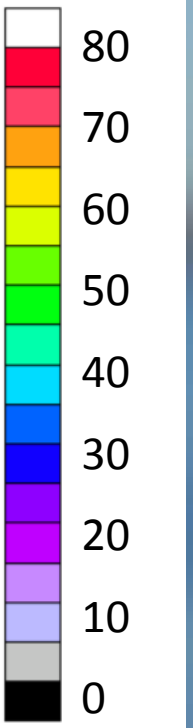


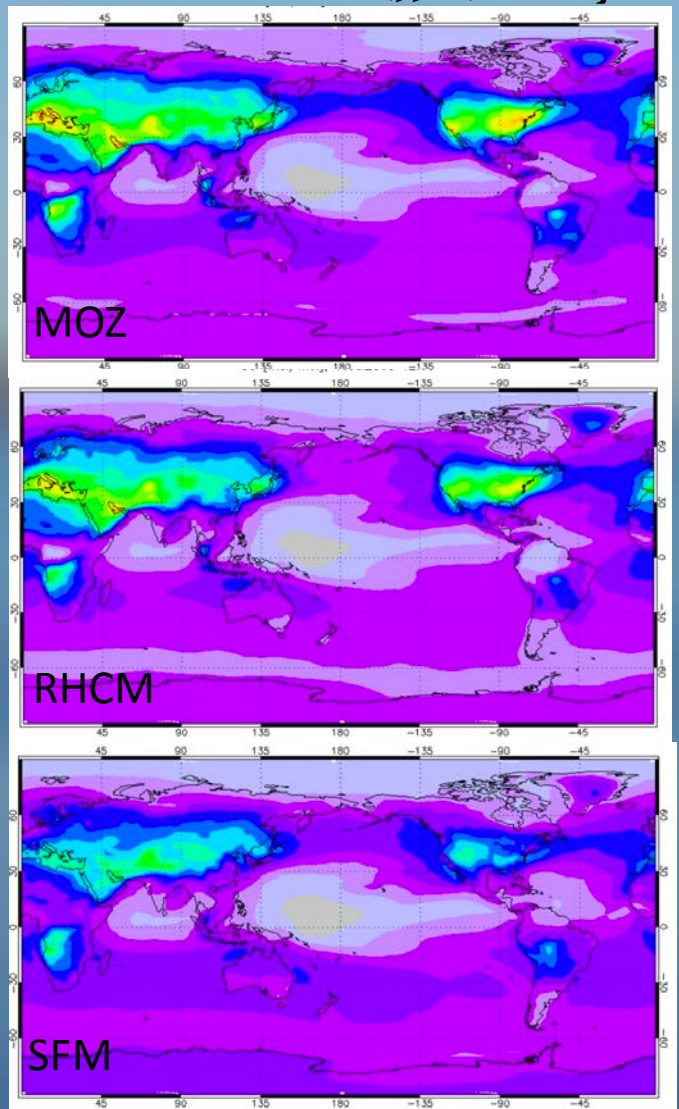
CAM-Chem	GEOS5	MOZART	MOZ
CAM-Chem	GEOS5	Reduced HCs	RHCM
CAM-Chem	GEOS5	Superfast	SFM
CAM-Chem	GEOS5	BAM	BAM

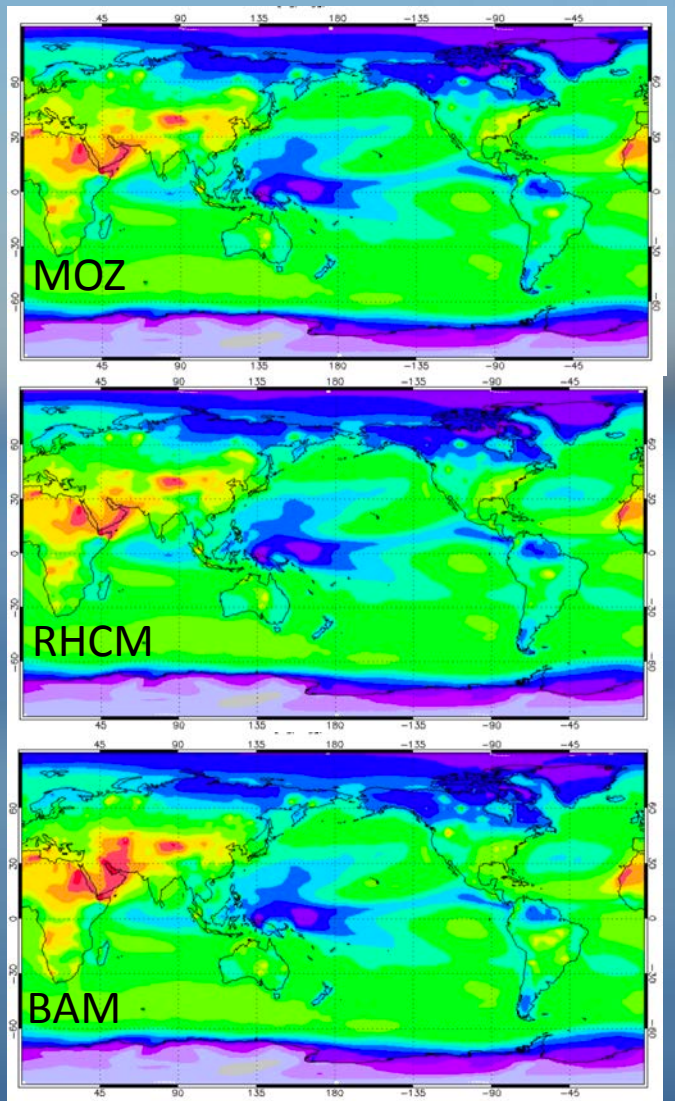
Comparing Mechanisms

Summertime (JJA) Daily Surface Average, 2004 - 2007

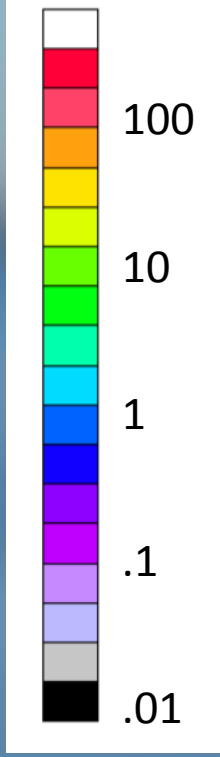
O3 ppb







PM2.5 ug/kg



CAM-Chem	GEOS5	MOZART	MOZ
CAM-Chem	GEOS5	Reduced HCs	RHCM

RHCM

MOZ

Comparing Mechanisms

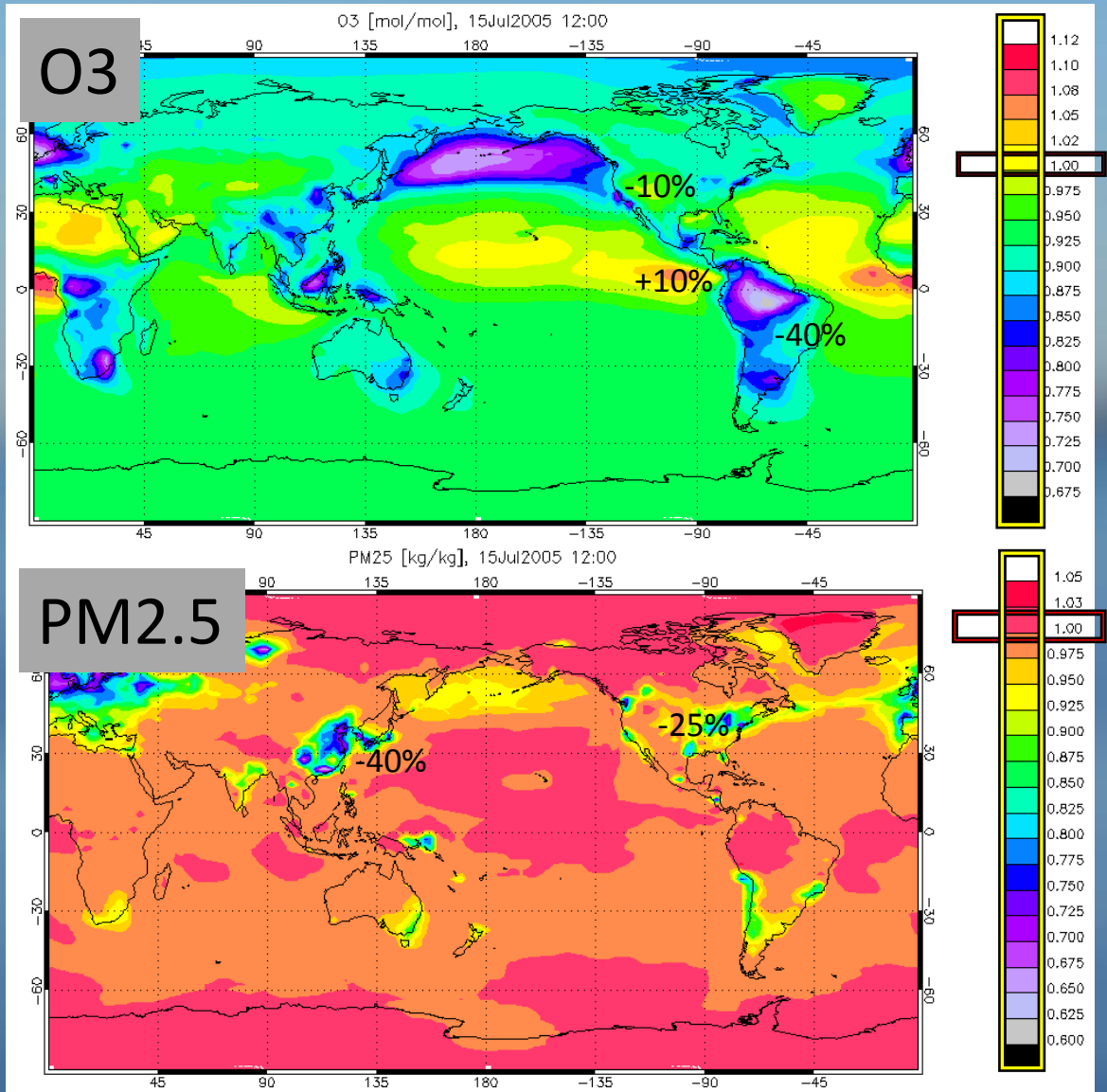
Relative Difference

Reduced Hydrocarbon Mechanism (Houweling et al., 1998)

