Regional Climate-chemistry Model Simulations of Ozone in the Lower Troposphere and its Climatic Impacts

Wen-Yih Sun
and
Kate J. Yang
Purdue University

Outline

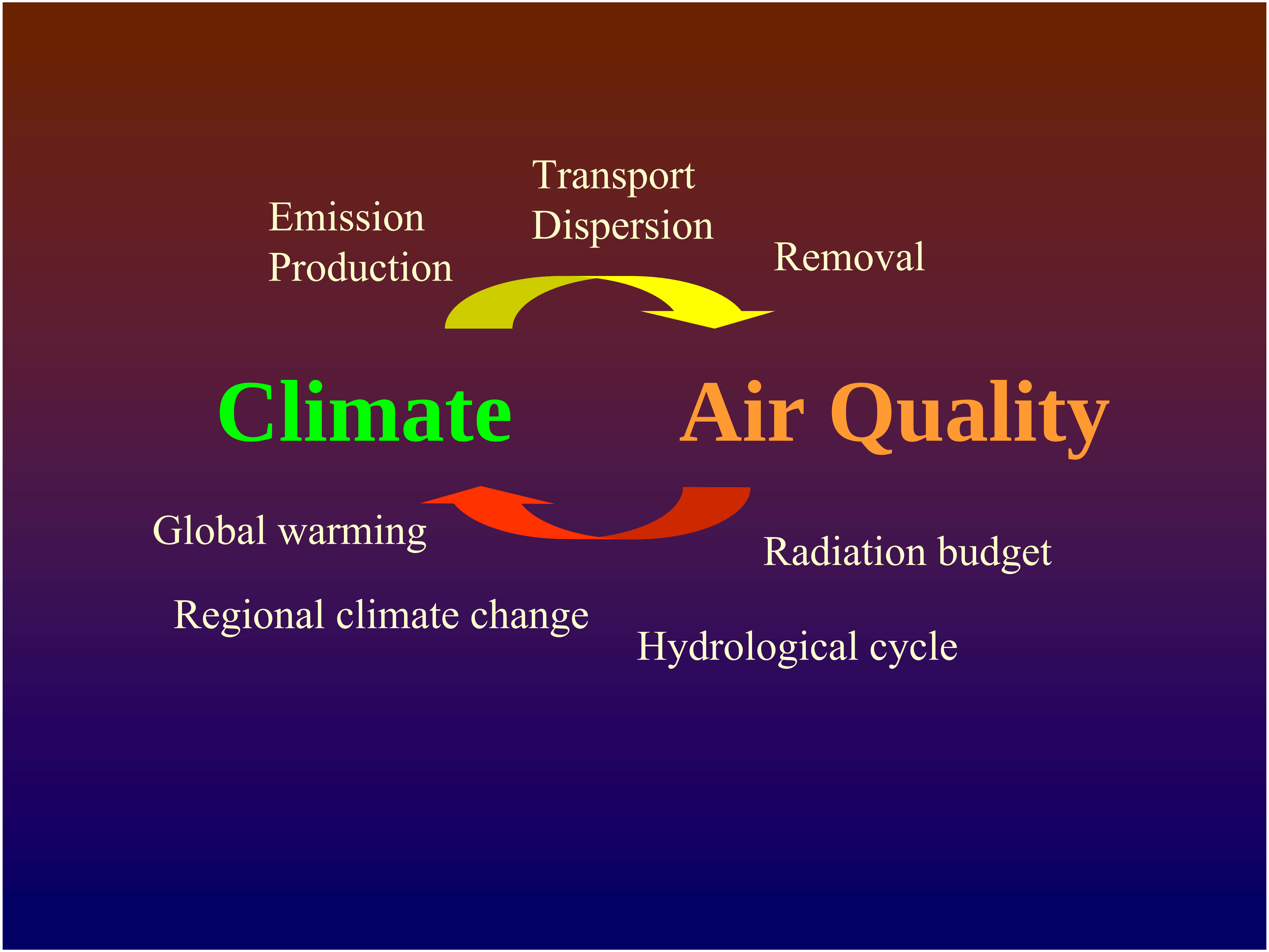
- *Background*
- *Research Objectives and Approach*
- *Model Descriptions - Purdue Regional Climate and Chemistry Model (PRCCM)*
- *Case Study*
- *Model Results*
- *Summary & Conclusions*

Outline

- *Background*
- *Research Objectives and Approach*
- *Model Descriptions - Purdue Regional Climate and Chemistry Model (PRCCM)*
- *Case Study*
- *Model Results*
- *Summary & Conclusions*

Background

- Air quality problems, such as the urban smog, aerosols, dusts, and acid rain, can affect human health, ecological environment, agriculture, businesses and climate.
- Air quality is related to many aspects of the earth environment and living beings on the Earth.
- One particular aspect that has been much emphasized in the research community for the past three decades due to the increased evidence is **climate change**.



Transport
Dispersion
Emission
Production
Removal
Climate
Air Quality
Global warming
Radiation budget
Regional climate change
Hydrological cycle

Tropospheric ozone

- Tropospheric ozone is a major photochemical pollutant.
- It is harmful to human health, agriculture and buildings.
- High ozone concentrations in the lower troposphere is one of the most important issues of air quality.
- Tropospheric ozone also plays an important role in climate change as a greenhouse gas.
- Global-scale modeling studies estimated the global annual mean radiative forcing due to tropospheric ozone to be 0.2 ~ 0.55 w/m^2 (eg. *De Froster et al.*, 1996; *Portmann et al.*, 1997; *Haywood et al.*, 1998).

Outline

- *Background*
- *Research Objectives and Approach*
- *Model Descriptions - Purdue Regional Climate and Chemistry Model (PRCCM)*
- *Case Study*
- *Model Results*
- *Summary & Conclusions*

Research Objectives

- **To perform air quality modeling with climate model**
  - Simulate tropospheric ozone distribution and transport accurately at the regional scale
- **To investigate the impacts of tropospheric chemistry on climate modeling**
  - Should chemistry be included in regional climate modeling?
- **To investigate the regional climatic impacts of tropospheric ozone**
  - Direct radiative forcing and warming effects
  - Indirect effects on moisture distribution
  - Influence on atmospheric stratification and the regional atmospheric dynamics

Approach

- Development of a ***on-line*** coupled climate-chemistry model at the regional scale that is capable of regional weather/climate forecasts and of describing the evolution of tropospheric ozone.
- Considerations of the interactions between tropospheric ozone and regional weather/climate.
- Model validation and evaluation with a case study.
- Regional climatic impact analyses with numerical simulation results.

Off-line and On-line Modeling

Off-line

- Using archived meteorological data from historical weather data or another model as the input to the photochemical model.
- Only a fraction of meteorology information is available and interpretation is necessary.
- Potential inconsistency and incompatibility.
- No interaction between meteorology and chemistry.
- Efficient in computation.
- Easier to operate.

On-line

- Using dynamic fields generated from the imbedded meteorological model as the input to the photo-chemical model.
- All meteorological information is available at each time step.
- Chemistry feedback can be considered in meteorological modeling.
- Requires extensive computation resources.
- Integration must be comprehensive

Recommended in recent reviews and research.
[eg. *Byun and Ching*, 1999; *Seaman*, 2000]

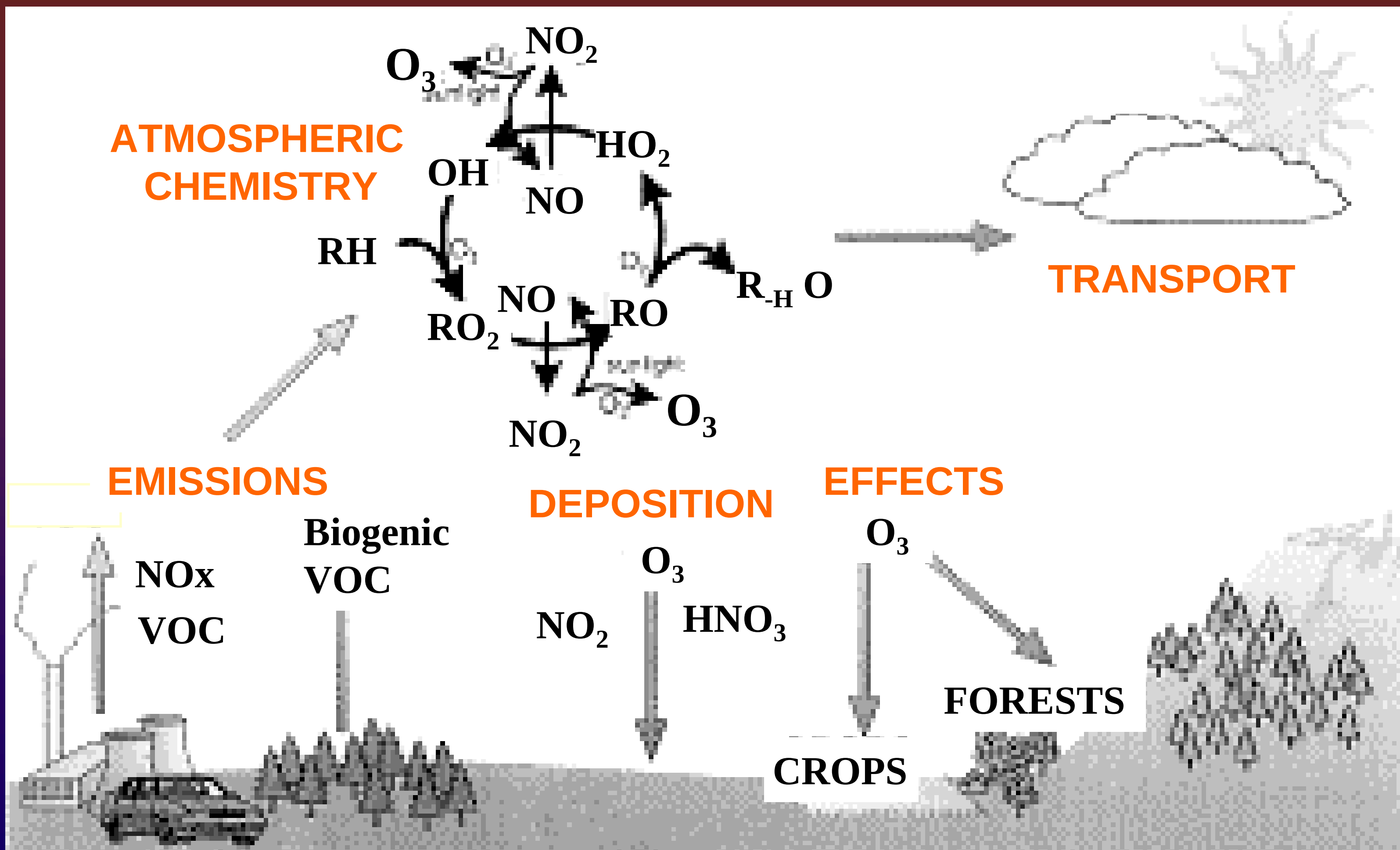
Approach

- Development of a ***on-line*** coupled climate-chemistry model at the regional scale that is capable of regional weather/climate forecasts and of describing the evolution of tropospheric ozone.
- Considerations of the interactions between tropospheric ozone and regional weather/climate.
- Model validation and evaluation with a case study.
- Regional climatic impact analyses with numerical simulation results.

Outline

- *Background*
- *Research Objectives and Approach*
- *Model Descriptions: Purdue Regional Climate and Chemistry Model (PRCCM, Yang, 2004)*
- *Case Study*
- *Model Results*
- *Summary & Conclusions*

Processes in Photochemical Pollution

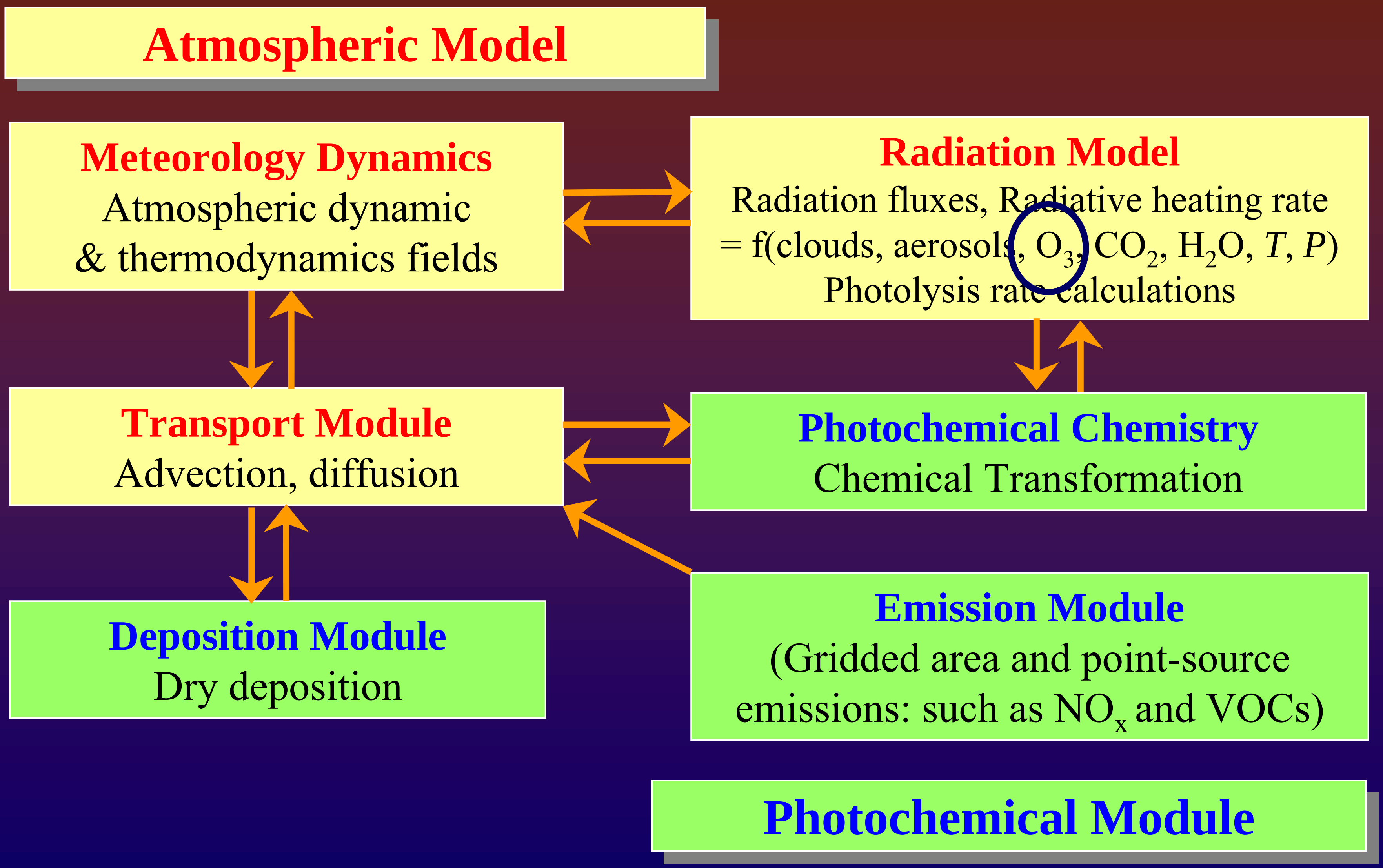


(Fowler,1999)

