Effects Of Using The CB05 vs. SAPRC99 vs. CB4 Chemical Mechanism On Model Predictions

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International Conference on Chemical Mechanisms
December 6, 2006

Questions we wanted to answer…

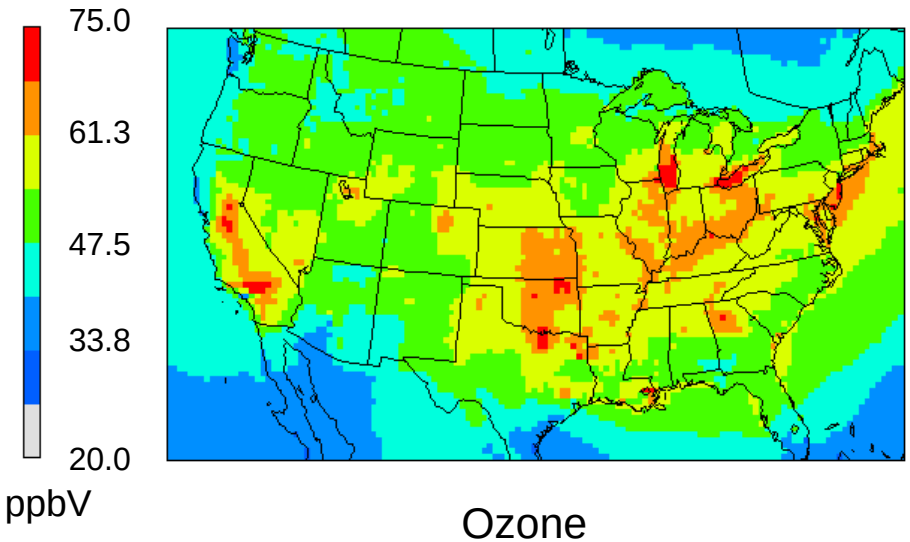
- Does using CB05 instead of CB4 in an air quality model give us different predictions? Are they consistent with SAPRC99 predictions?
  - Focus on ozone and other gas-phase species
  - Focus on large-scale, monthly predictions
- Are there spatial variations in the differences?
- Do the different mechanisms vary in their results for emission changes? (i.e. do they give the same relative reduction)

This work is part of a large study looking at sensitivities, evaluation, comprehensive comparison

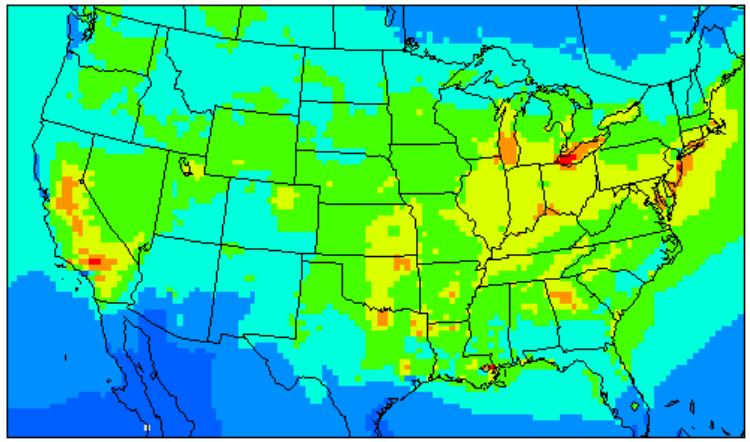
What we did: modeling scenarios

- Used the Community Multi-Scale Air Quality Modeling System (CMAQ v4.5.1)
- 36-km (continental U.S.) and12-km (Eastern US) domain
- January and July, 2001 meteorology from MM5
- CB4, CB05 and SAPRC99 (with cloud chemistry and aerosols)
- Emissions from 2001 NEI