Simplified treatment of hydrocarbons

Different Lumping:
Alkanes – Paraffins
Alkenes - Olefins

Additionally:
Removed Halogen Species (as Stratosphere is Specified),which results in 40%+ faster simulations with only small differences at the surface compared to “full” Reduced Hydrocarbon Mechanism



CAM-Chem	GEOS5	MOZART	MOZ
CAM-Chem	GEOS5	Superfast	SFM
CAM-Chem	GEOS5	BAM	BAM

SFM or BAM

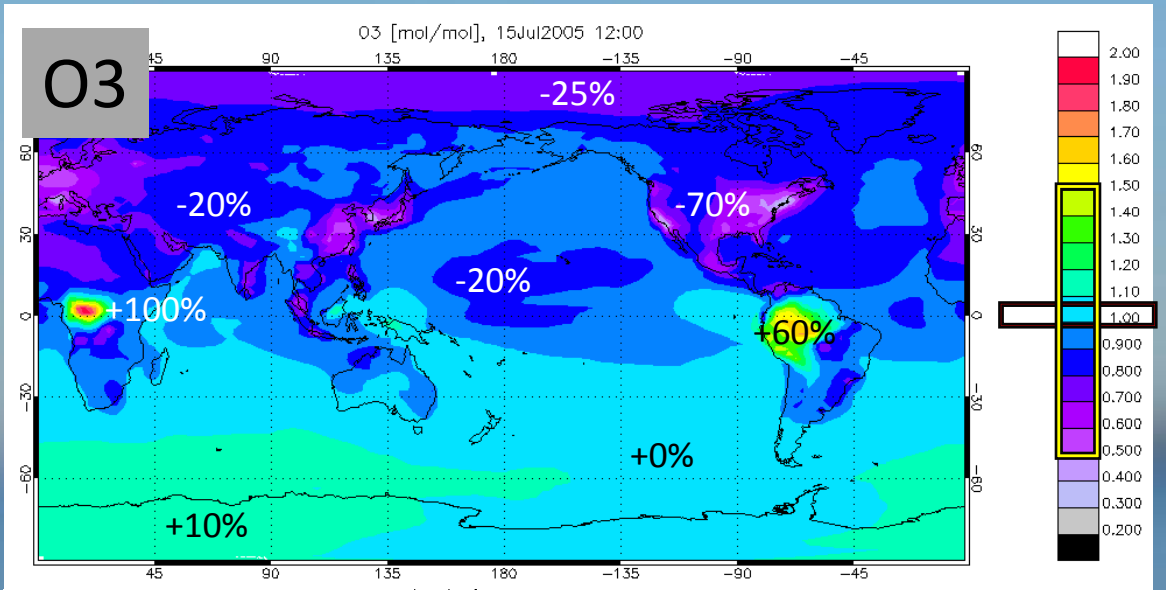
MOZ

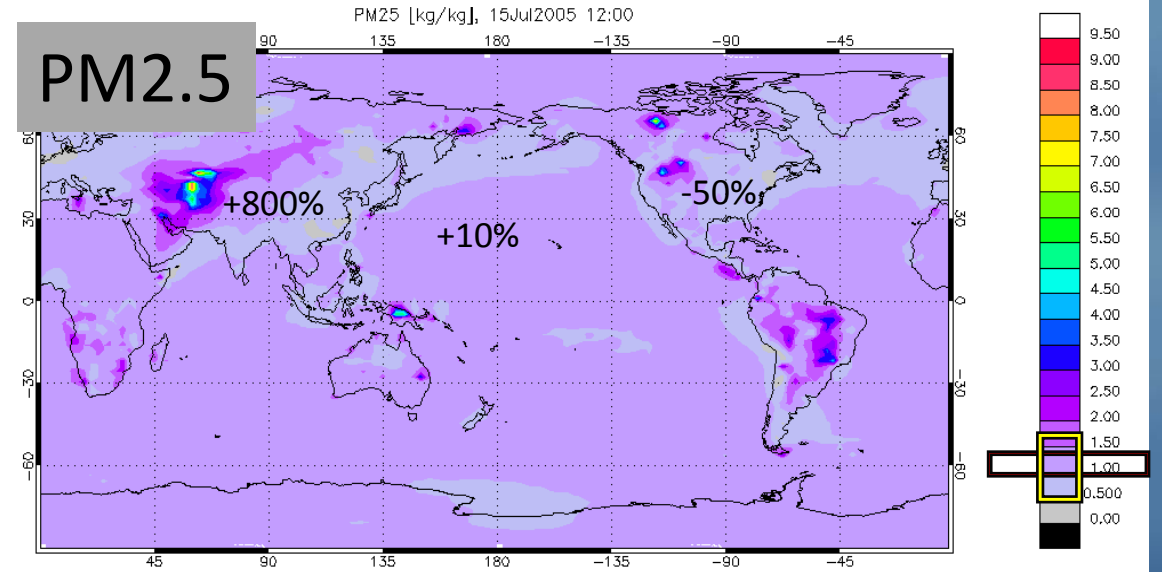
Comparing Mechanisms

Relative Difference

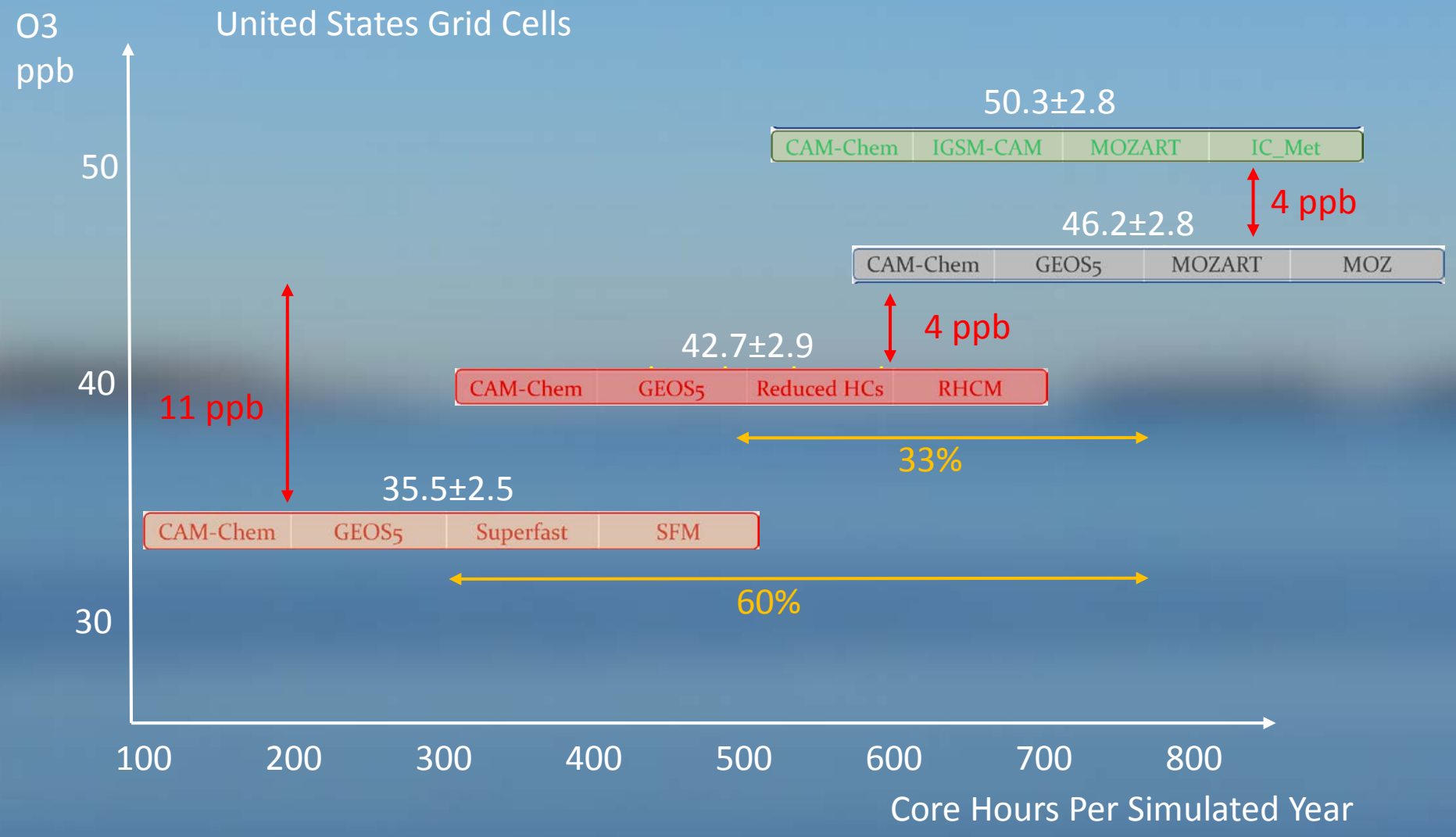
For Ozone:
Superfast Mechanism
(Cameron-Smith et al., 2006, Lamarque et al. 2013, others)