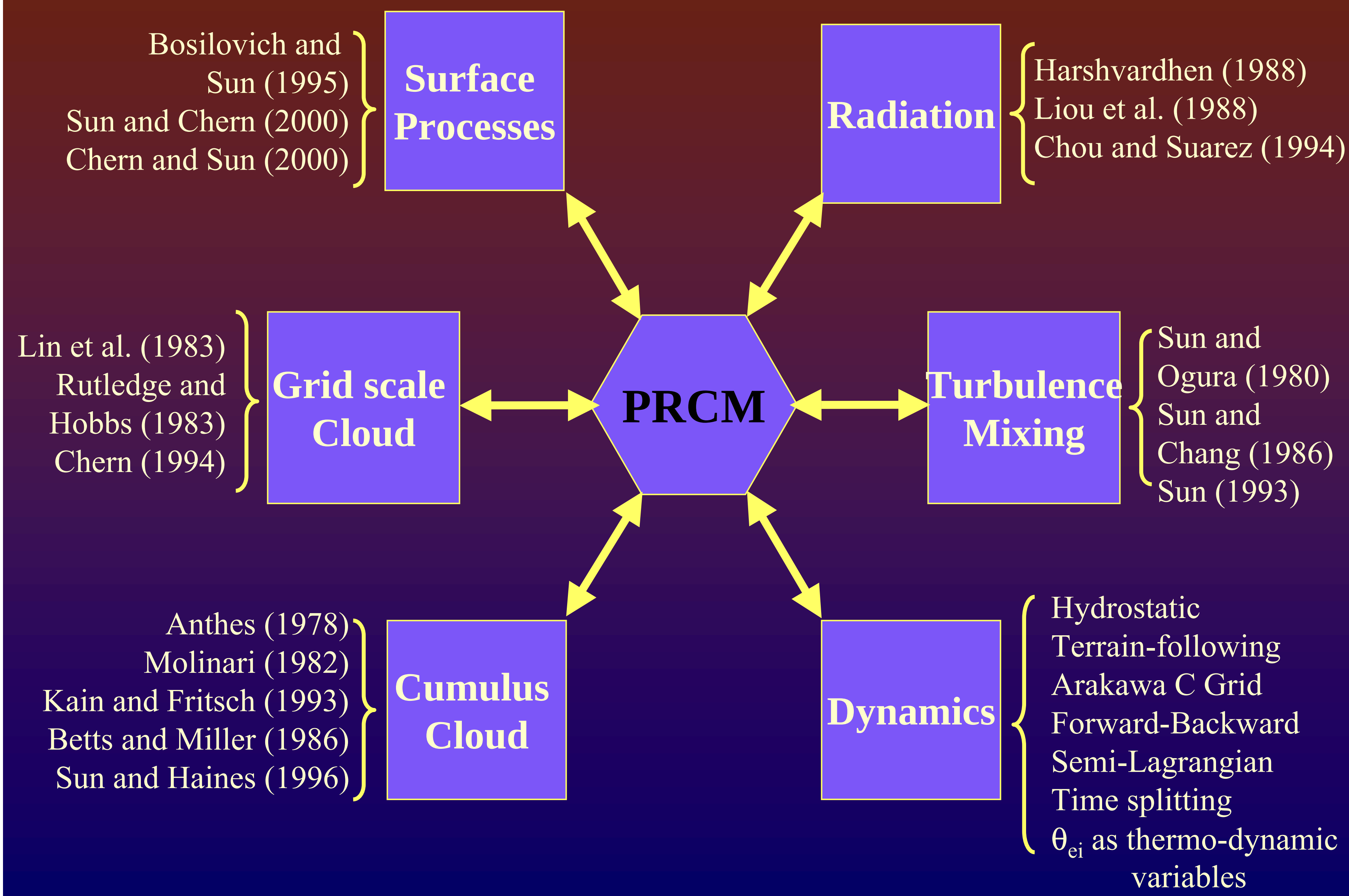
Model Descriptions

- Coupled climate-chemistry model **PRCCM** (Purdue Regional Climate and Chemistry Model)
- Atmospheric modeling - a regional-scale climate model that is based on the **PRCM** (Purdue Regional Climate Model)
- Photochemical Modeling
- Climate-Chemistry Interactions

Purdue Regional Climate and Chemistry Model (PRCCM, *Yang*, 2004)



Purdue Regional Climate Model
(PRCM, *Purdue Mesoscale Modeling Lab*)



Photochemical Module

Gas-phase Chemistry mechanism - SAPRC97 (*Carter*, 1995, 1997)

- **184 reactions and 76 species**
- **39 species are treated as "state species", 33 are treated as radicals, and 4 are treated as constants (water vapor, CH_4, O_2 and air).**

Gas-phase Chemistry solvers: Modified IEH (Implicit-Explicit Hybrid)

On-line photolysis calculation:

- **Modified radiation model in the PRCM calculates photolysis rates with an empirical parameterization scheme**

Coupling: *climate-chemistry interactions*

$$\frac{\partial c_i}{\partial t} = \left(\frac{\partial c_i}{\partial t}\right)_{adv} + \left(\frac{\partial c_i}{\partial t}\right)_{diff} + \left(\frac{\partial c_i}{\partial t}\right)_{\substack{dry\\dep}} + \left(\frac{\partial c_i}{\partial t}\right)_{emission} + \left(\frac{\partial c_i}{\partial t}\right)_{chemistry}$$

Tracer transport
with atmospheric modeling

photochemistry

In the lower 15 model layers, photochemistry, chemical tracer transport and the radiative feedback of tropospheric ozone are performed ***on-line*** with the atmospheric modeling processes.

The radiation code drives the photochemistry by providing photolysis rates and takes account for the radiative effects of tropospheric ozone in atmospheric modeling.

Outline

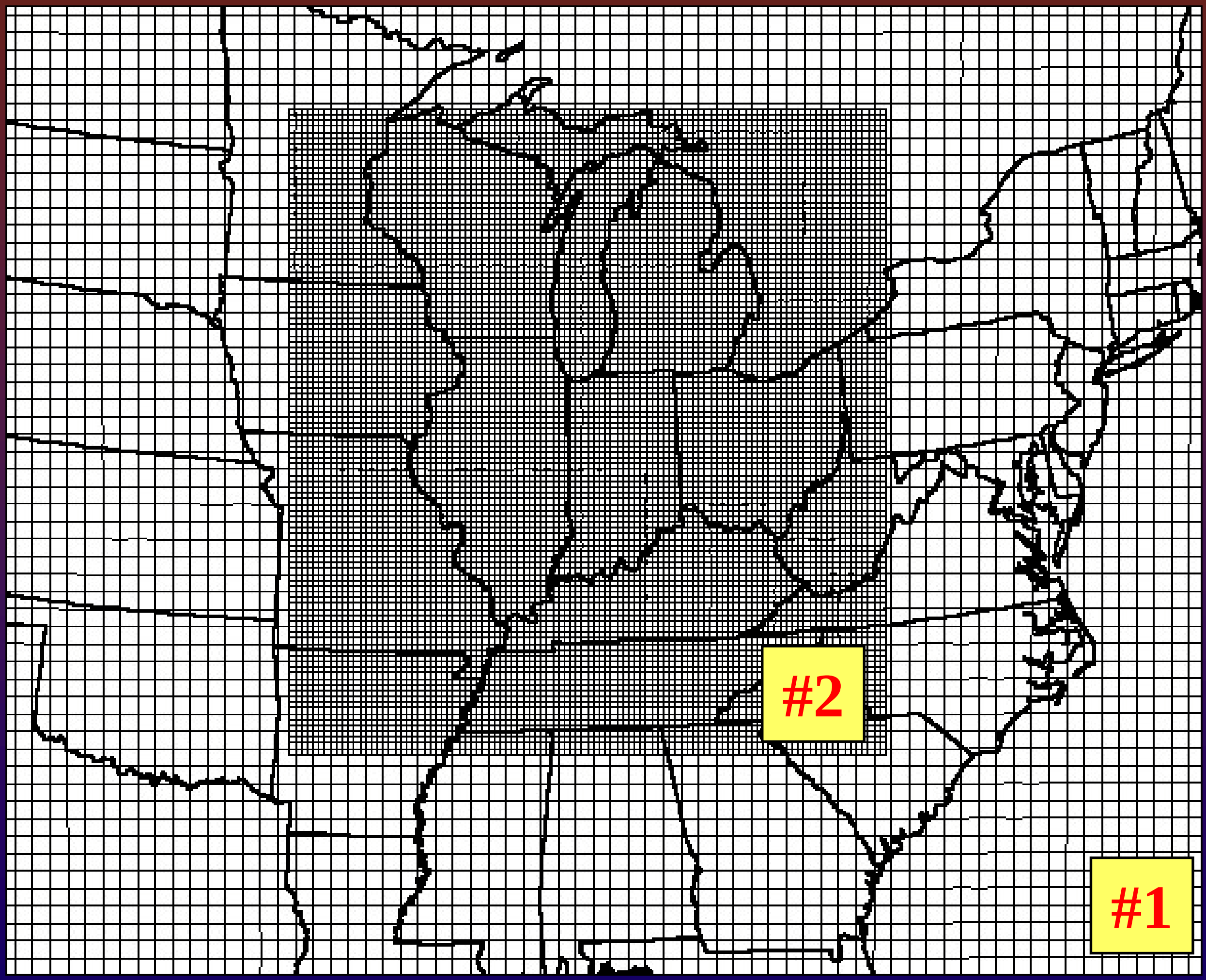
- *Background*
- *Research Objectives and Approach*
- *Model Descriptions - Purdue Regional Climate and Chemistry Model (PRCCM)*
- *Case Study*
- *Model Results*
- *Summary & Conclusions*

Model Validation: Case Study

The July 1998 Ozarks Isoprene Experiment (OZIE)

- Modeling time period: July 16~22, 1998
- Model domain (Based on the Eastern-Unified Grids)
- Emission Data: EPA NET99 and biogenic emissions (provided by the Lake Michigan Air Director Consortium)
- Surface-level and aircraft measurements of tropospheric ozone are available for comparison.

Model Domains



Domain #1:

79x68 grid points
with 36km resolution

Domain #2:

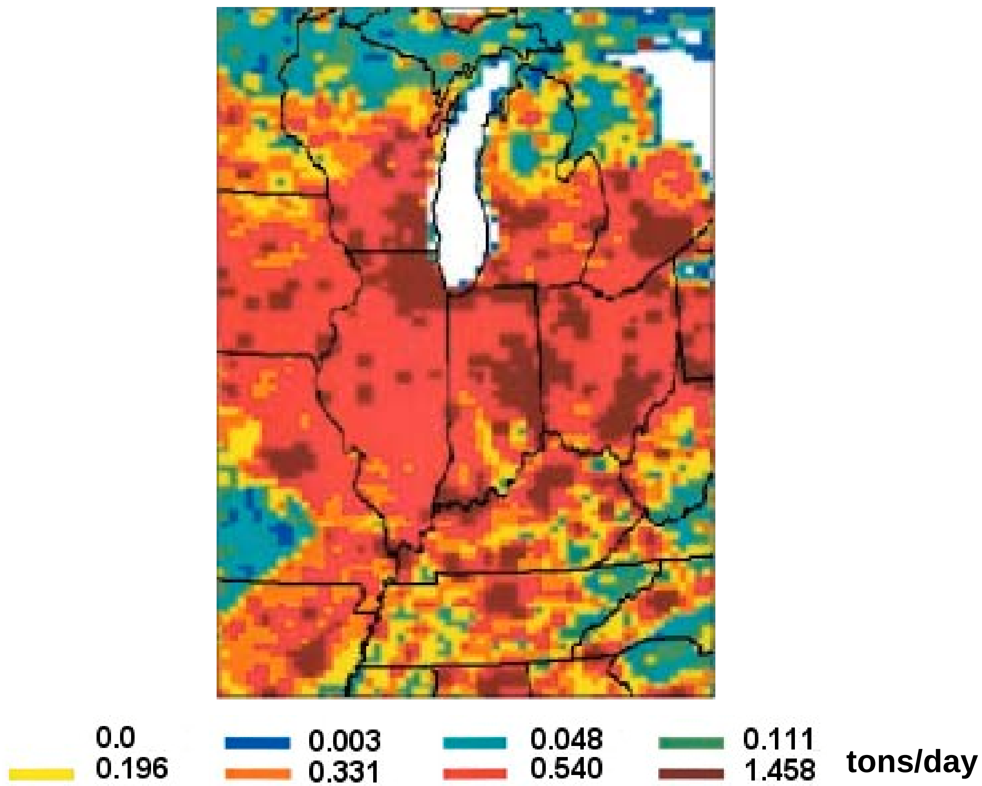
102x111 grid points
with 12km resolution

28 vertical levels

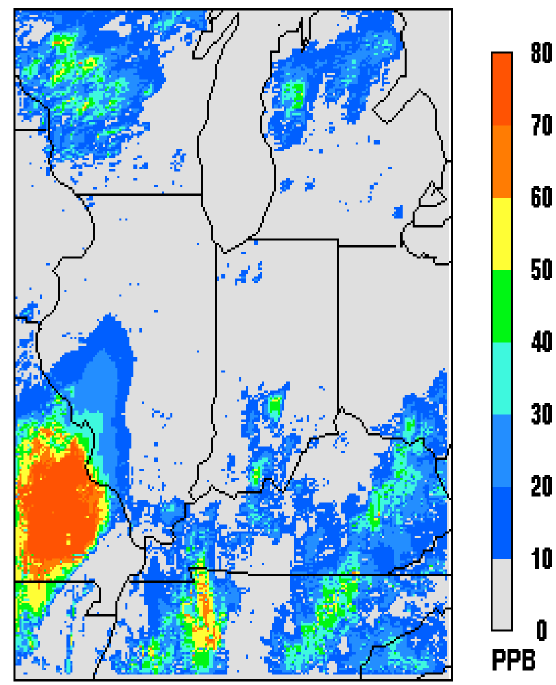
soil 4 layers

Emissions

Low-level NOx Emissions (Tons/day)



BEIS2 Modeled Hourly Isoprene Concentrations(ppb)



Model Setup

- ***Case 1***: Chemistry-free PRCM control run for domain#1

  Case 2: Chemistry-free PRCM control run for domain#2

  Case 3: Interactive climate-chemistry **PRCCM**(*Yang*, 2004) run for domain#2

- Time steps: 100 seconds and 30 seconds in atmospheric modeling for domain #1 and #2, respectively.
- Photochemistry is calculated every 10 minutes with photolysis rates updated every 30 minutes with the radiation calculation
- Emissions are added every 1.5 minutes.