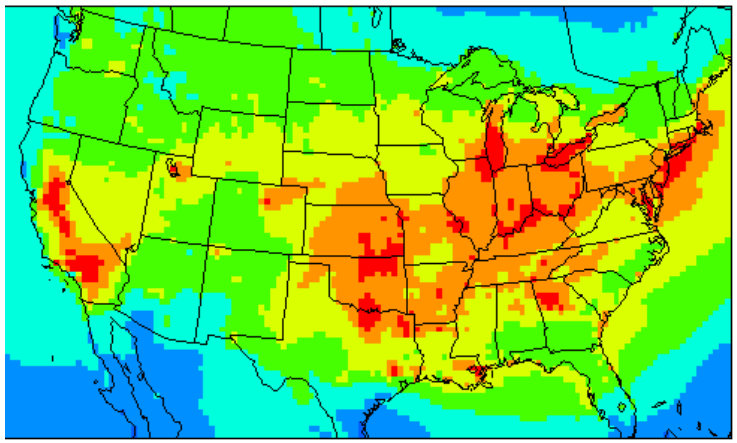
Ozone
CB05



Ozone
CB4



Ozone
SAPRC99

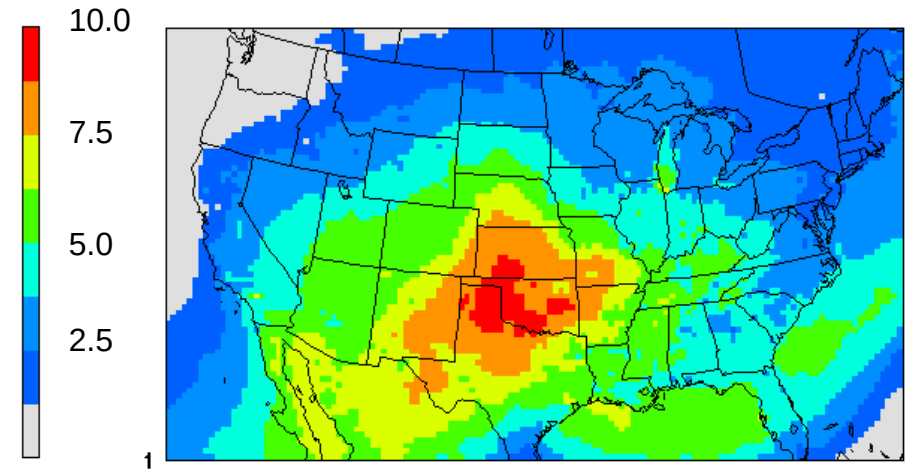


Ozone

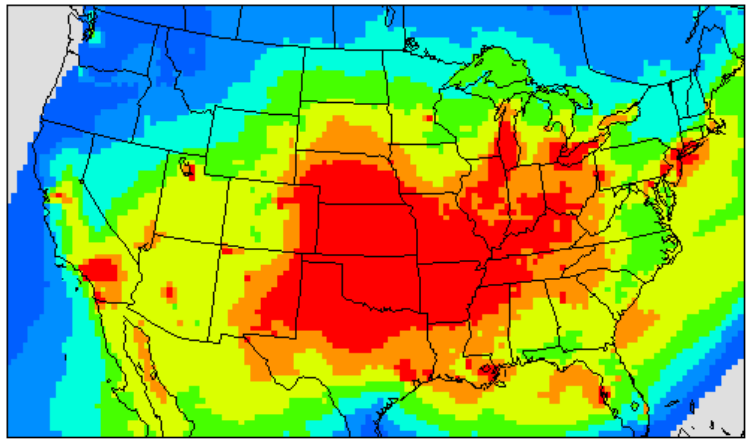
Concentration, July monthly avg of daily 8-hr max