For PM2.5:
BAM-Only





Computational Advantages



Quantifying RHCM Acceptability

Difference in Means Test
To determine is RHCM is
Different from MOZART
(taken from Wilks, 2006)

$$z = \frac{\bar{x}_{MOZ} - \bar{x}_{RHCM}}{\sqrt{\frac{{s_{MOZ}}^2}{n_{MOZ}} + \frac{{s_{RHCM}}^2}{n_{RHCM}}}}$$

H_o: underlying means are equal
H_A: not equal

As surface time series data for O3 and PM2.5 are highly autocorrelated (ρ_1 ~ 0.7 – 0.9)
I use the effective sample size (n')
instead of the
full sample size (n = 368)

$$n' = n\frac{1-\rho_1}{1+\rho_1}$$

Using n’

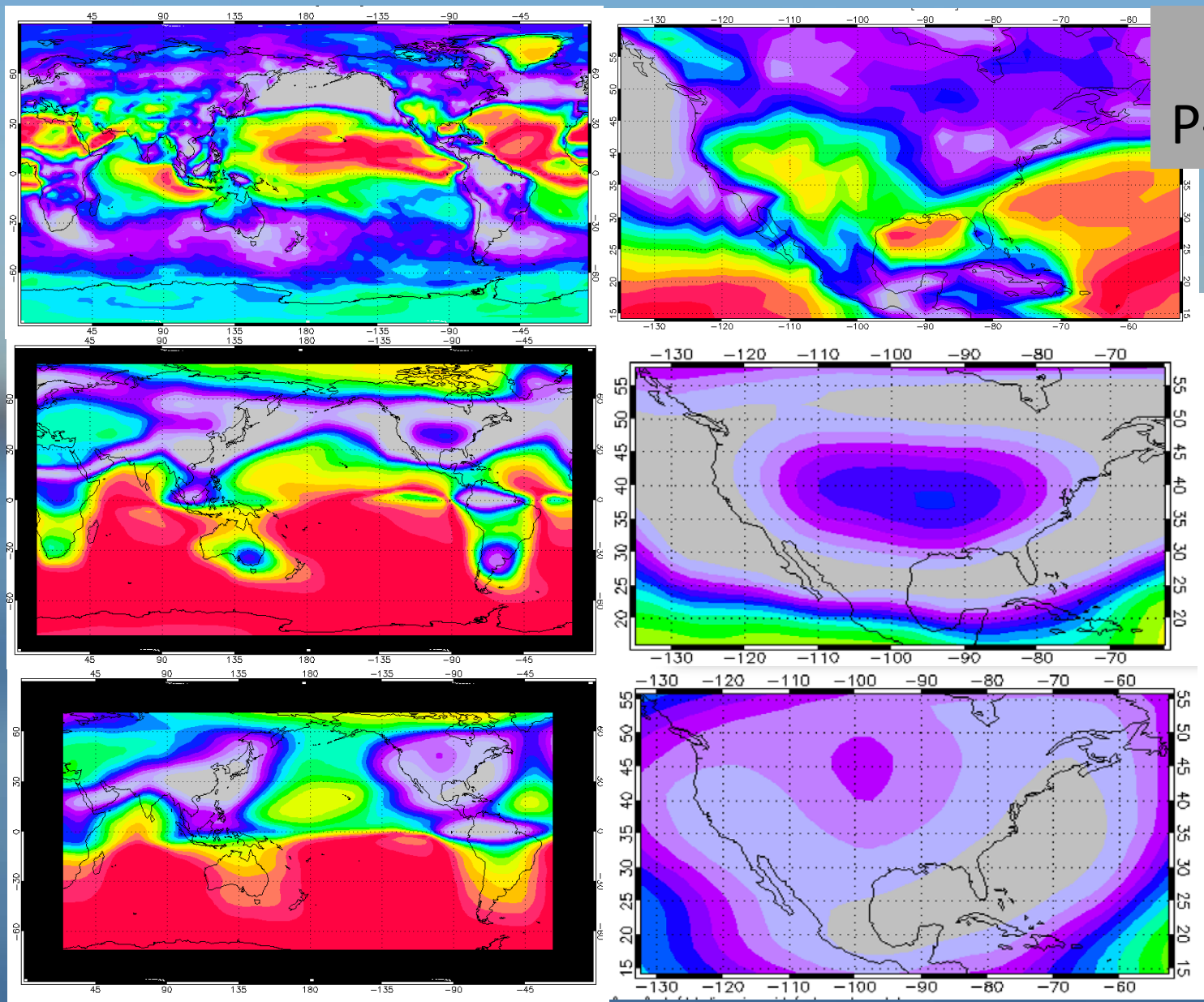
CAM-Chem	GEOS5	MOZART	MOZ
CAM-Chem	GEOS5	Reduced HCs	RHCM

p-values for: (Ho:no difference in mean between MOZ and RHCM)

each grid cell

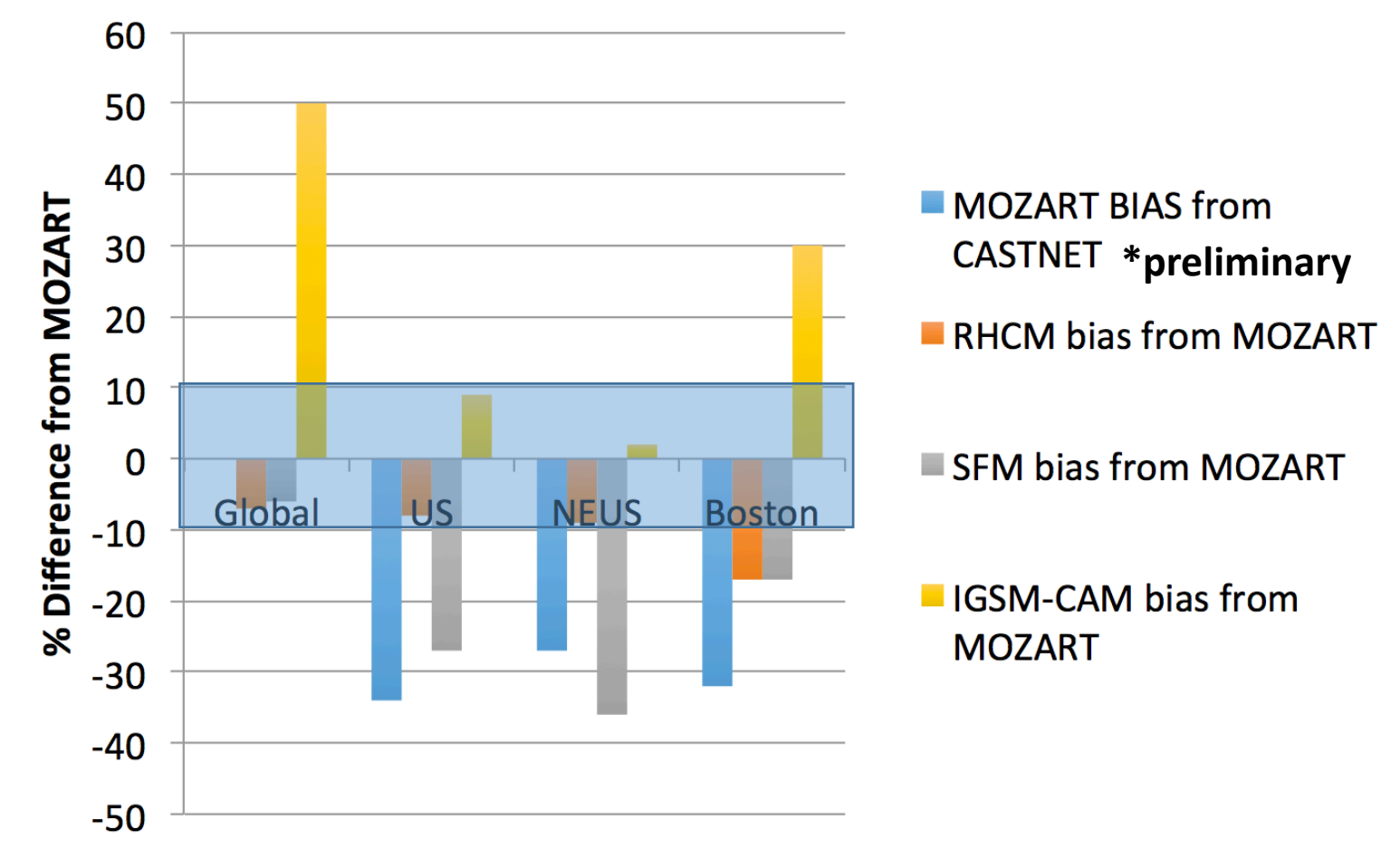
5 cells in every direction

10 cells in every direction



How do they all compare?