- **85%** computational time is spent in photochemical modeling.

Outline

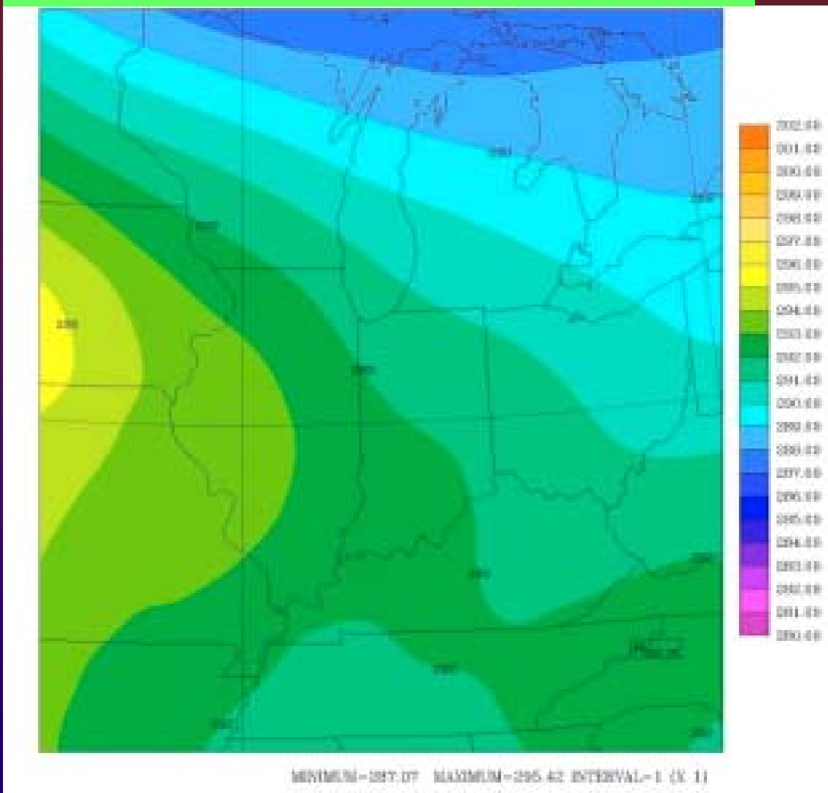
- Background
- Research Objectives and Approach
- Model Descriptions - Purdue Regional Climate and Chemistry Model (PRCCM)
- Case Study
- Model Results
- Summary & Conclusions

Model Results

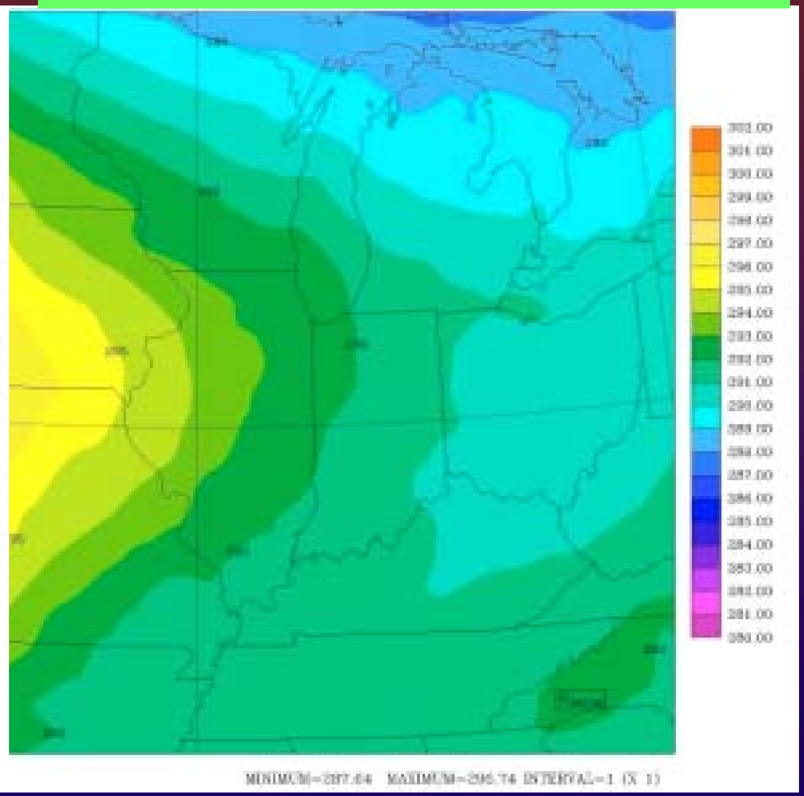
- ❖ **Atmospheric variables from chemistry-free control run results**
- ❖ **Tropospheric ozone:**
  - ❖ Surface-level Ozone
  - ❖ Aloft ozone
- ❖ **Improvement of climate-chemistry modeling**
- ❖ **Climatic impact analyses**

Chemistry-free Control Run Results

ECMWF weekly mean
850mb Air Temperature Field (K)
during July 16-22 episodic simulation

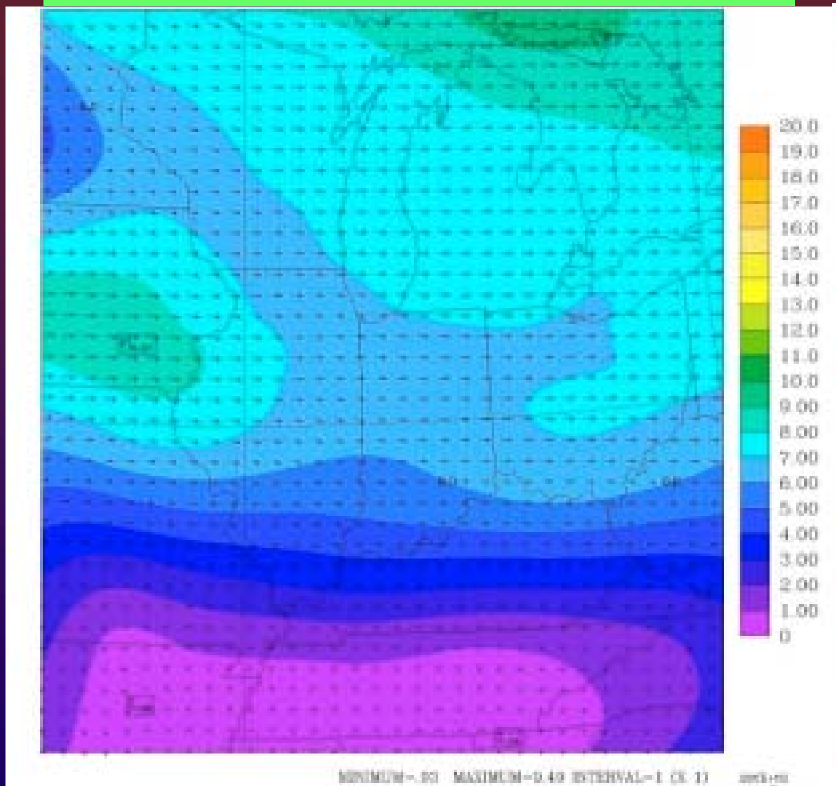


PRCM weekly mean
850mb Air Temperature Field (K)
during July 16-22 episodic simulation

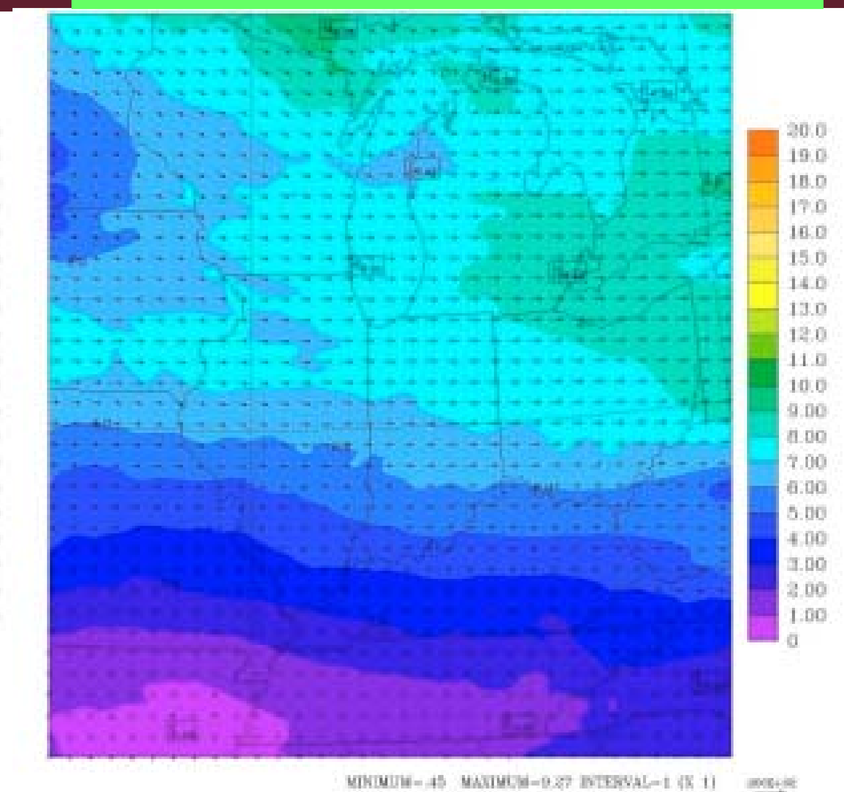


Chemistry-fee Control Run Results (cont.)

ECMWF weekly mean
850mb Wind Field (m/s)
during July 16-22 episodic simulation



PRCM weekly mean
850mb Wind Field (m/s)
during July 16-22 episodic simulation



PRCM Model Evaluation

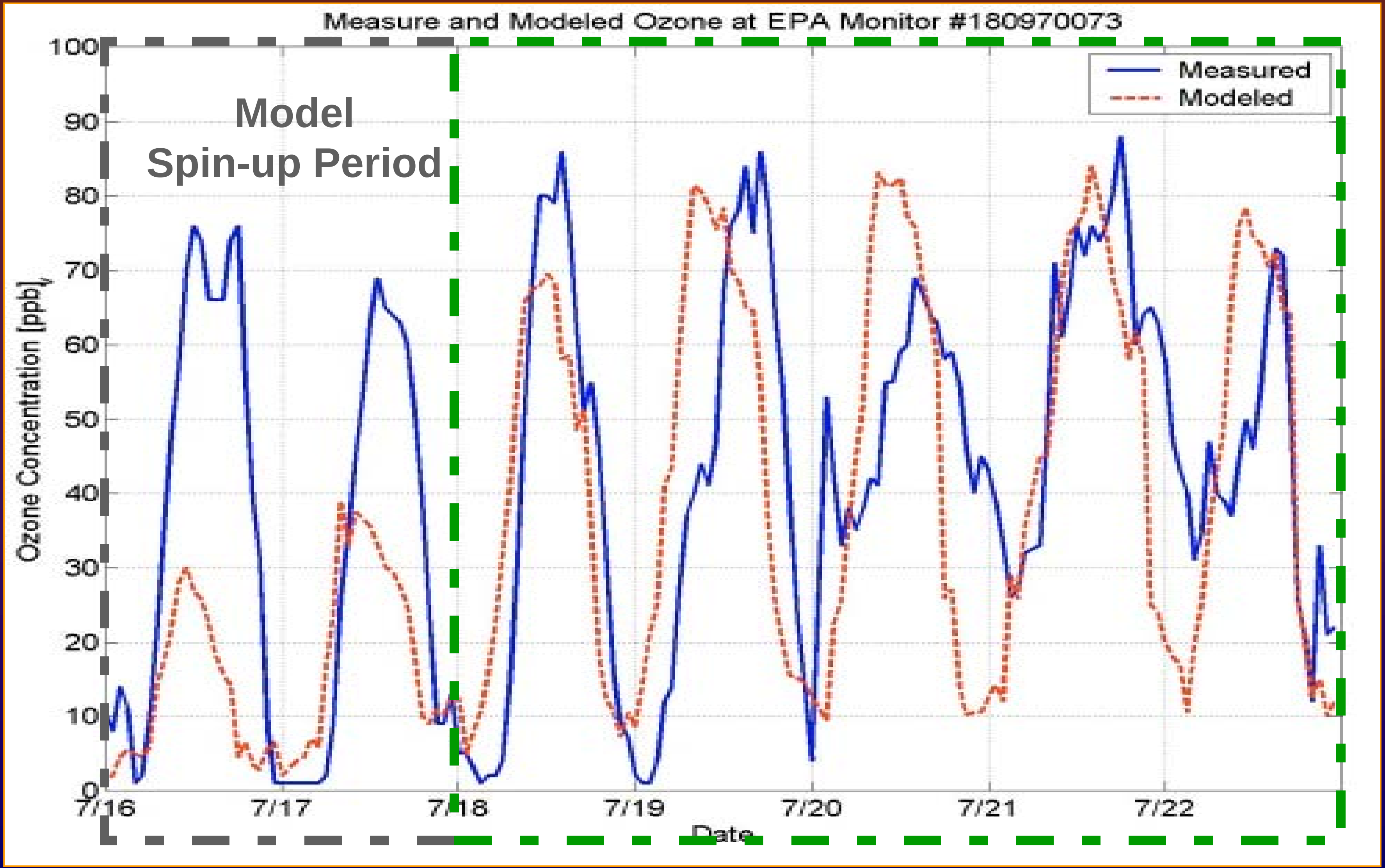
(No chemistry)

	Episodic simulation during July 16 ~ 22, 1998		Episodic simulation during July 16 ~ 22, 1998	
	Model Bias	Mean	COR	Mean
Surface Air Temperature (K)	1.49 ~ 2.39	1.73	0.79 ~ 0.88	0.84
Surface Wind ($m\ s^{-1}$)	- 0.710 ~ - 1.12	-0.931	0.47 ~ 0.77	0.63
Surface Water Vapor($kg\ kg^{-1}$)	3.61E-03 ~ 4.62E-03	4.19E-03	0.52 ~ 0.76	0.66
850mb Air Temperature (K)	0.385 ~ 0.807	0.587	0.91 ~ 0.98	0.96
850mb Wind ($m\ s^{-1}$)	- 0.228 ~ 0.967	0.177	0.82 ~ 0.95	0.89
850mb Water Vapor($kg\ kg^{-1}$)	9.94E-04 ~ 1.66E-03	1.22E-03	0.48 ~ 0.81	0.63

With the quality assured meteorology, one can proceed with photochemical modeling as well as use these chemistry-free meteorological fields as the ***base-case*** in climatic impact analyses.