SAPRC99 predicts highest concentrations, CB4 predicts the lowest

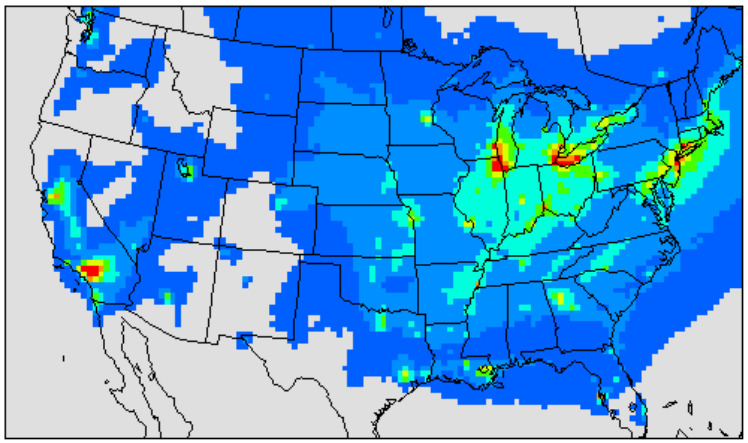
Difference in O3
CB05 – CB4



Difference in O3
SAPRC – CB4



Difference in O3
SAPRC99 – CB05

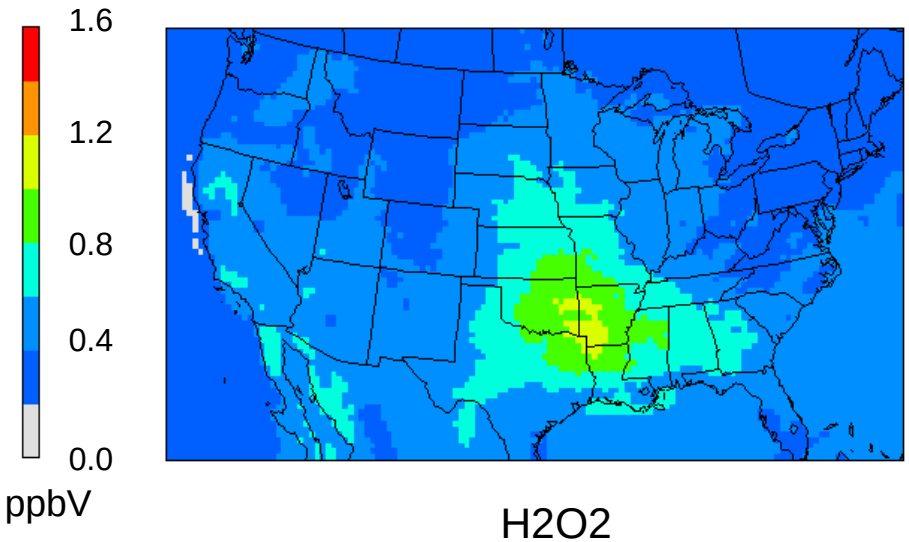


Ozone

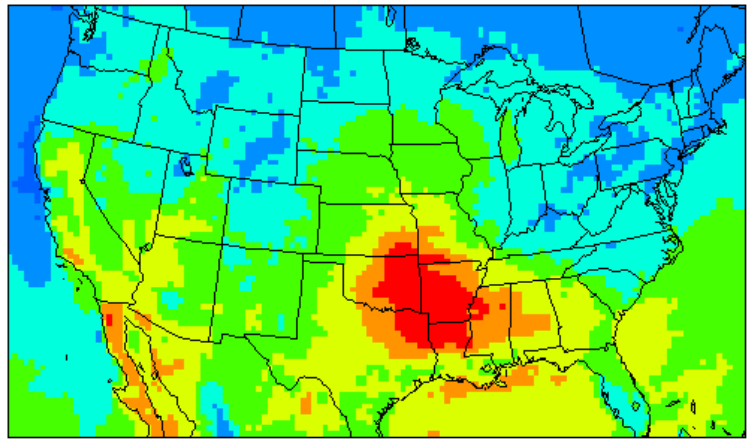
Differences in July monthly avg of daily 8-hr max

Largest differences occur in the central-southern part of the U.S. There are differences between CB05 and SAPRC in some urban areas.