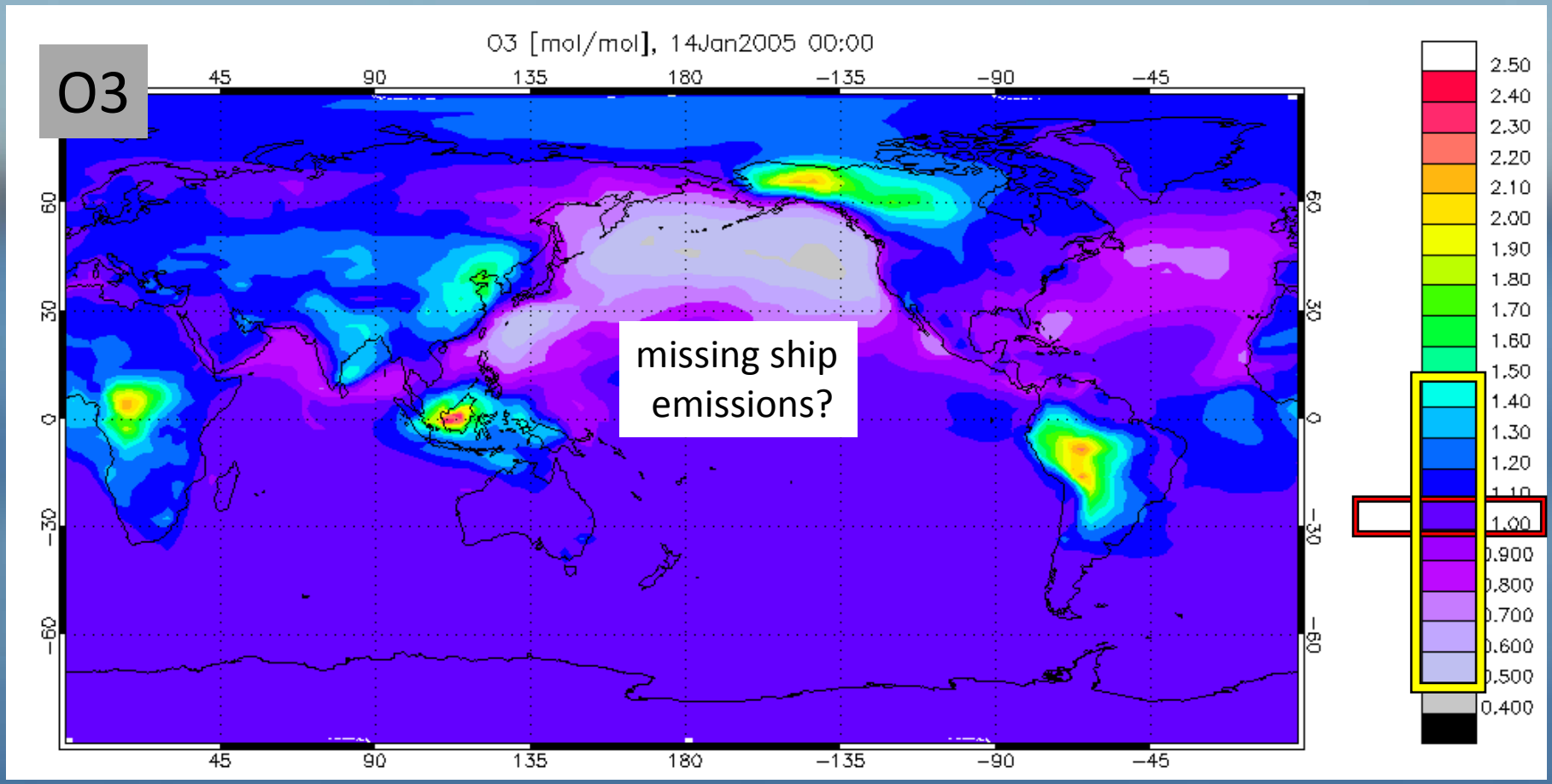
Percent Difference from MOZART Ozone Simulations



GEOS-Chem | GEOS5 | MOZART | CC_w_GC

First Pass: using GEOS-Chem's emissions in CAM-Chem
Near Future: GEOS-Chem simulations, direct comparison

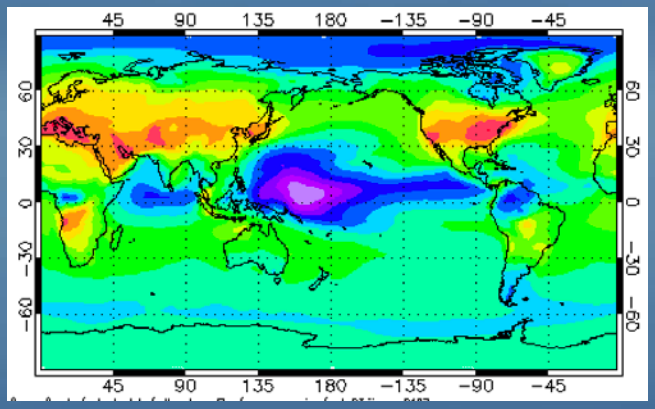
- Relative Difference: $\frac{\text{CAM-Chem with GEOS-Chem Emissions}}{\text{CAM-Chem with CAM-Chem Emissions}}$

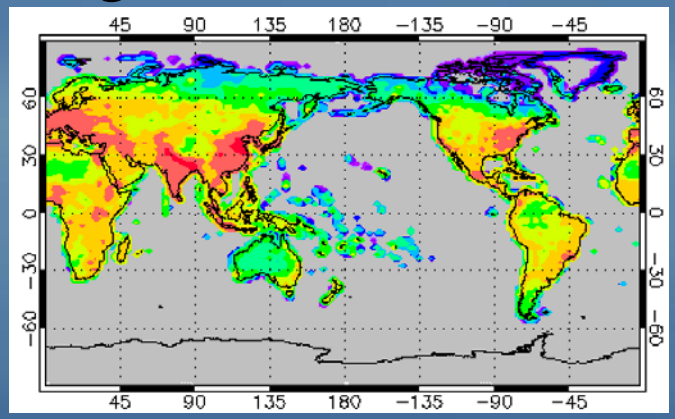


Next Steps

- GEOS-Chem Simulations → Structural Uncertainties
  - standard full tropospheric chemistry
    - GEOS5 and IGSM-CAM meteorology
- 4x5 degree (maybe T31?) simulations
  - (CAM-Chem and GEOS-Chem)
  - Aiming for maximum efficiency/ensemble sizes
- Comparison to Observations
- Population-Weighted Statistics
  - for Human Health Impacts (e.g. via BenMAP)

MOZART





population weighted MOZART

Thanks!

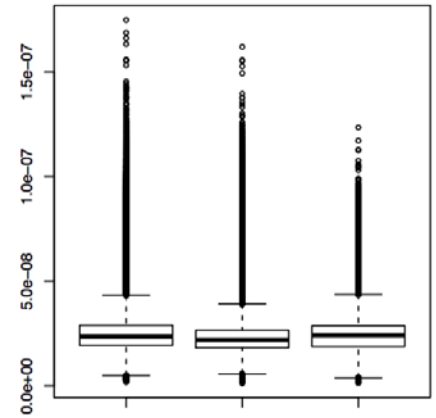
- MIT:
  - Noelle Selin, Ron Prinn, Erwan Monier, Fernando Garcia-Menendez + many others
- NCAR:
  - Louisa Emmons, Simone Tilmes, Gabi Pfister + others
- LLNL:
  - Philip Cameron-Smith

Extra Slides

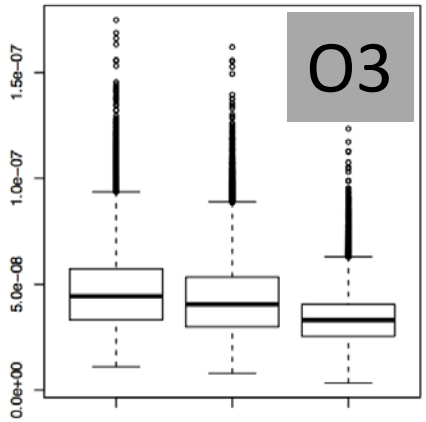
CAM-Chem	GEOS5	MOZART	MOZ
CAM-Chem	GEOS5	Reduced HCs	RHCM
CAM-Chem	GEOS5	Superfast	SFM
CAM-Chem	GEOS5	BAM	BAM

daily JJA
2004 - 2007

Global | US | NEUS | Boston Grid Cell



MOZ RHCM SFM



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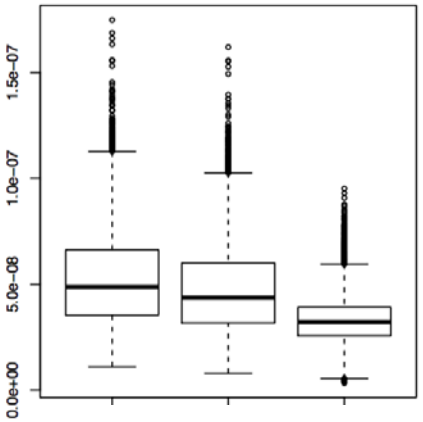