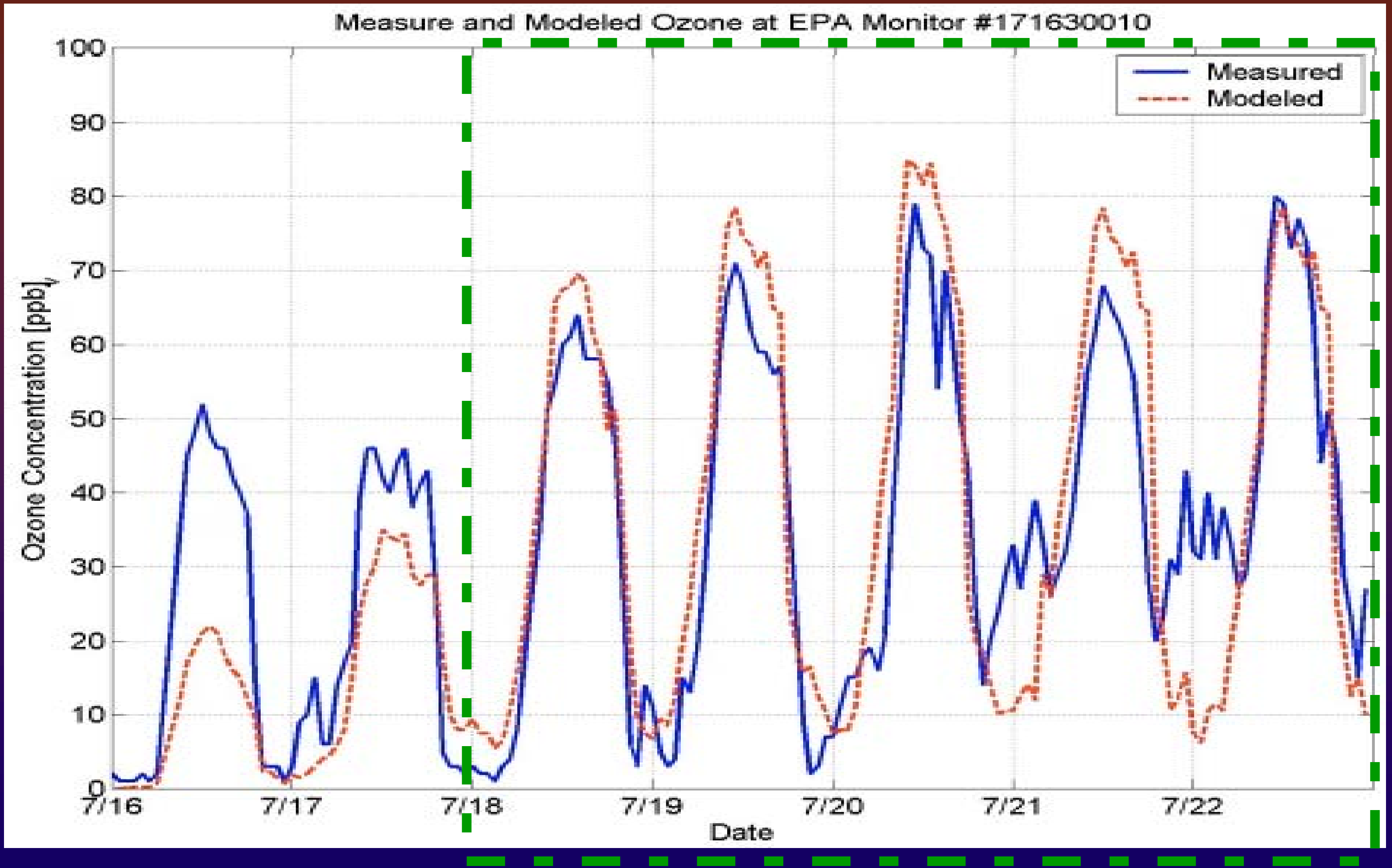
PRCCM Surface-level Ozone Prediction

Indianapolis, IN (86.06 W, 39.79° N, EPA monid: 18-097-0073-44201-1)



RMSE = 21.4 ppb

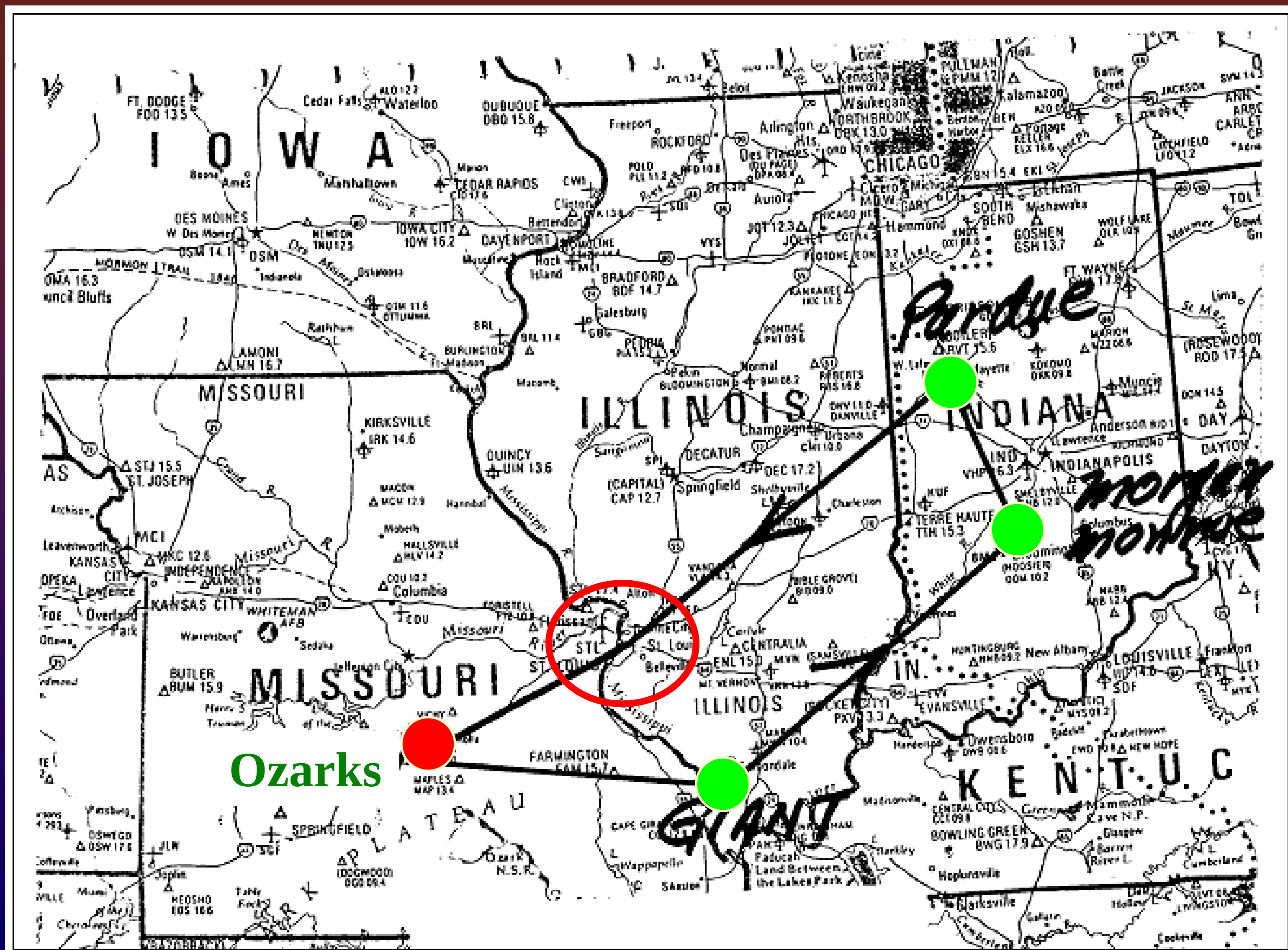
East St. Louis, IL (90.16 W, 38.36º N, EPA monid: 17-163-0010-44201-1)



RMSE = 12.5 ppb

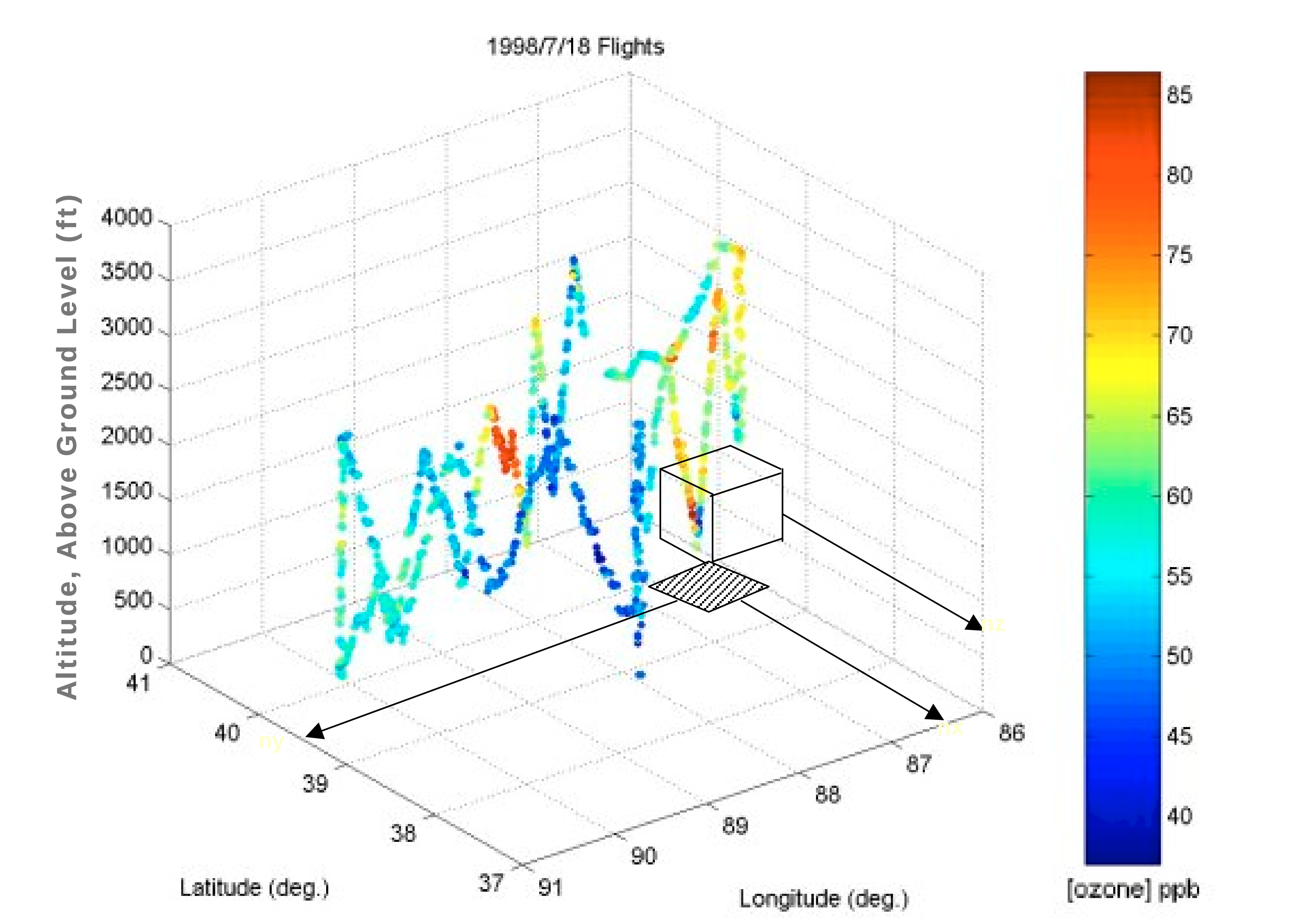
1998 Aircraft Ozone Measurement Mission

(On July 18 ~ 21, 1998)