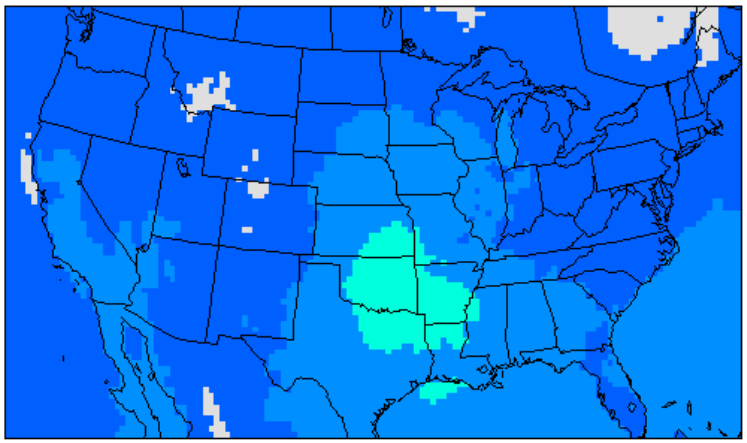
H2O2
CB05



H2O2
CB4



H2O2
SAPRC99

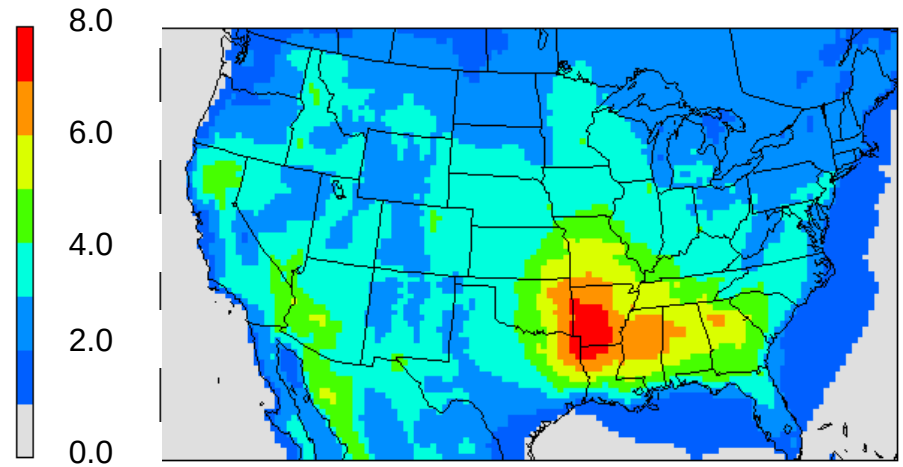


Hydrogen Peroxide

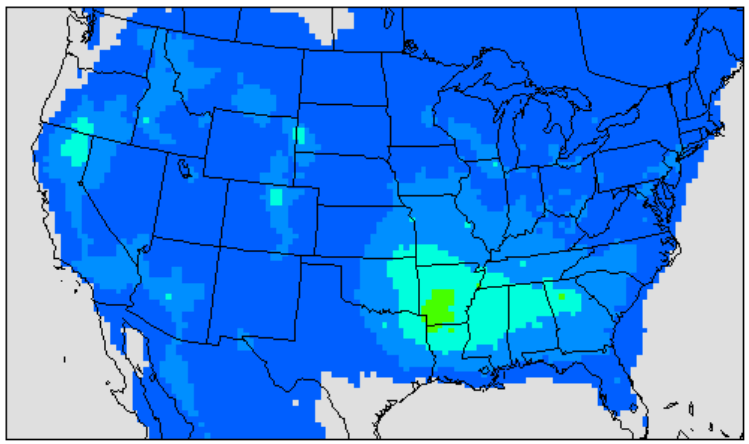
Monthly avg conc

CB4 gives significantly higher concentrations than CB05 or SAPRC

Acetaldehyde
CB05



Acetaldehyde
SAPRC99

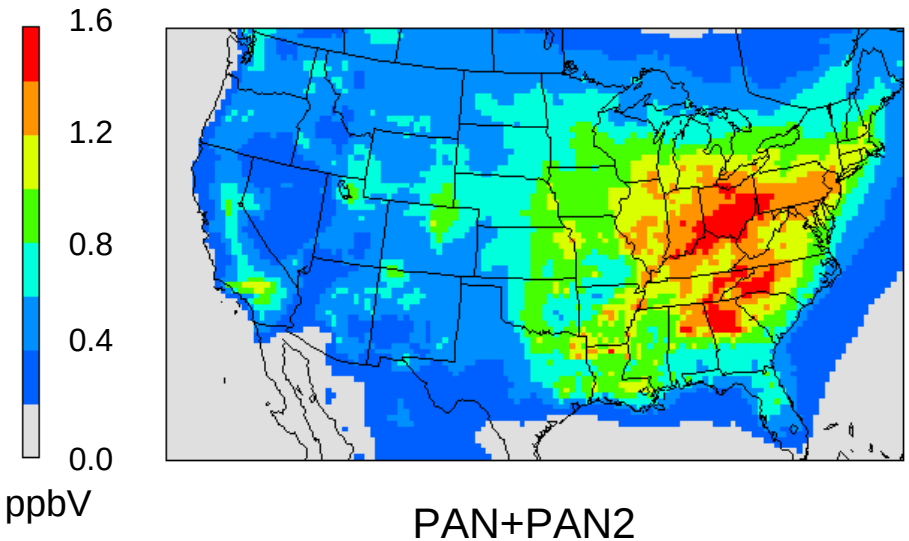


Acetaldehyde

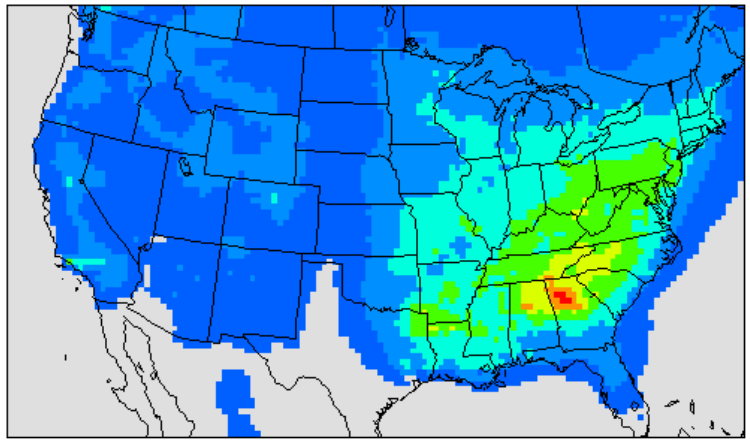
Monthly avg conc

CB05 produces more acetaldehyde as SAPRC99, mostly through alkene/O3 reactions.