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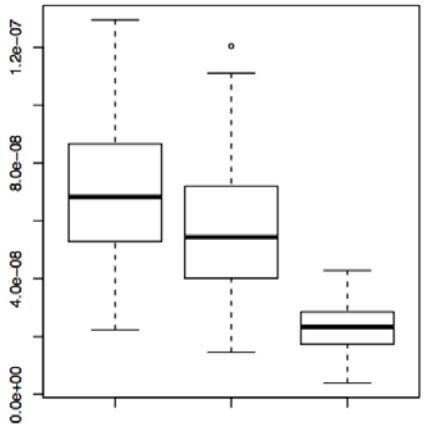

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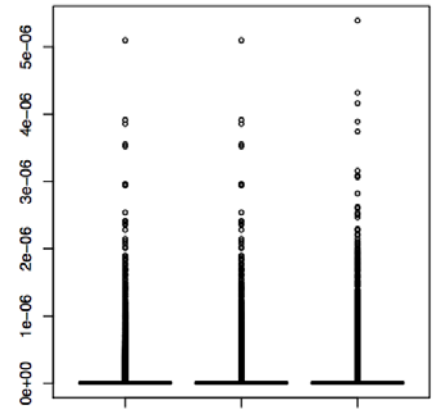
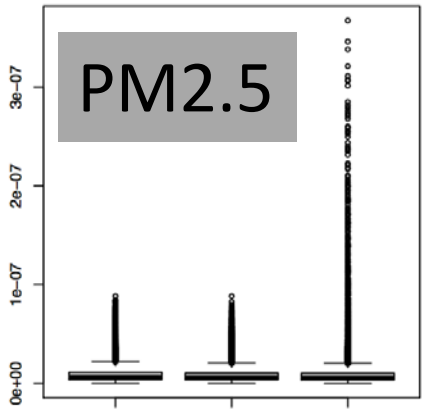
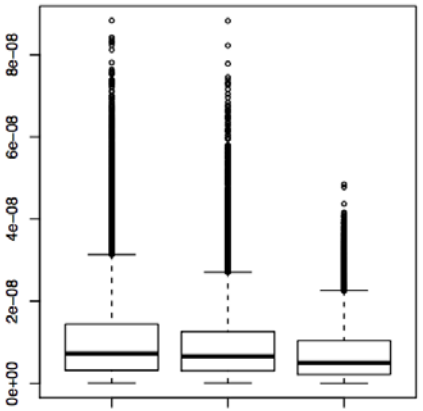


MOZ RHCM BAM



MOZ RHCM BAM



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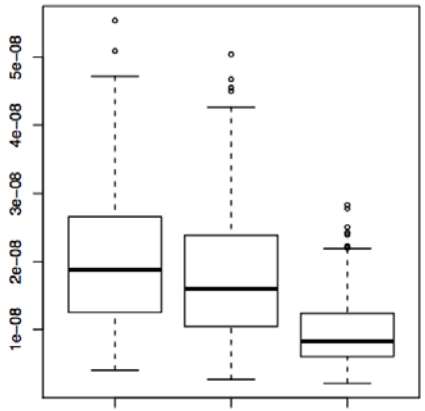