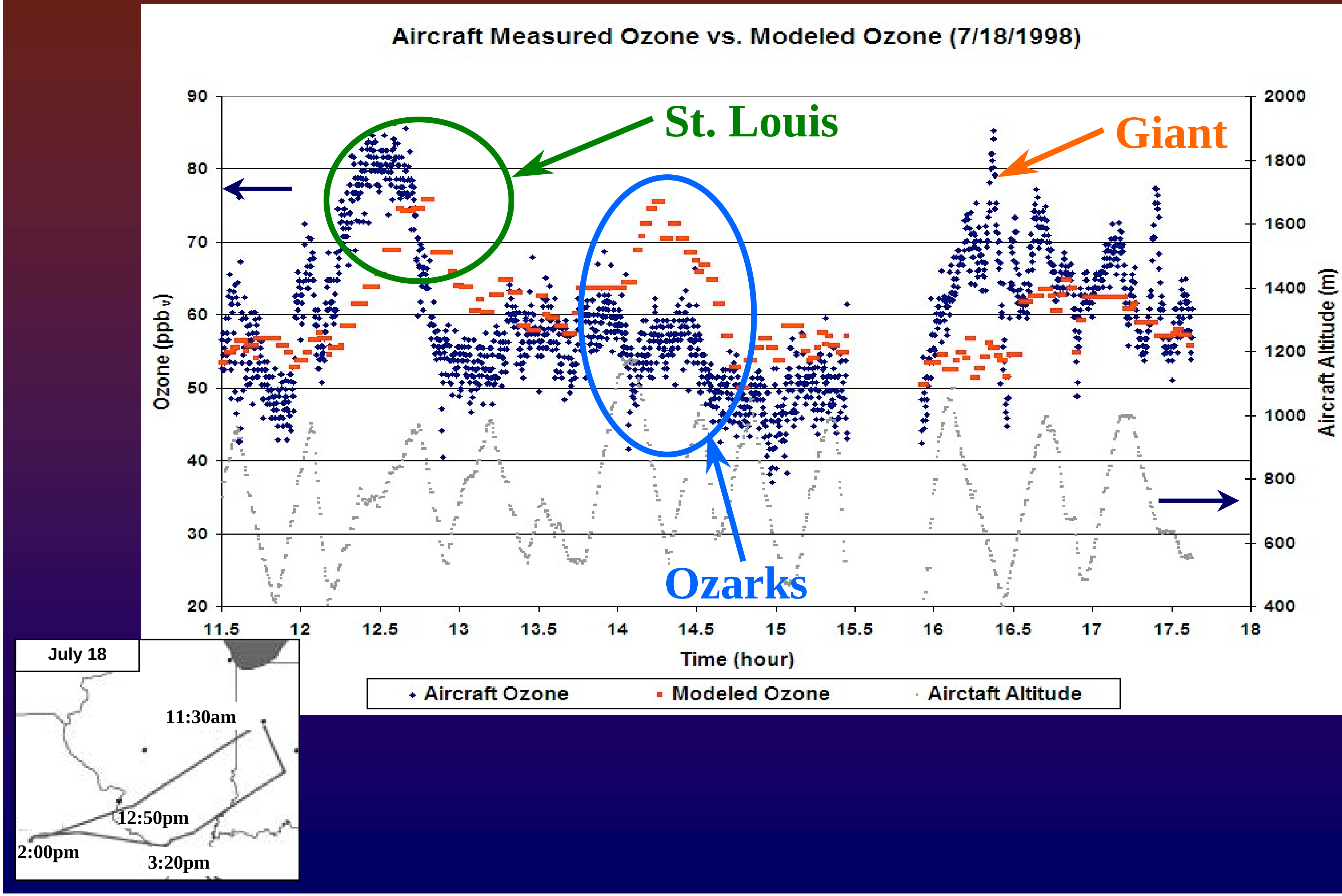


Aircraft Measurements vs. PRCCM Modeled Ozone

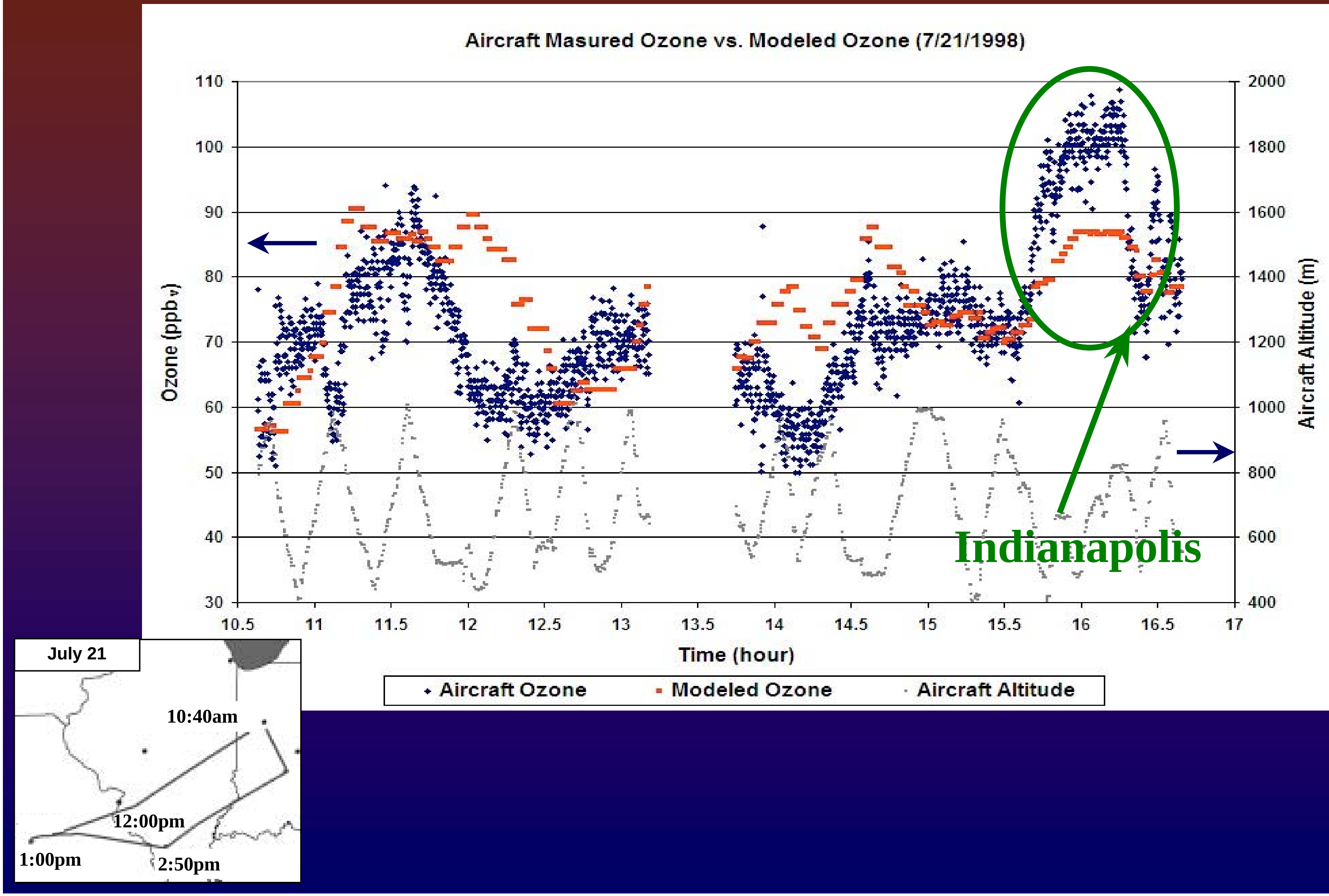
Comparison Methodology



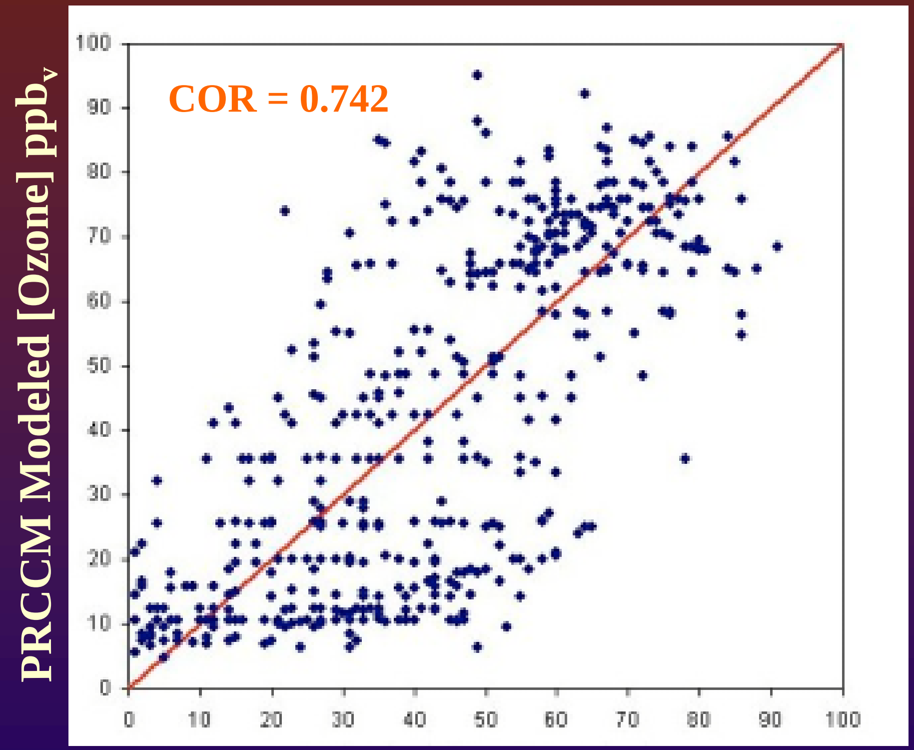
Aircraft Measurements vs. PRCCM Modeled Ozone



Aircraft Measurements vs. PRCCM Modeled Ozone

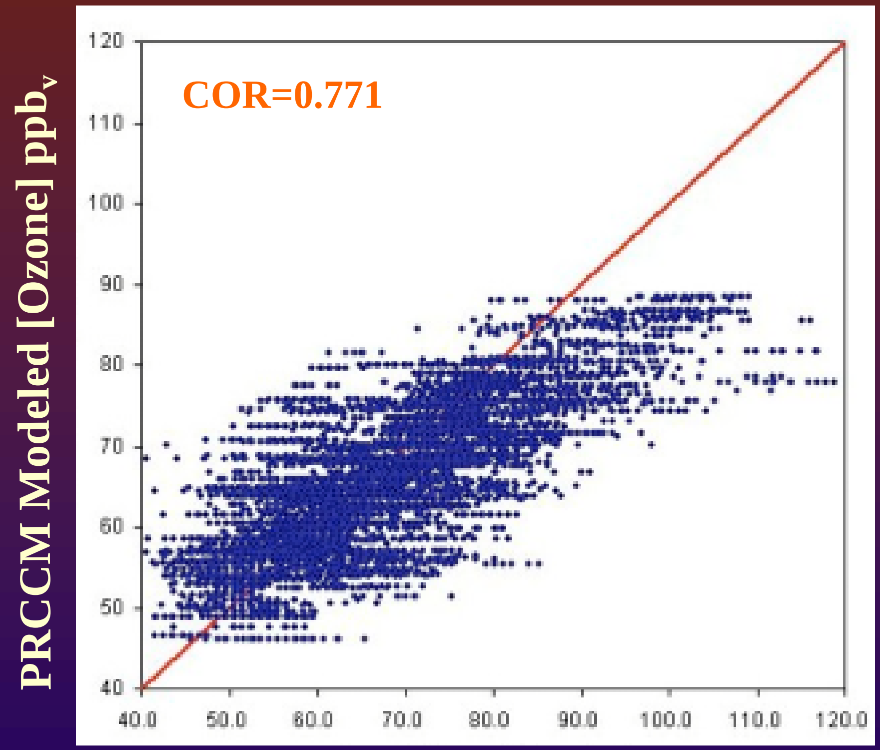


Measurements vs. PRCCM Modeled Ozone



Surface-level Measurement [Ozone] ppb$_v$

at four EPA monitoring stations
during July 18~22, 1998



Aircraft Measurement [Ozone] ppb$_v$

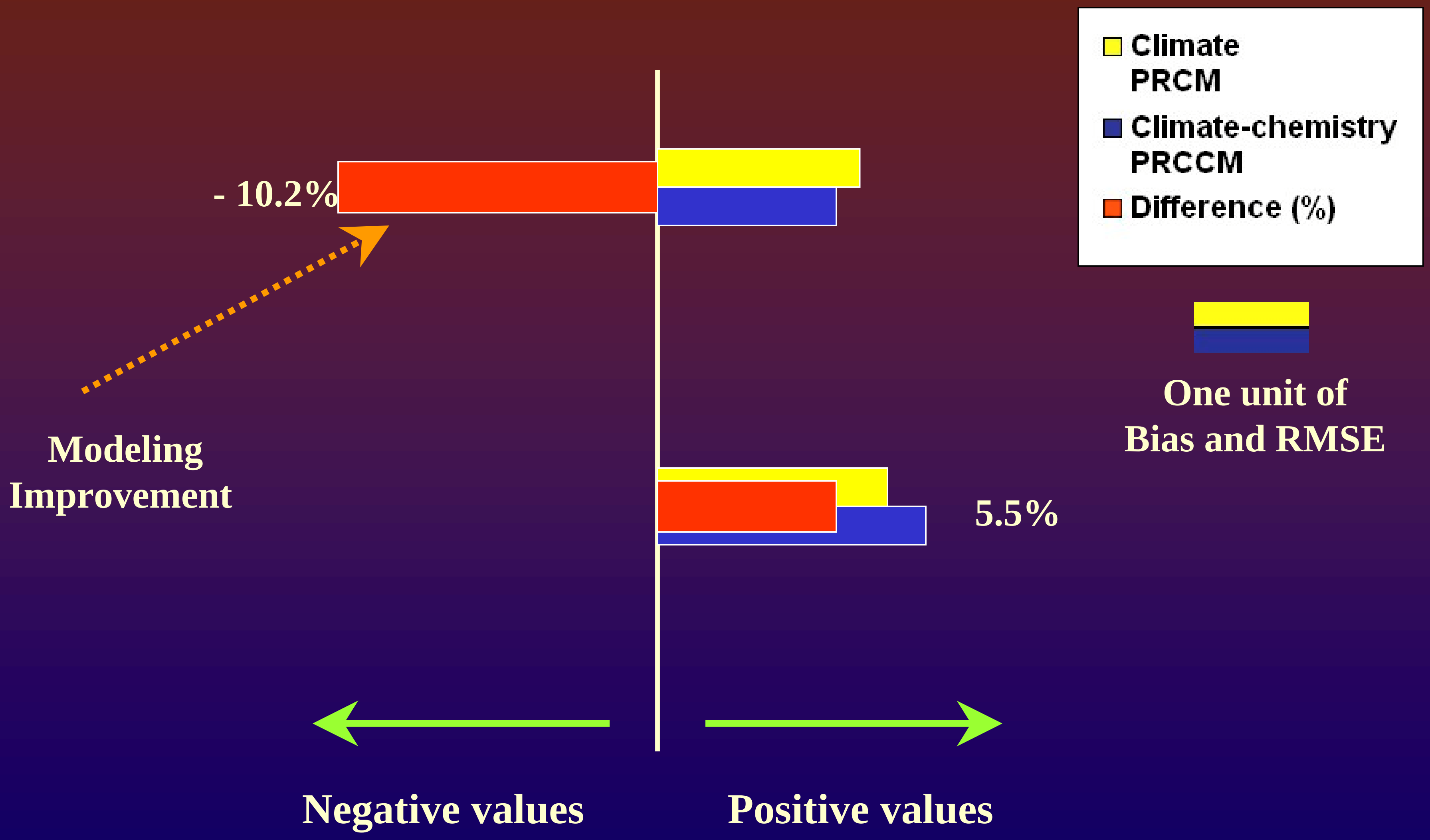
from four aircraft ozone measurement
missions on July 18~21, 1998

Coupled Climate-chemistry modeling

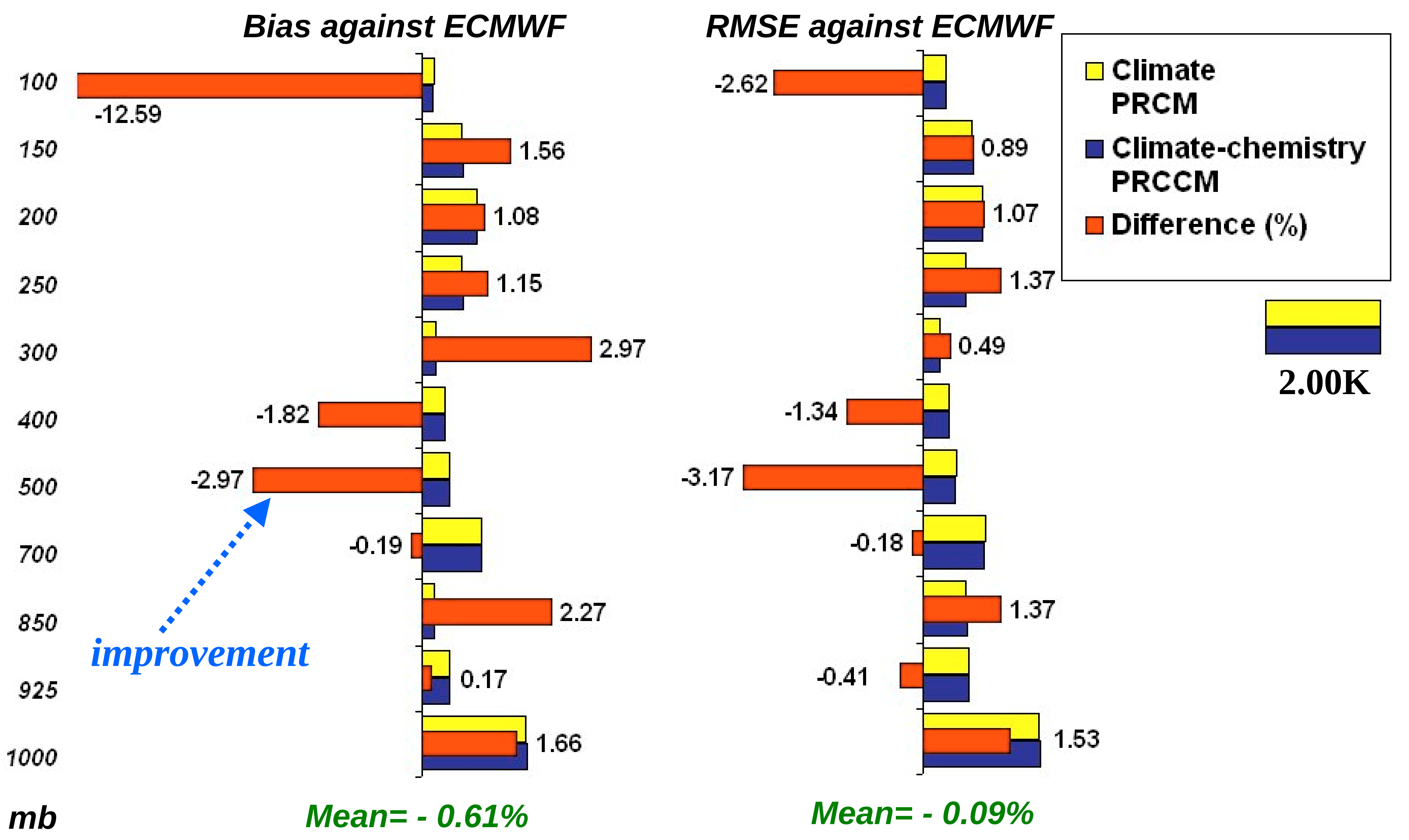
Improvements in climate/atmospheric modeling with tropospheric chemistry?