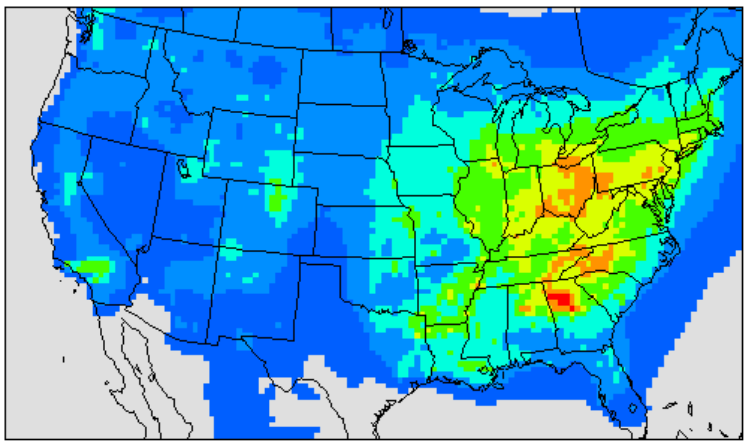
PAN+PANX
CB05



PAN
CB4



PAN+PAN2
SAPRC99



PANs (PAN+PPN+…)

Monthly avg conc

There are significant differences in PAN concentrations and distributions.

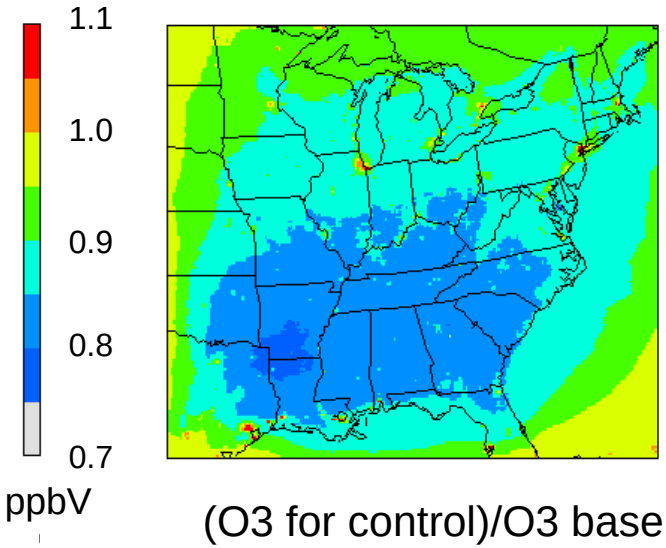
Sensitivity Studies

Focus on these two

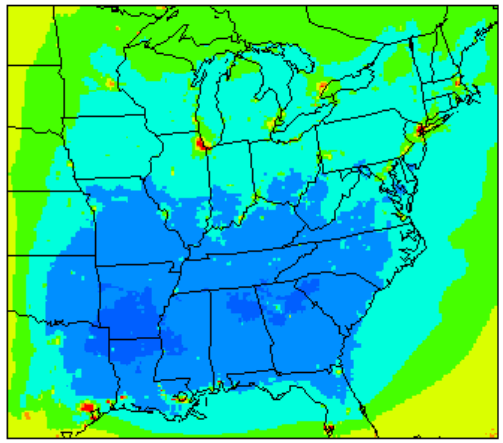
	CB4	CB05	SAPRC99
Sensitivity Studies, 12km, based on base case			
50% NOx decrease	January July	January July	January July
50% SO2 decrease	January July	January July	January July
50% NOx and 50% SO2 decrease	January July	January July	January July
25% VOC decrease	January July	January July	January July
50% NOx and 25% VOC decrease	January July	January July	January July
25% NH3 decrease	January July	January July	January July