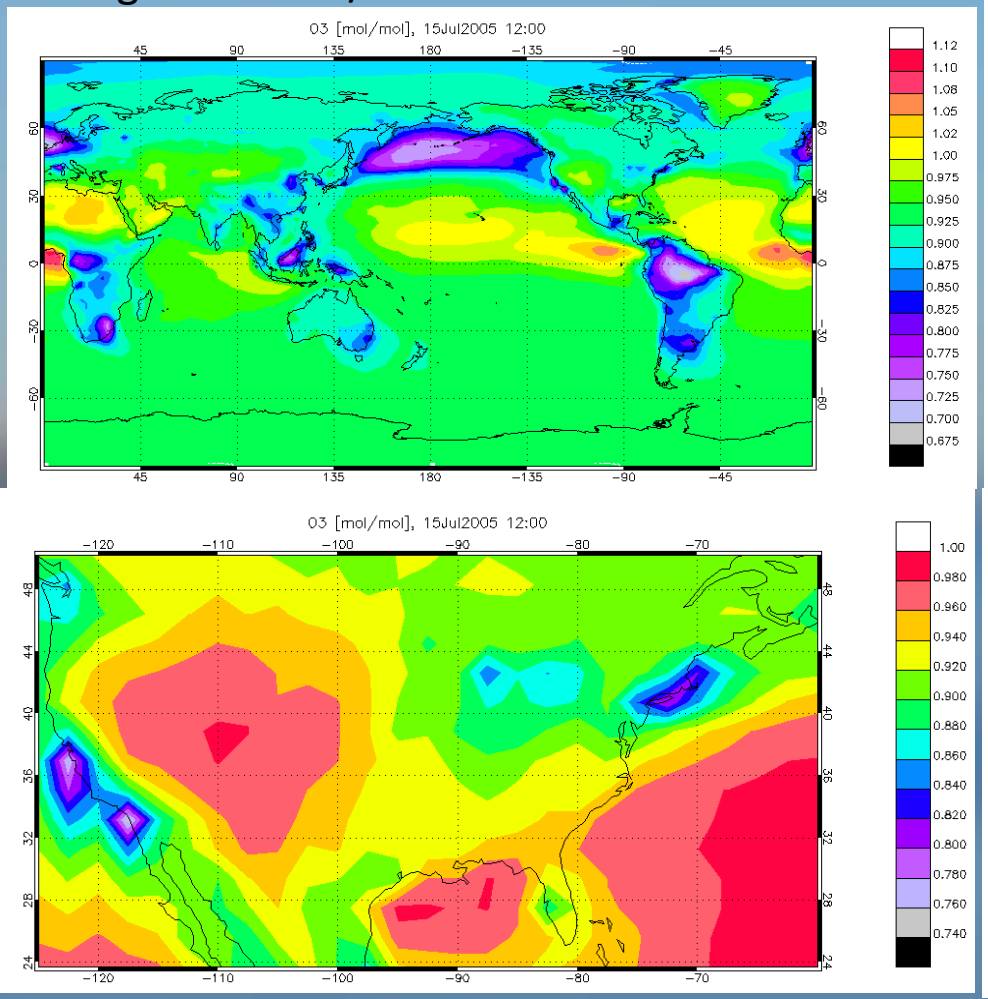
MOZ RHCM BAM

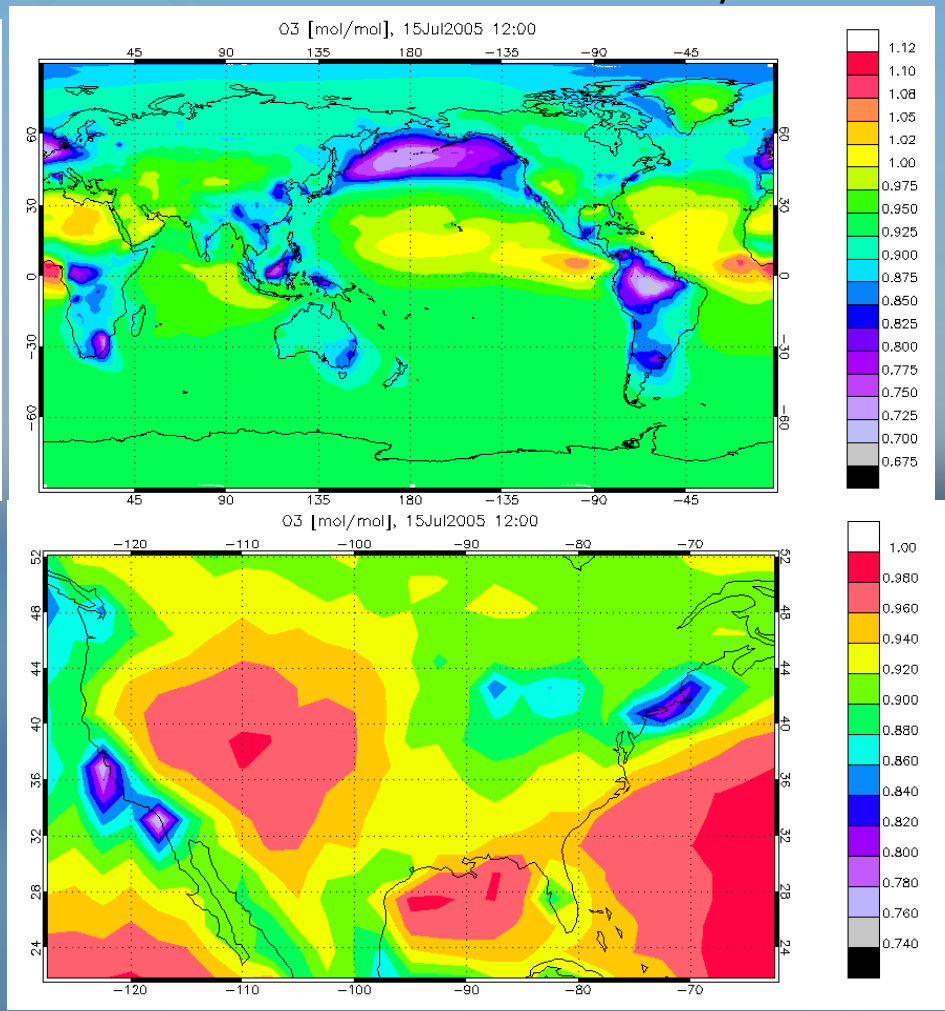
More Details About the “Reduced” RHCM

All these Plots:
RHCM Mechanism/MOZART

Regular RHCM/MOZART

Reduced RHCM/MOZART

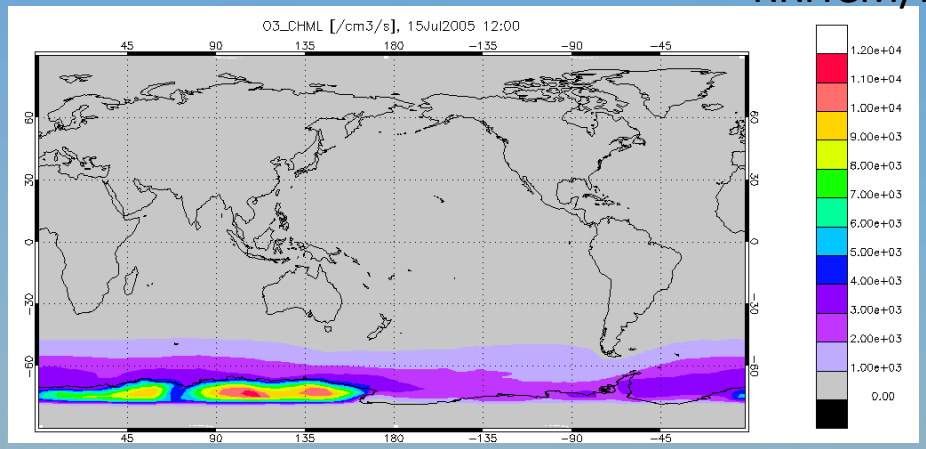


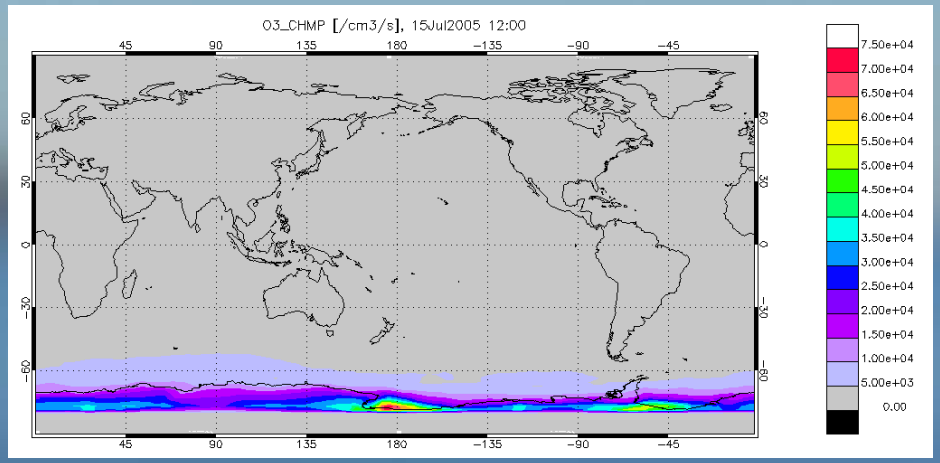


Surface Values, Average JJA, Daily, 2004 - 2007

Difference Between Regular RHCM and Reduced RHCM:

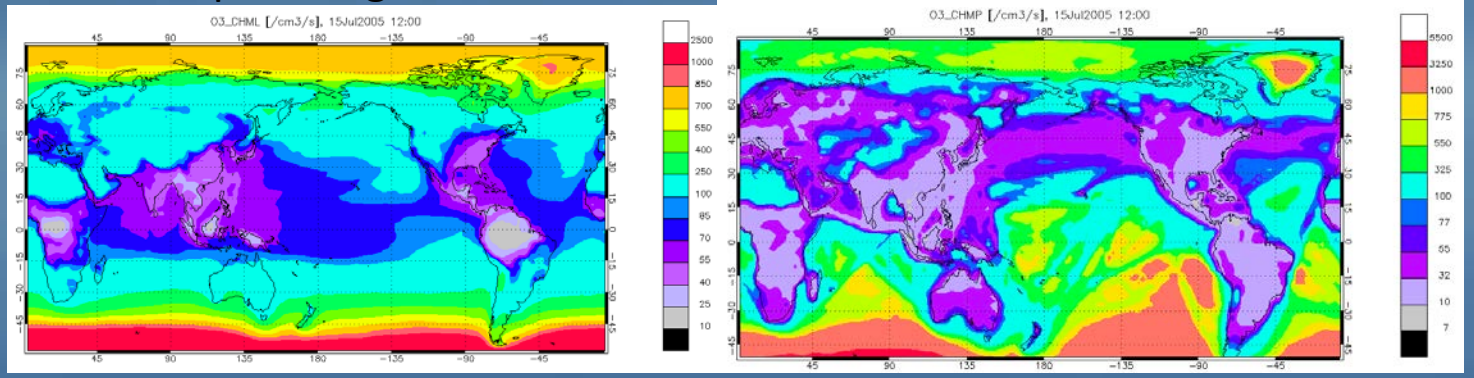
RRHCM/MOZART





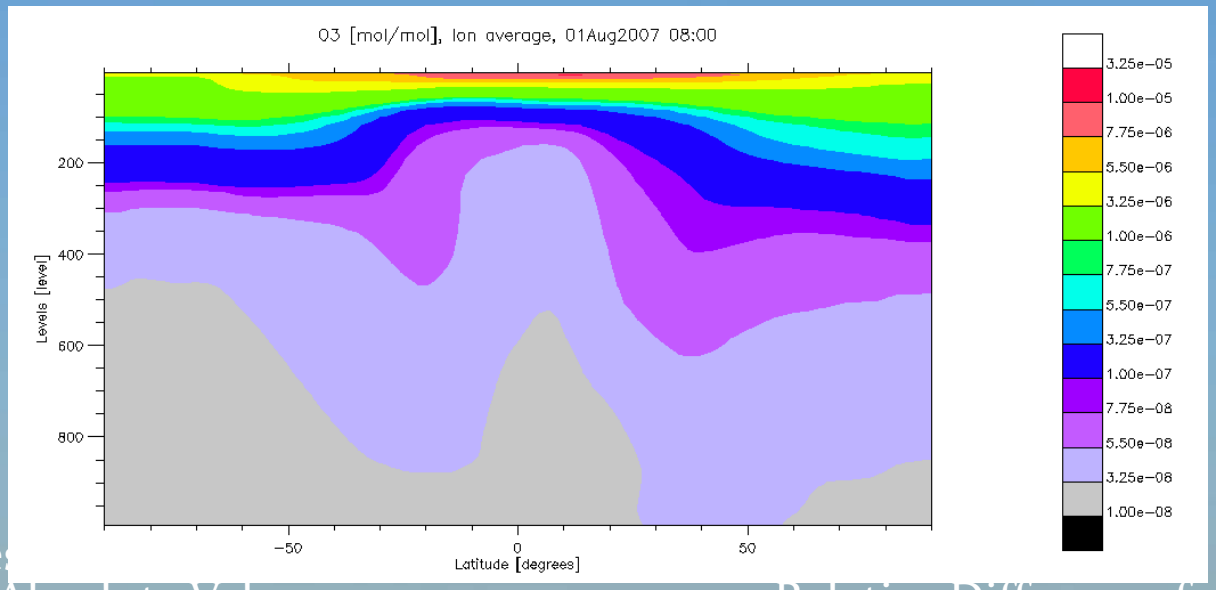
- Not surprising, as we've removed much of the halogen chemistry, which strongly impacts ozone chemistry over Antarctica
- Everywhere else, there does not seem to be a significant difference in O3 chemistry

If I exclude the southern polar region:



O_3

MOZART

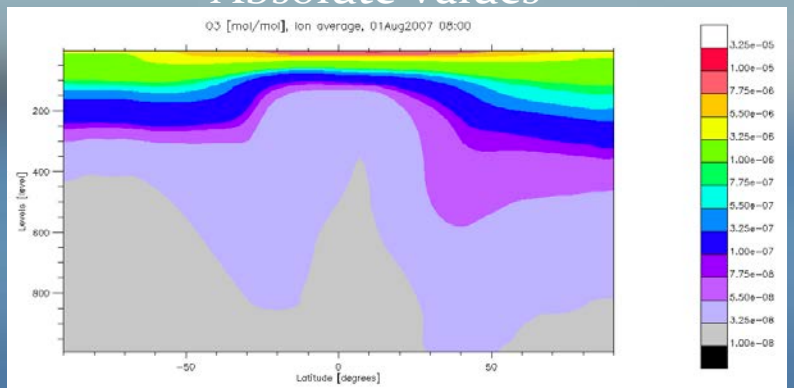


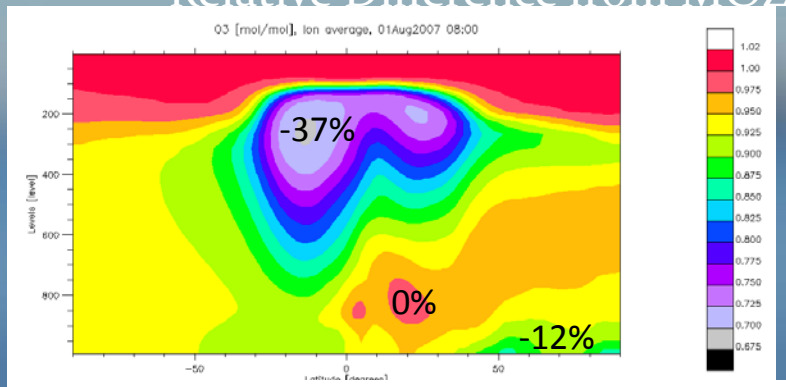
NOTE:
same
color scales

Absolute Values

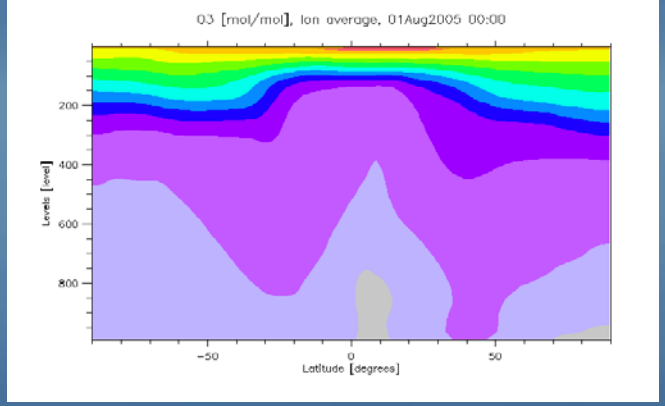
Relative Difference from MOZART

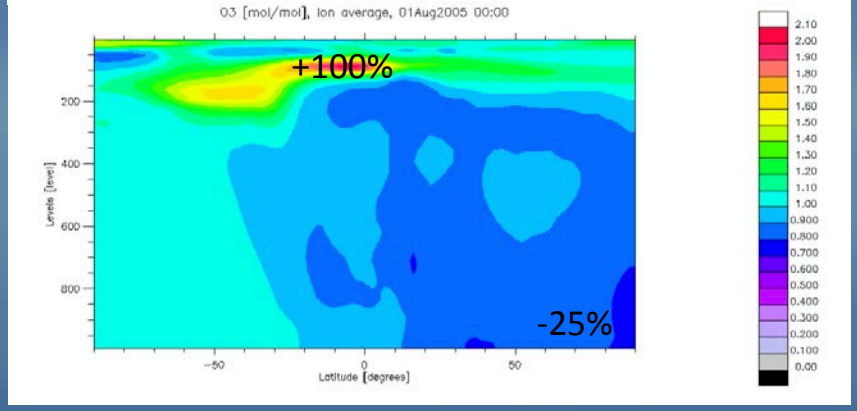
Reduced Hydrocarbon





Superfast



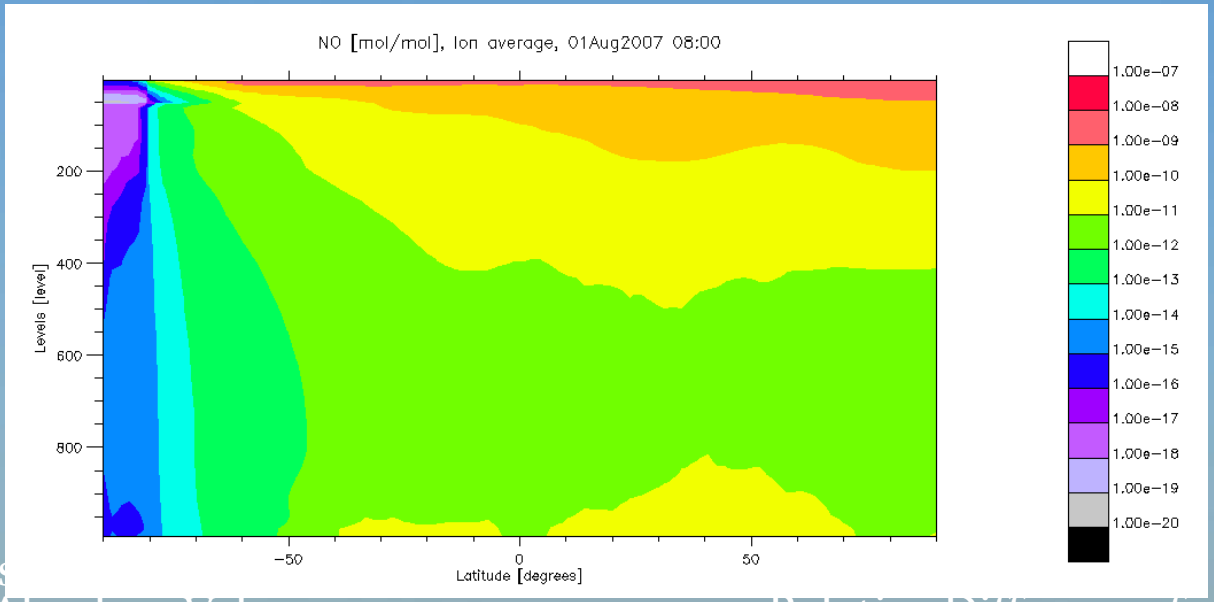


NOTE:
different
color
scales

NO

MOZART

NOTE:
same
color scales

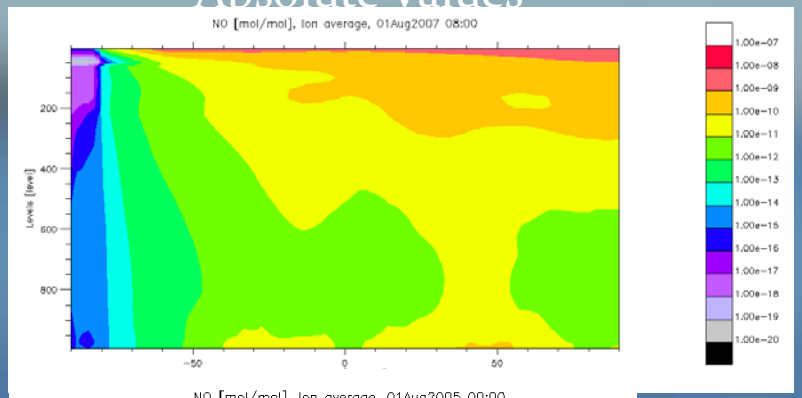


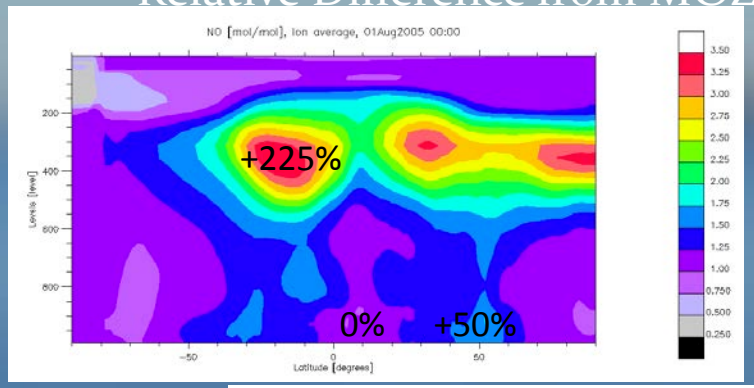
Absolute Values

Relative Difference from MOZART

Reduced Hydrocarbon

Superfast





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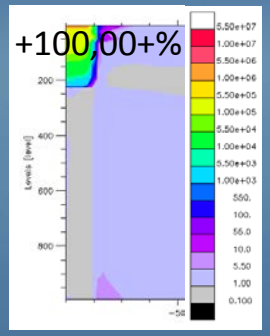
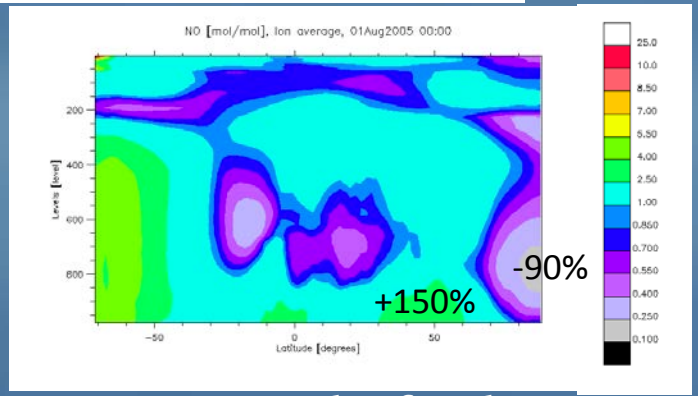