Regional climatic Impacts due to increased tropospheric ozone from the photochemical pollution?

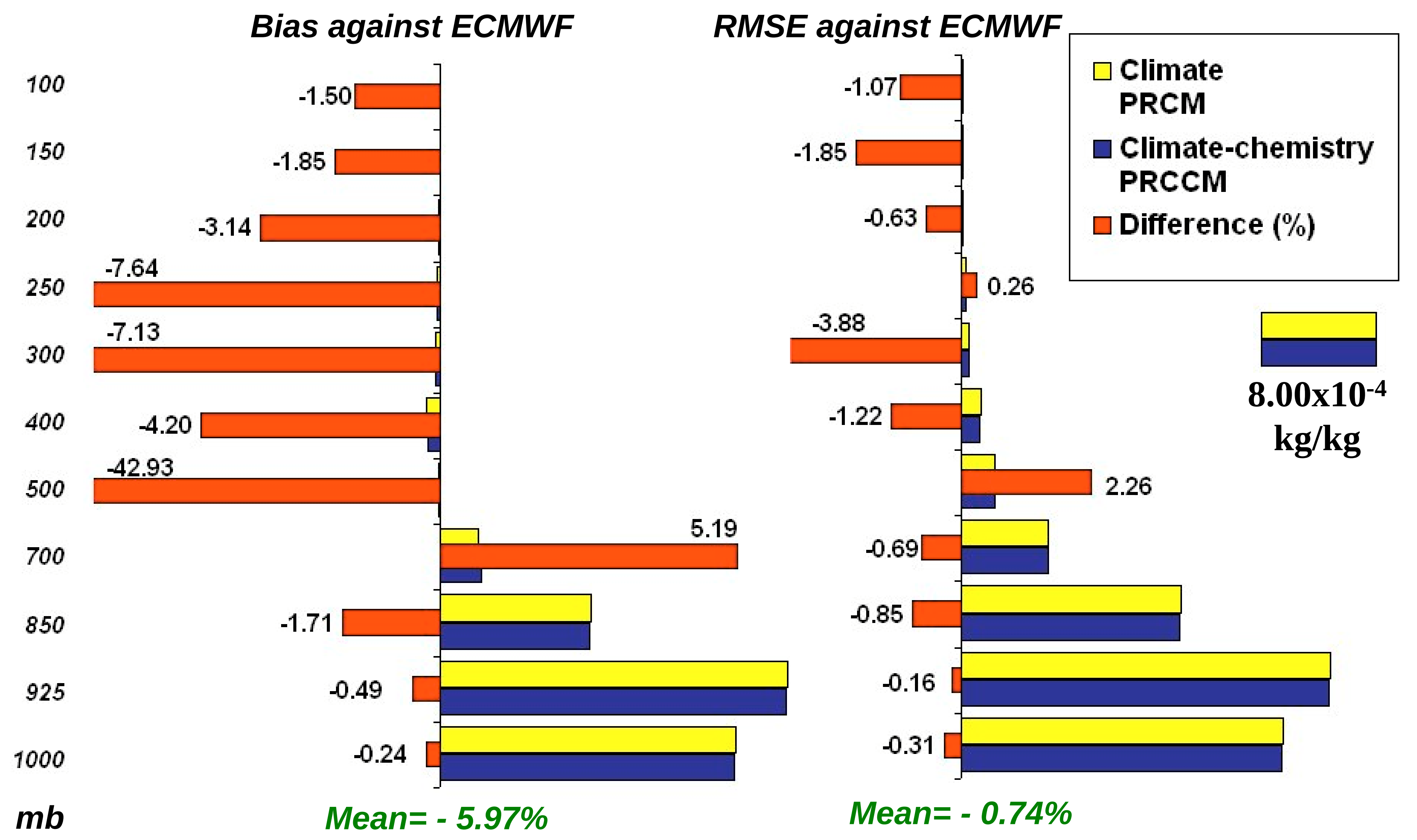
Model bias and RMSE against ECMWF



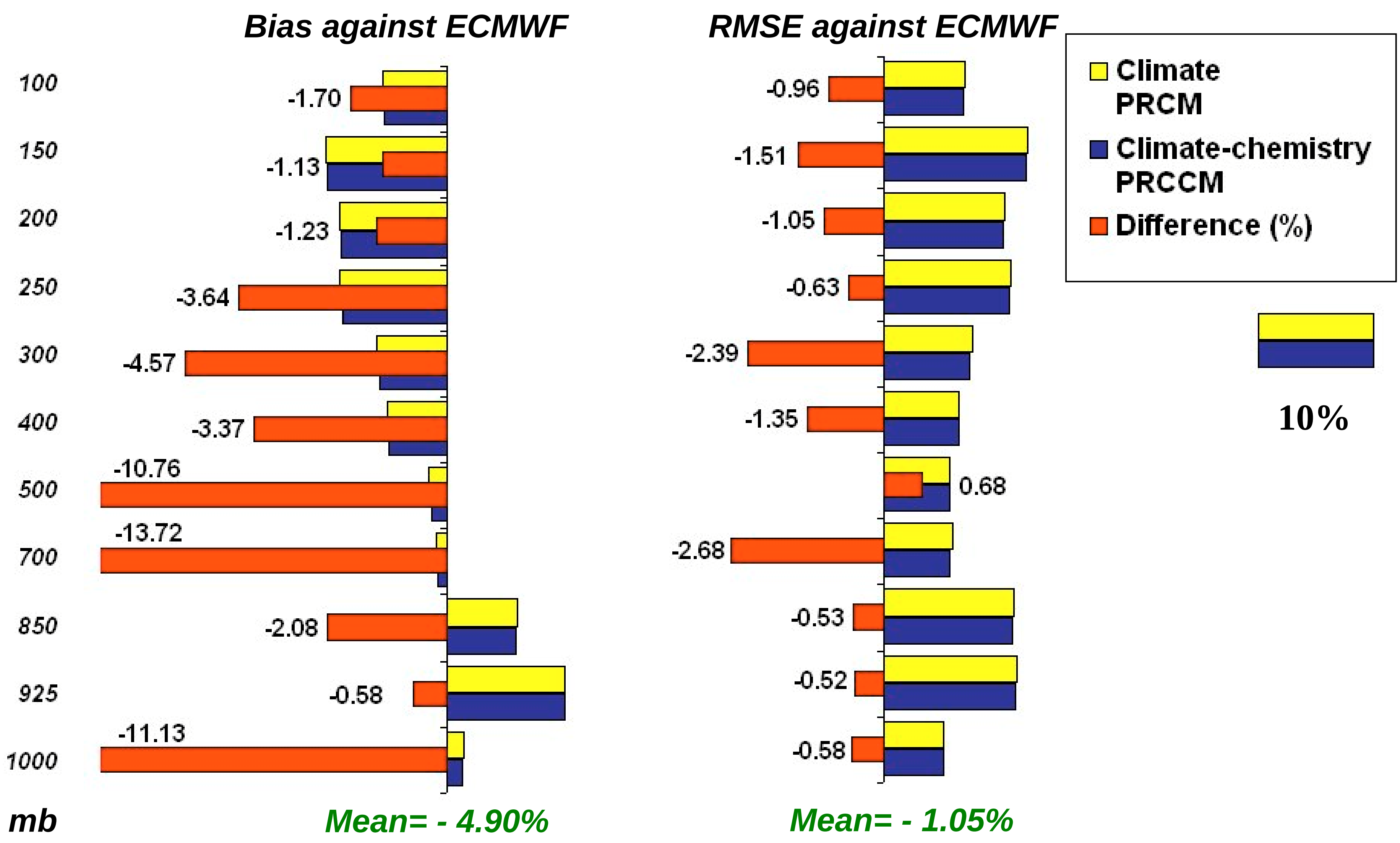
Air Temperature Predictions



Atmospheric Moisture Qv Predictions



Atmospheric RH Predictions

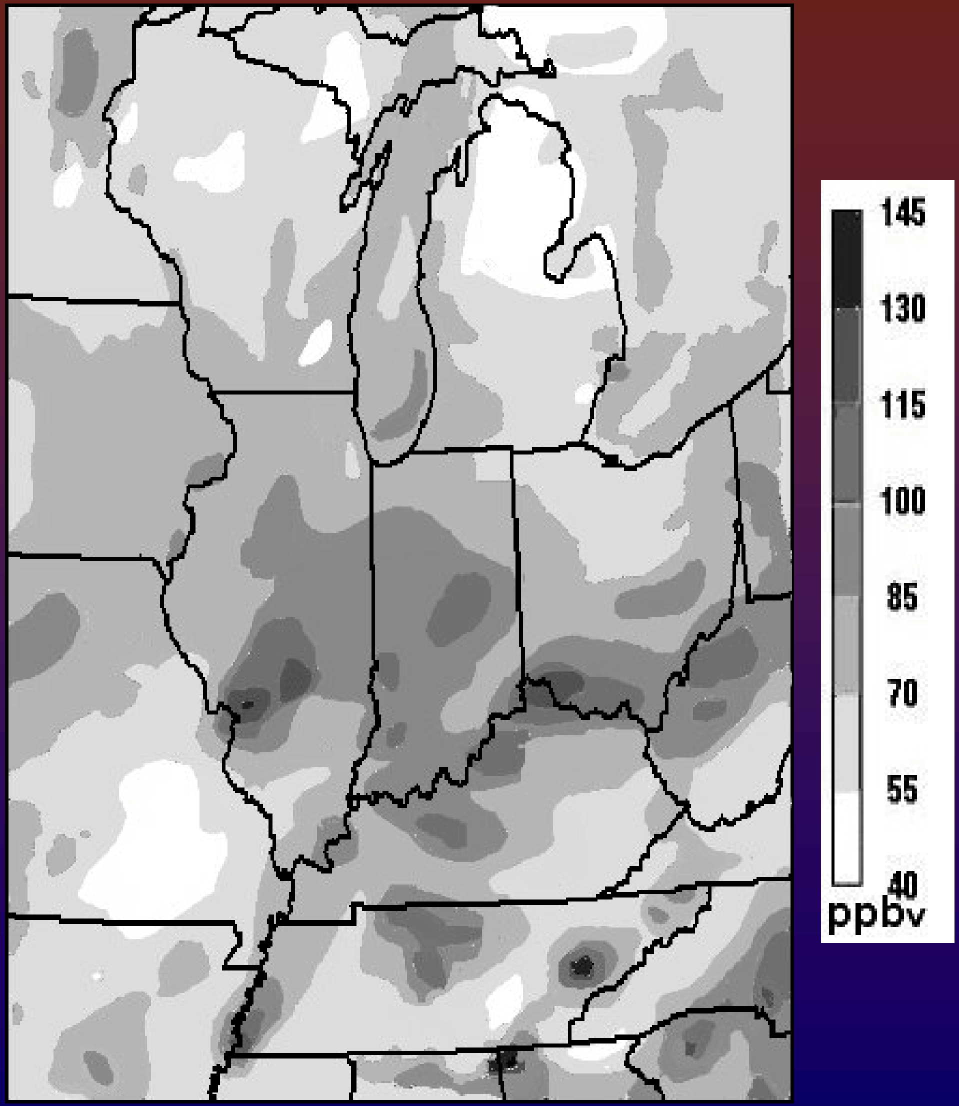


Climatic Impact Analysis Methodology

- Analyses are carried out with the modeled meteorological fields from the interactive climate-chemistry ***PRCCM*** run and from the chemistry-free ***PRCM*** control run.
- The only modification in atmospheric modeling processes from two computer runs is real-time updated tropospheric ozone in the radiation calculation of the ***PRCCM***.
- Therefore, the differences between two model run results can be regarded as the impacts due to the increased tropospheric ozone.