Reductions made across-the-board, and only in anthropogenic emissions

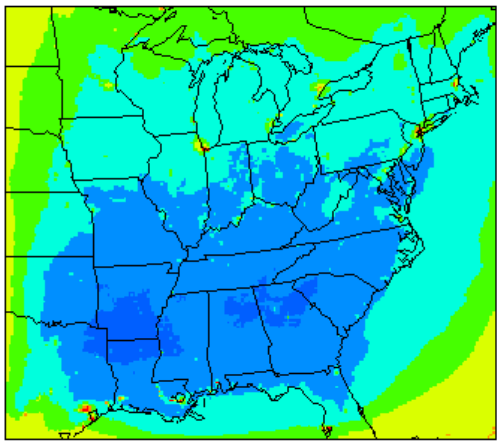
(O3 for control)/O3 base
CB05



(O3 for control)/O3 base
CB4



(O3 for control)/O3 base
SAPRC99

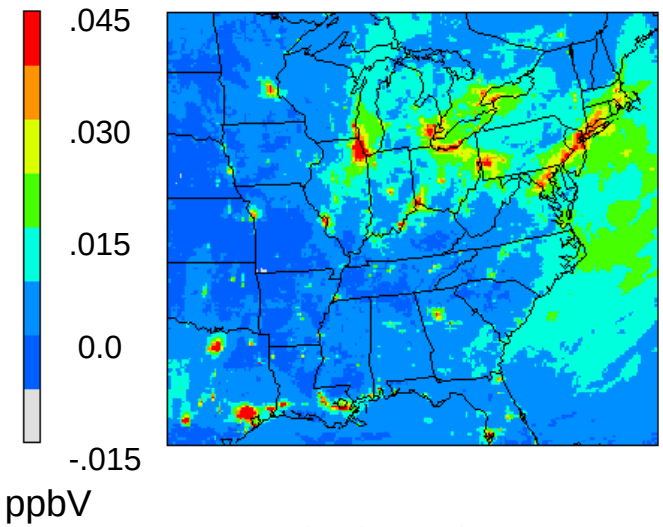


O3 for 50% NOx + 25% VOC reduction

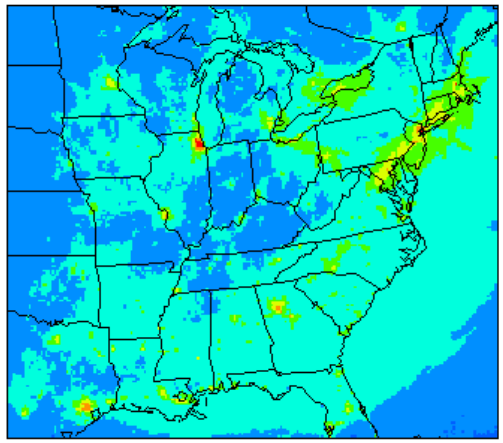
Ratio of O_3 in reduction scenario divided by O_3 in the base case. Based on average of 8-hr daily max concentrations.

All three mechanisms show similar patterns in the ratio.