south of 50 lat



north of 50 lat

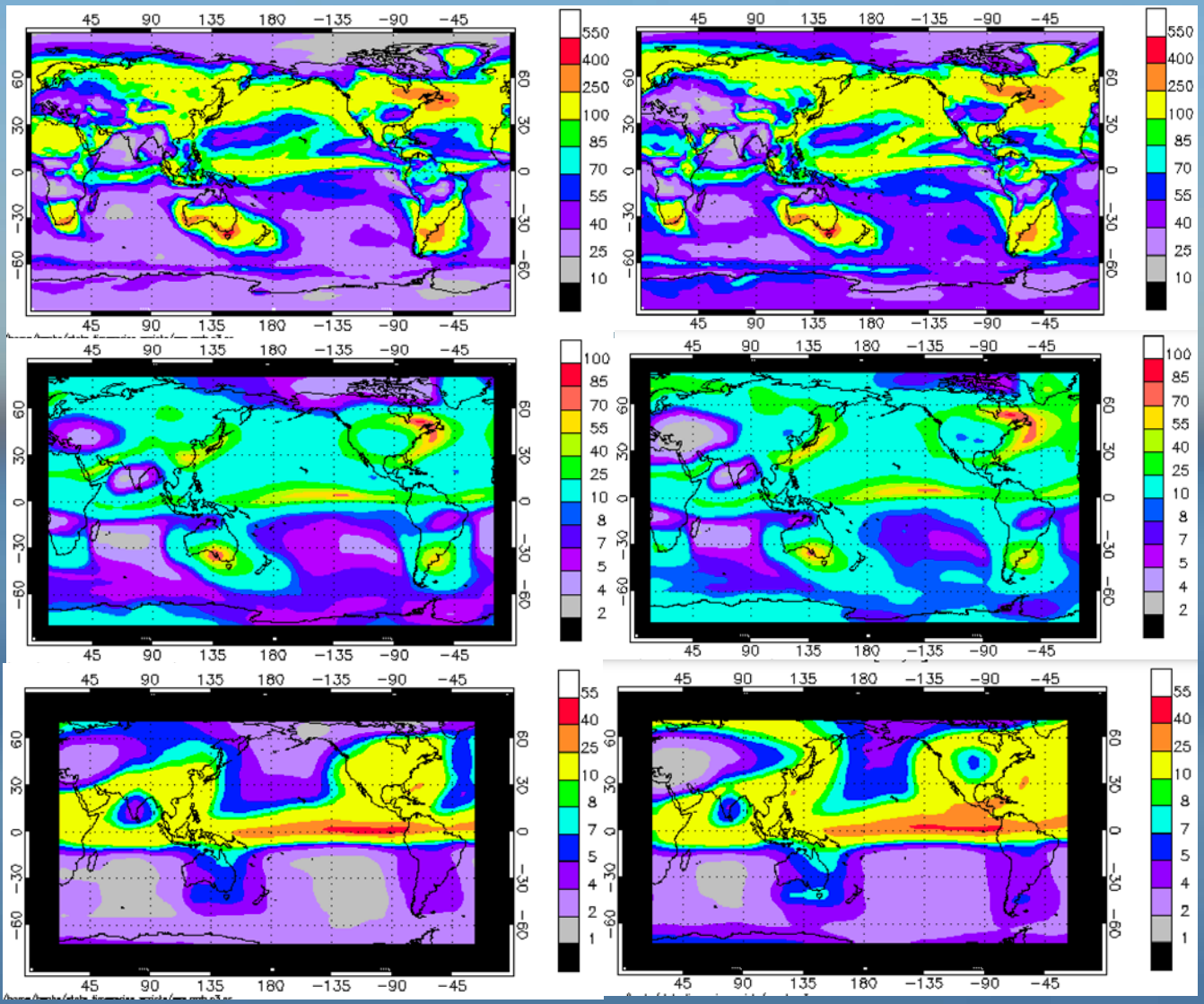
CAM-Chem	GEOS5	MOZART	MOZ
CAM-Chem	GEOS5	Reduced HCs	RHCM

n=368

MOZ

n' for O3

RHCM



each grid cell

n' < 250

5 cells in every direction

n' < 100

10 cells in every direction

n' < 40

use n=368

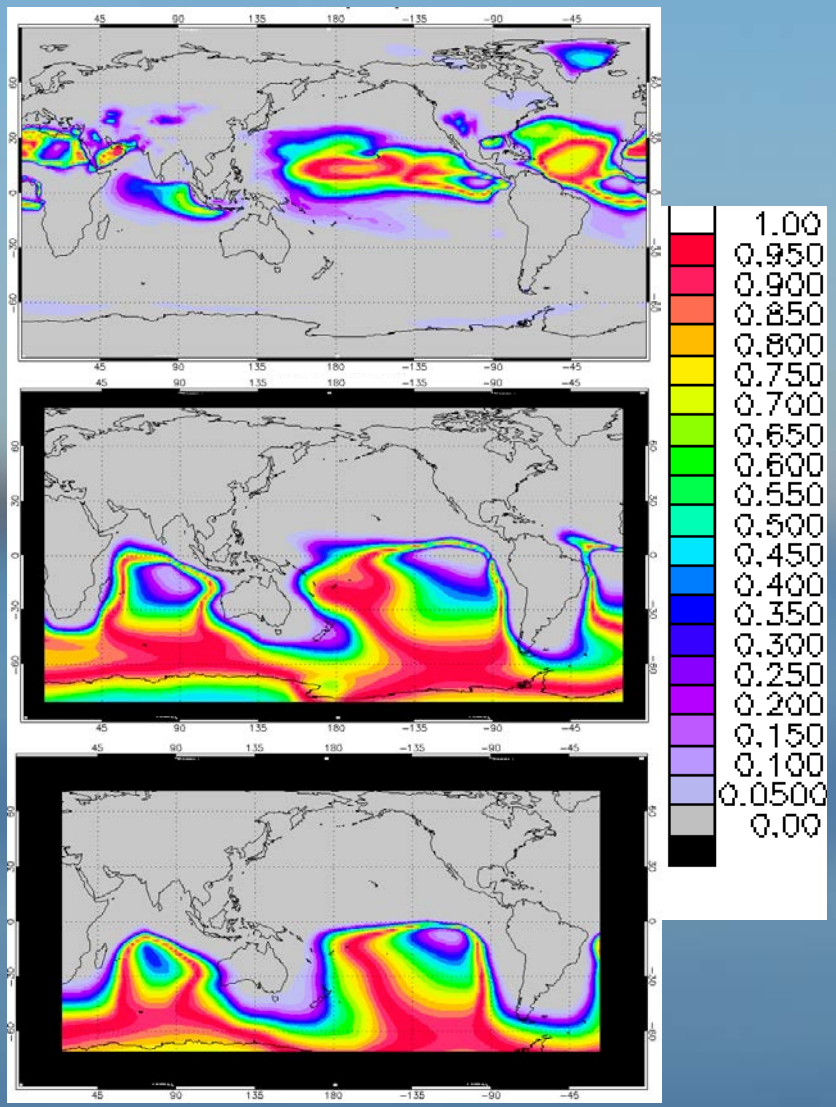
CAM-Chem	GEOS5	MOZART	MOZ
CAM-Chem	GEOS5	Reduced HCs	RHCM

p-values for: (H0:no difference in mean between MOZ and RHCM)

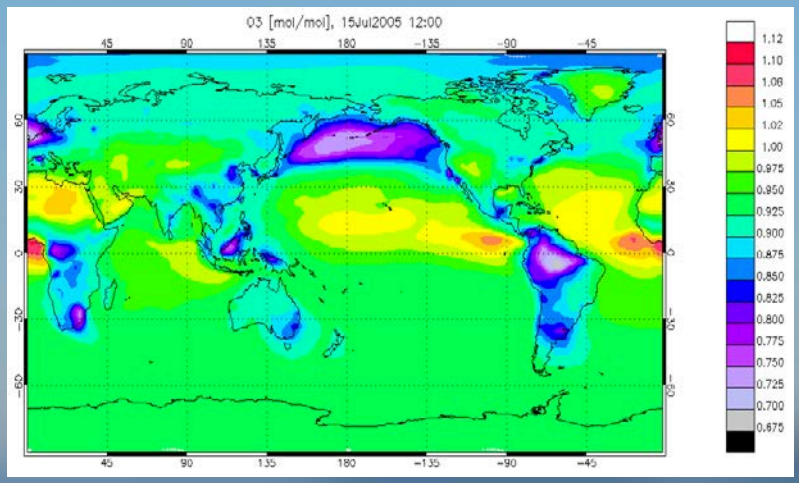
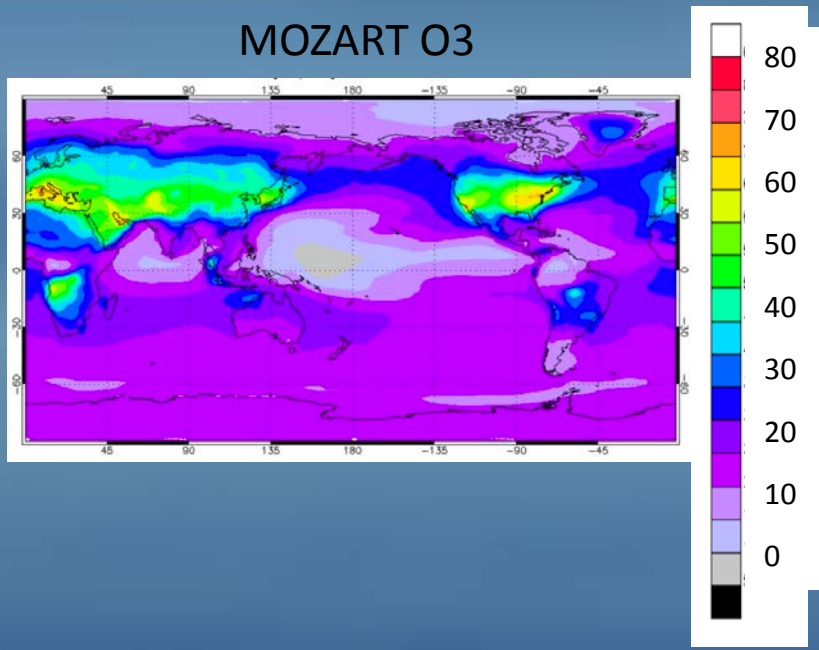
each grid cell

5 cells in every direction

10 cells in every direction



relative difference (RHCM/MOZ)



MOZART O3