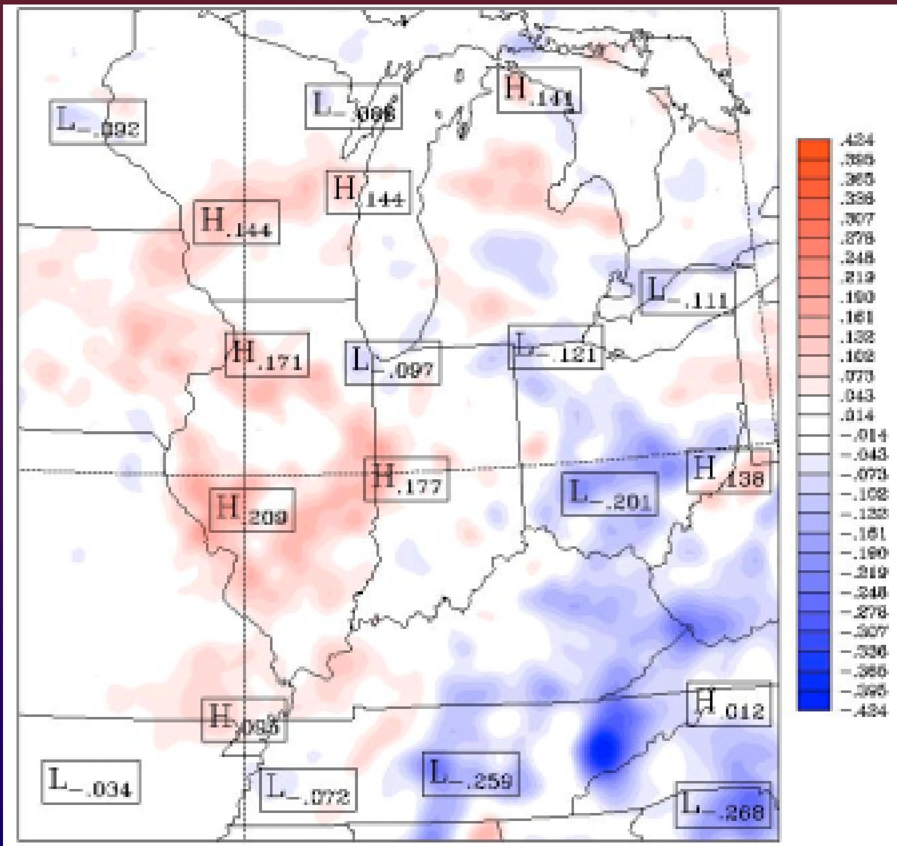
Climatic Impacts = PRCCM results - PRCM results

Mean Daily Peak Surface-level Ozone



Surface Flux Change

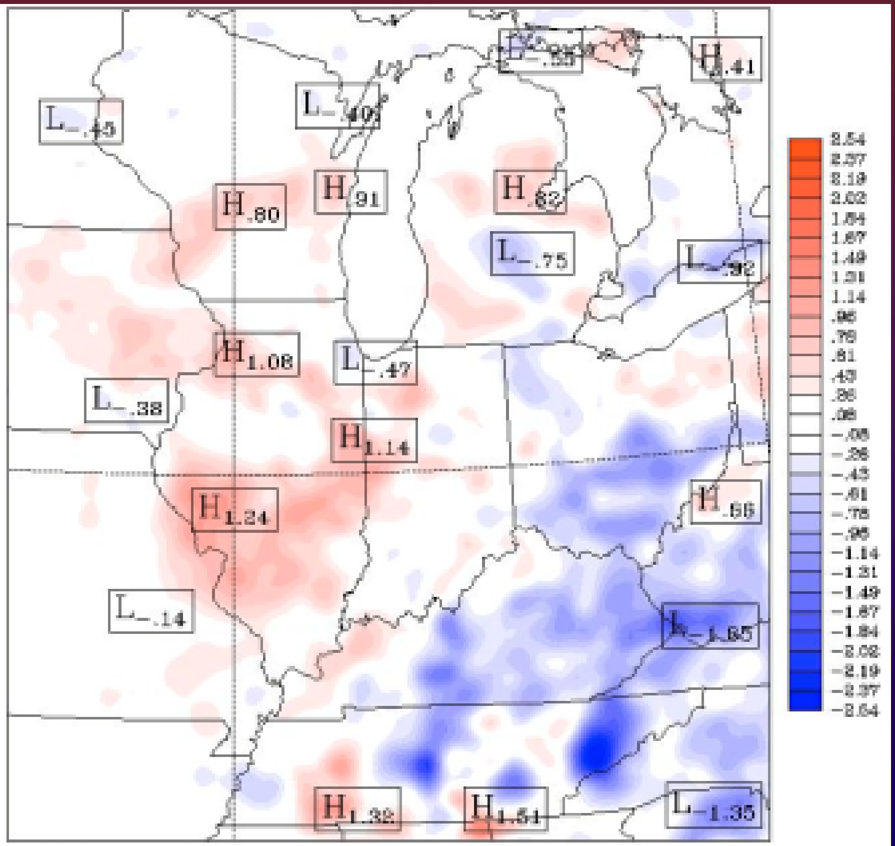
(PRCCM run- PRCM control run)
Mean Surface Air temperature (k)



Min. = -.424 Max. = .209 Interval=.029

Domain average= - 3.85×10^{-3} k

(PRCCM run- PRCM control run)
Mean Longwave upward Radiation (w/m^2)

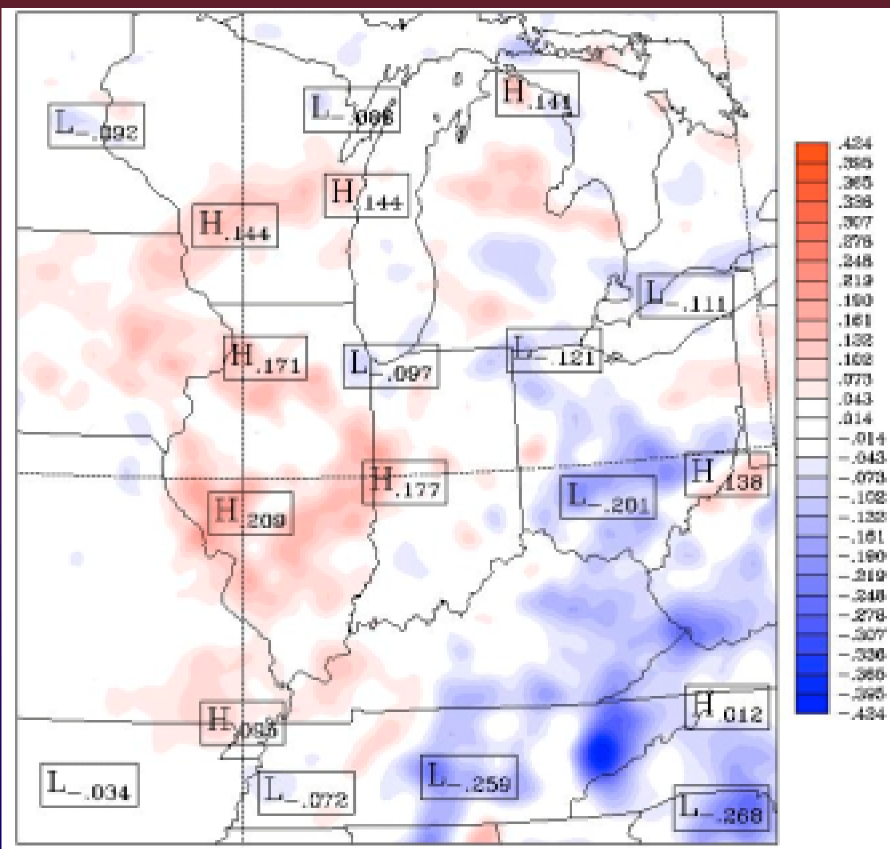


Min. = -2.54 Max. = 2.51 Interval=17

Domain average= - 0.025 w/m^2

Surface Flux Change

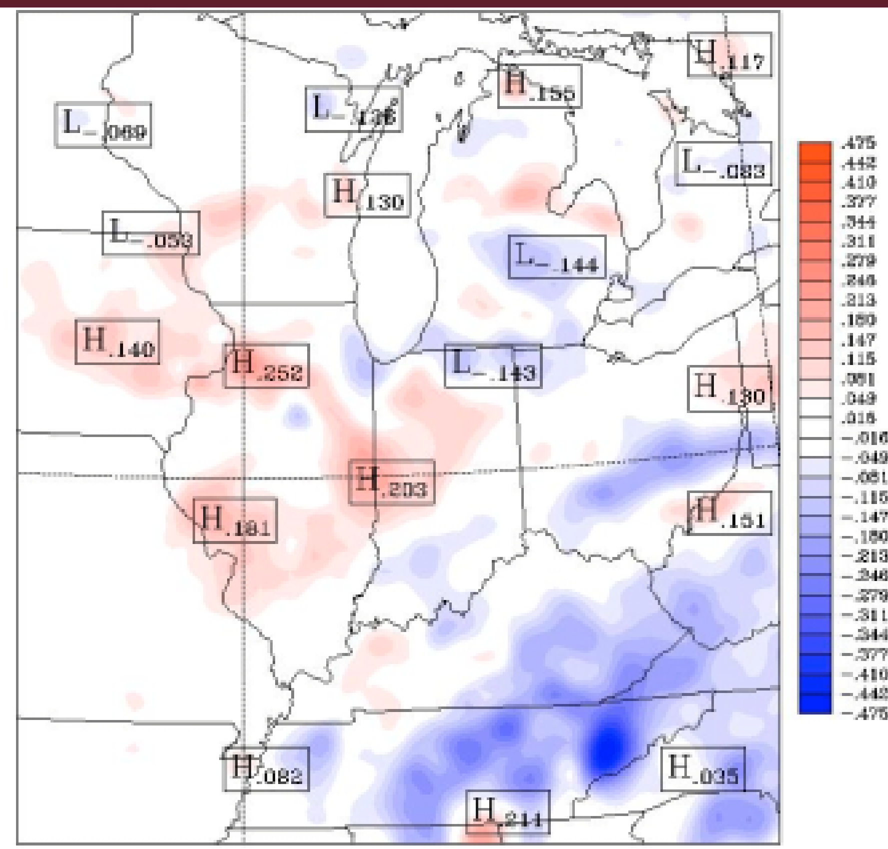
(PRCCM run- PRCM control run)
Mean Surface Air temperature (k)



Min. = -.424 Max. = .209 Interval=.029

Domain average= - 3.85×10^{-3} k

(PRCCM run- PRCM control run)
Mean surface water vapor (kg/kg)

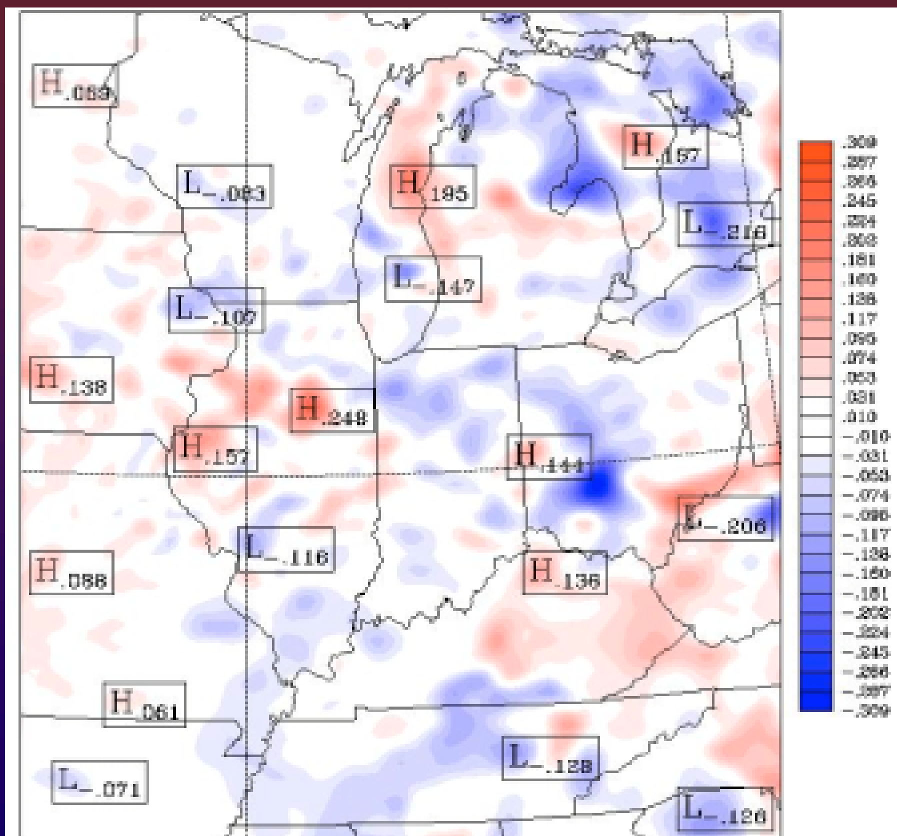


Min. = -.475 Max. = .252 Interval=.032x0.001

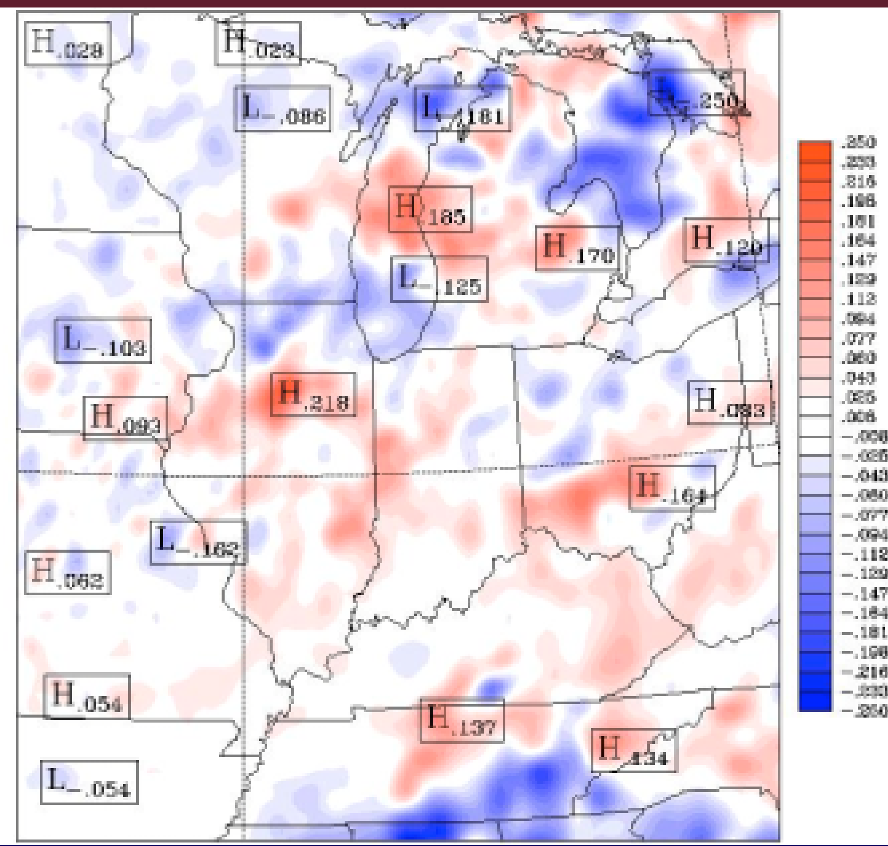
Domain average= - 1.22×10^{-5} w/m^2

Surface Wind Change

(PRCCM run- PRCM control run)
Mean Surface wind U comp.(m/s)