CB4 – SAPRC99

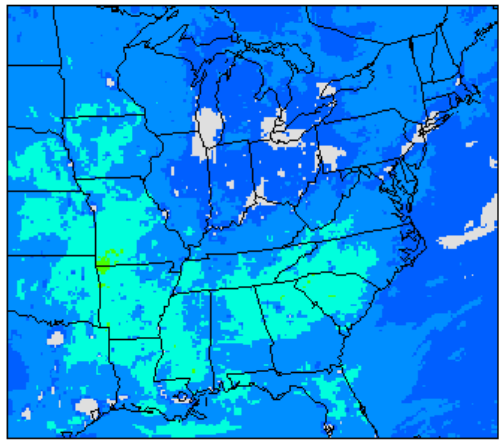


CB05 – SAPRC99



50% NOx + 25% VOC reduction

CB05 – CB4

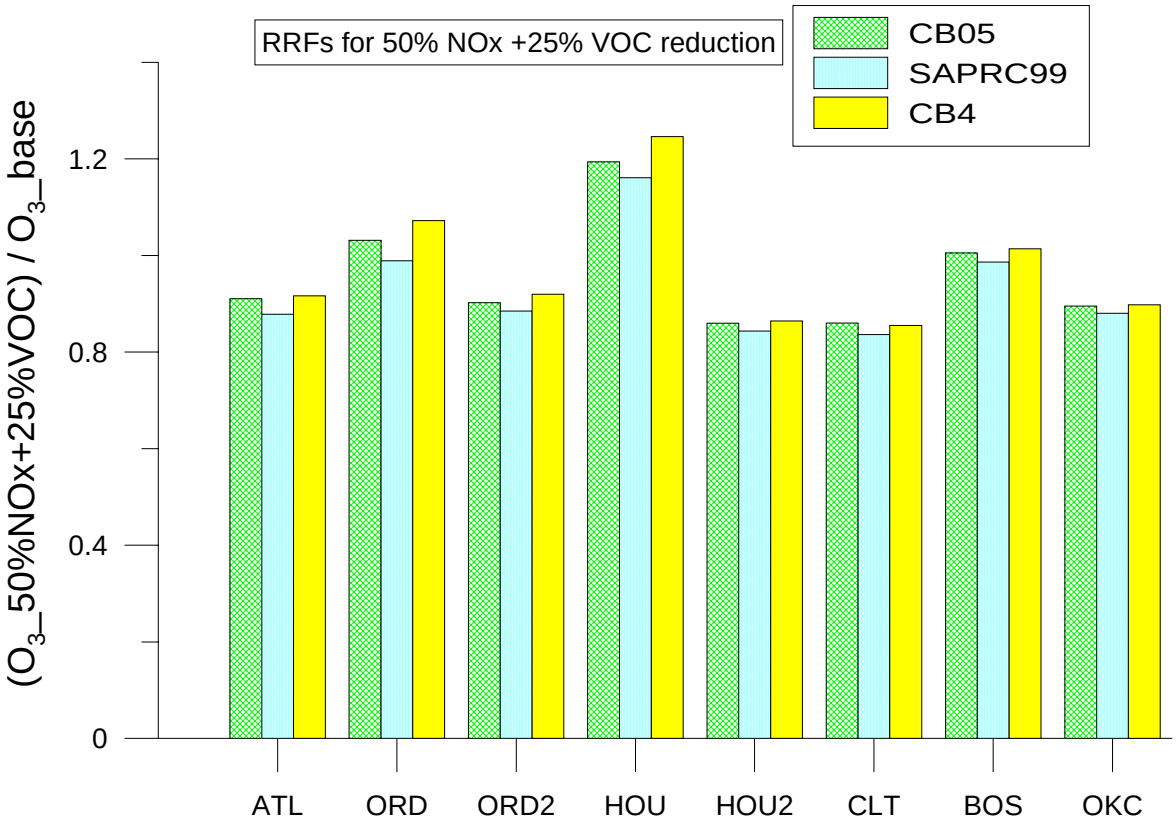


Differences in the ratio of O_3 in reduction scenario divided by O_3 in the base case

There are some differences in the relative reduction in some urban areas (especially Chicago and Houston area).

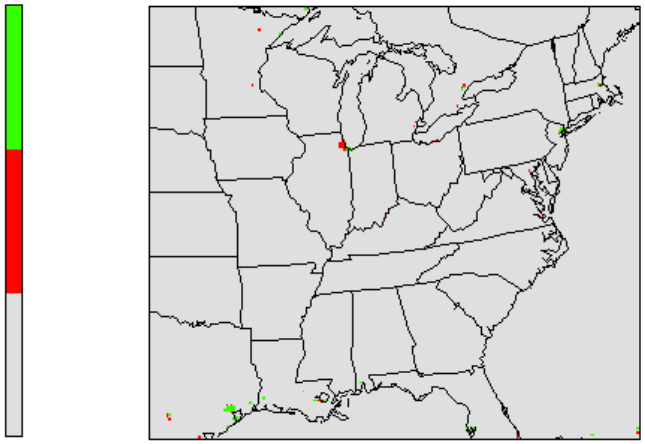
50% NOx + 25% VOC reduction

Ratios at select grids for each mechanism

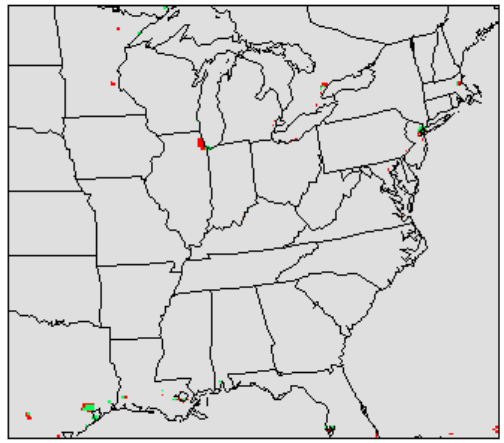


Differences in RRFS are not large. Example: if use SAPRC in Atlanta instead of CB05 might end up with 83 ppb instead of 80ppb.

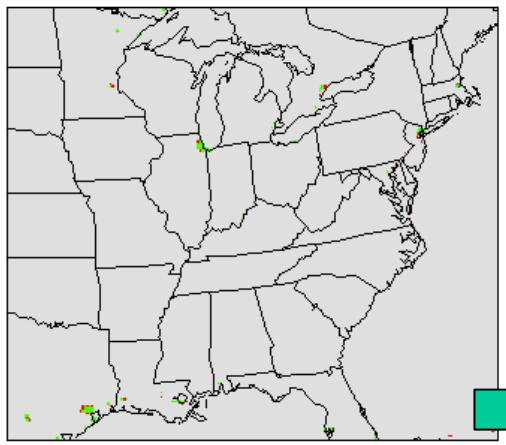
CB05 vs. SAPRC99



CB4 vs. SAPRC99



CB05 vs. CB4

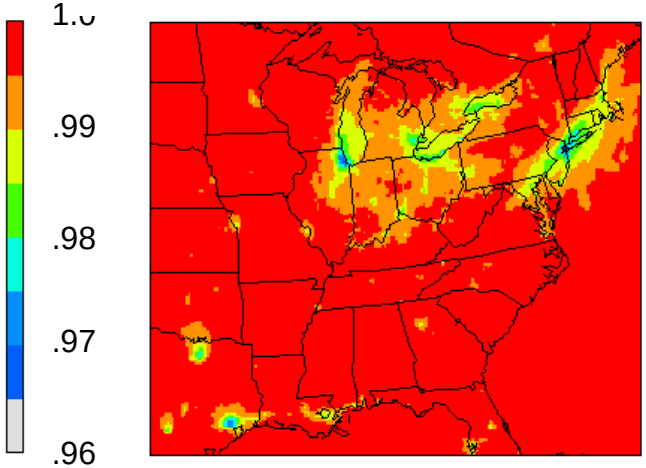


Are there differences in the direction of the ozone change?

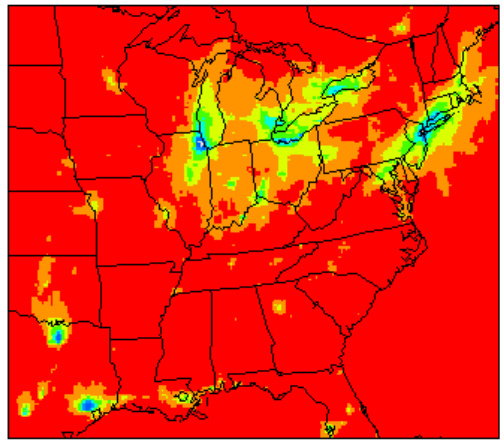
- both predict O3 increase
- one predicts increase, one decrease
- both predict O3 decrease

There are a few (but only a few) areas where the changes have opposite signs and these largely occur immediately outside of disbenefit grids.

(O3 for control)/O3 base
CB05

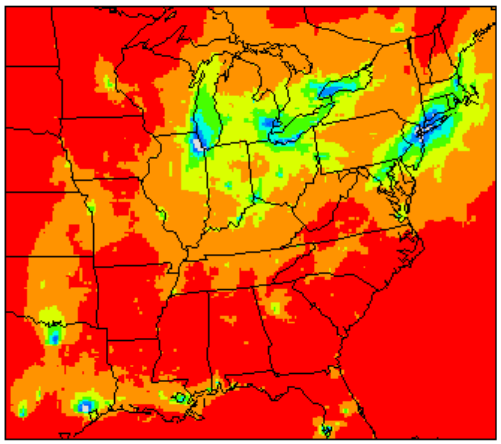


(O3 for control)/O3 base
CB4



25% VOC reduction

(O3 for control)/O3 base
SAPRC99



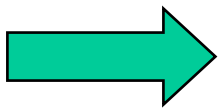
Scale is very compressed (from 0.96 to 1.0)

Ratio of O_3 in reduction scenario divided by O_3 in the base case

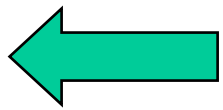
Ratios are close to one and differences among the mechanisms are very small

Effects of Emission Reductions on PM components

- Aerosol sulfate
- Aerosol nitrate



See poster by Sharon Phillips



Summary/Conclusions

- Does using CB05 instead of CB4 in an air quality model give us different predictions? Are they consistent with SAPRC99 predictions?
  - Ozone concentration and distribution is different between CB4 and the other mechanisms. SAPRC predicts slightly higher ozone predictions than CB05
  - H2O2 is significantly different between CB4 and other mechanisms
    - Affects sulfate production via aqueous oxidation of SO2
  - NOz distribution can be different among the 3 mechanisms
    - Affects nitrate production and $PM_{2.5}$ predictions
  - ➲ When you add more mechanisms to the comparison, the spread will likely increase
  - ➲ The mechanisms are trending closer to each other
  - ➲ Consistency in emissions should improve comparisons

- Are there spatial variations in the differences?
  - Large differences in ozone in the central U.S. between CB4 and others
  - Many of the differences occur in areas where biogenics are large

Summary/Conclusions (cont.)

- Do the different mechanisms vary in their results for emission changes?
  - The relative reductions in ozone are generally similar for most mechanisms in most areas
  - In some urban areas, there are slight differences in the sensitivities to emission reductions
  - ➲ Perhaps can use the differences identified between mechanisms to help account for uncertainty

Acknowledgements

- Other members of CB4-05 evaluation workgroup:
  - Golam Sarwar
  - Alice Gilliland
  - Wyat Appel
  - Rob Pinder
- Air Toxics team:
  - Bill Hutzell
- CSC:
  - Nancy Hwang

***DISCLAIMER**: The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number* DW13921548. *Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their policies or views*