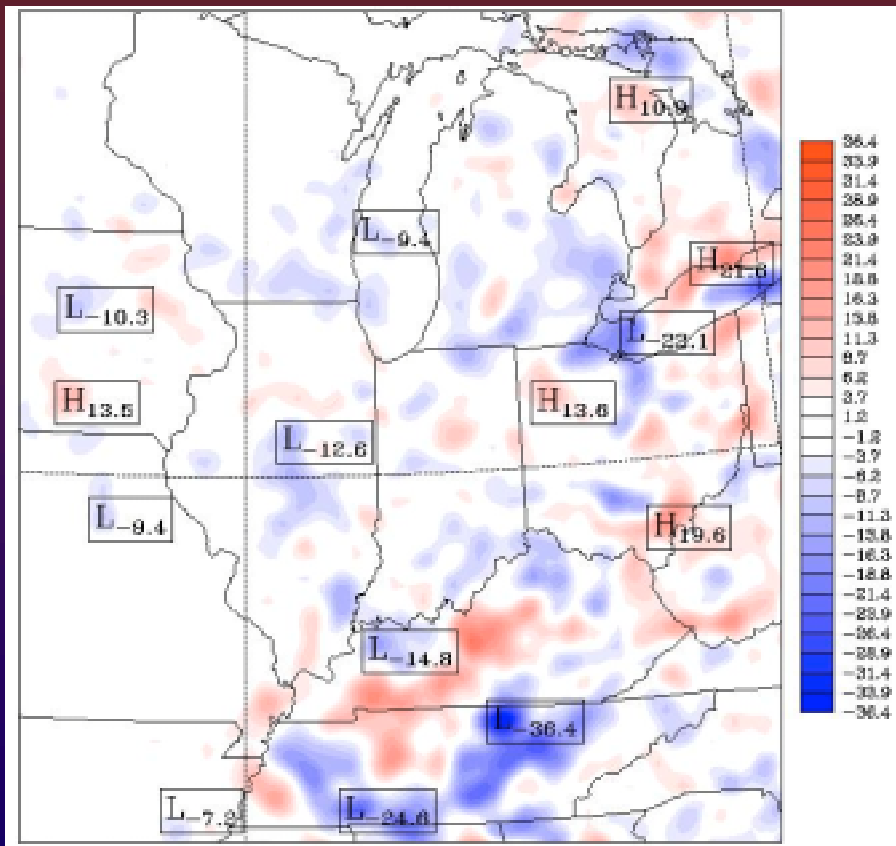


(PRCCM run- PRCM control run)
Mean Surface wind V comp.(m/s)



Radiation Change at TOA

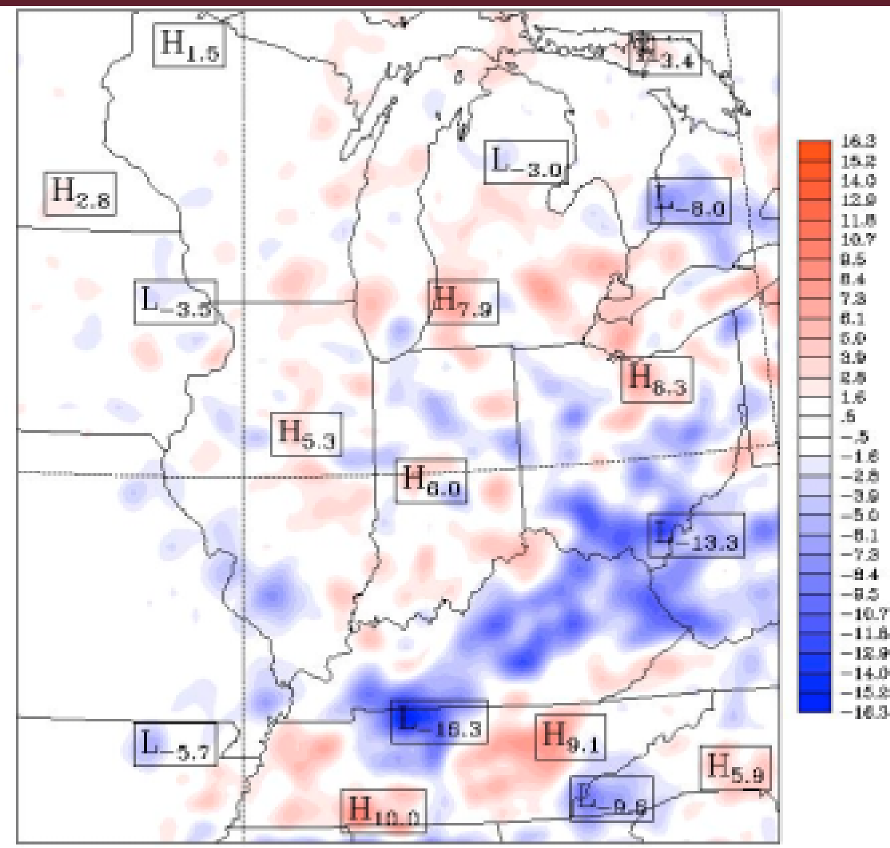
(PRCCM run- PRCM control run) mean Shortwave up. Radiation (w/m^2)



Min. = - 36.4 Max. = 24.5 Interval= 2.5

Domain average= - 0.658 w/m^2

(PRCCM run- PRCM control run) mean Longwave up. Radiation (w/m^2)



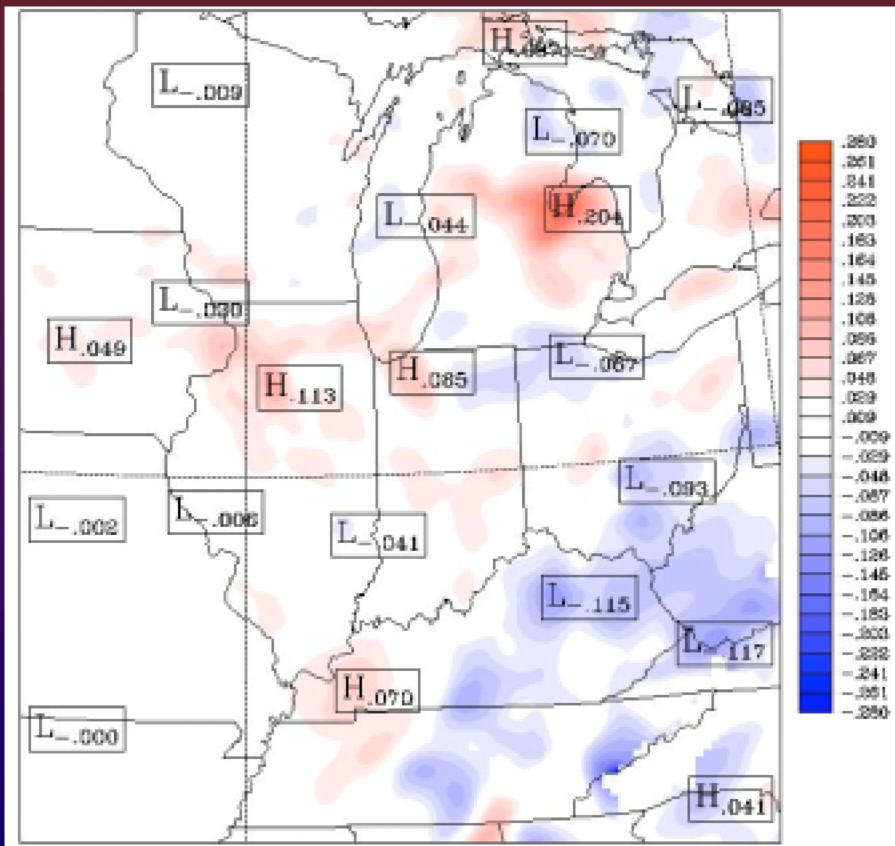
Min. = 16.3 Max. = 10.0 Interval= 1.1

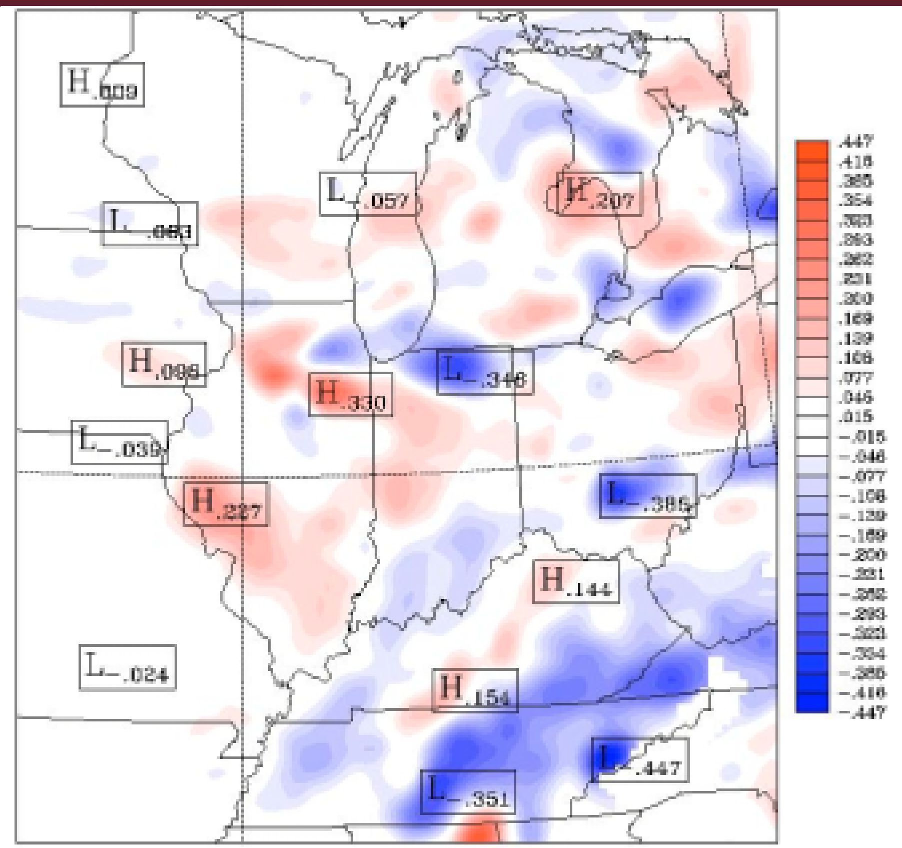
Domain average= - 0.363 w/m^2

Air temperature and Q_v at 925 mb

(PRCCM run- PRCM control run)
mean Air temperature (k)

(PRCCM run- PRCM control run)
mean water vapor mixing ratio (kg/kg)





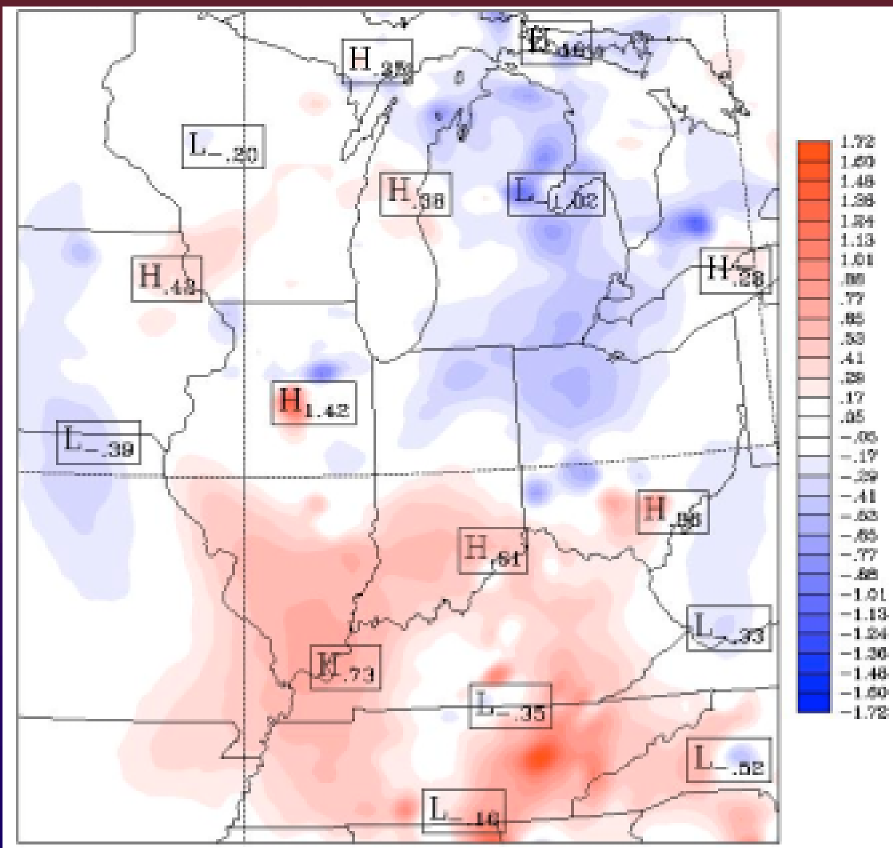
Domain average= 8.25×10^{-4} K

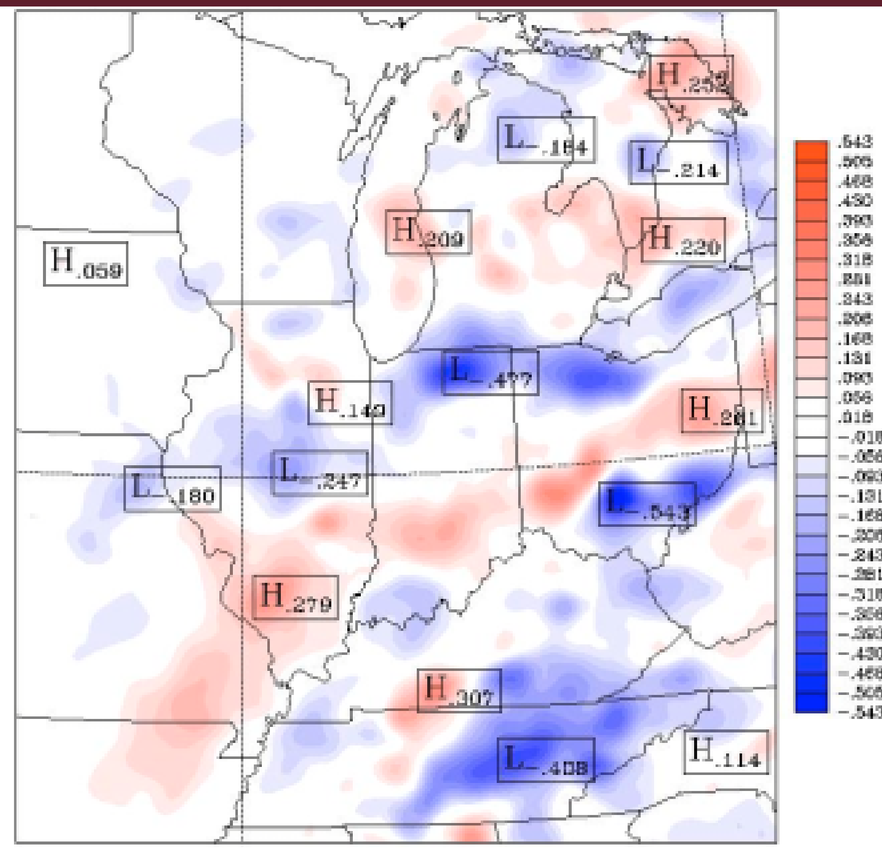
Domain average= - 1.18×10^{-5} kg/kg

Air temperature and Q_v at 850 mb

(PRCCM run- PRCM control run) mean Air temperature (k)

(PRCCM run- PRCM control run) mean water vapor mixing ratio (kg/kg)



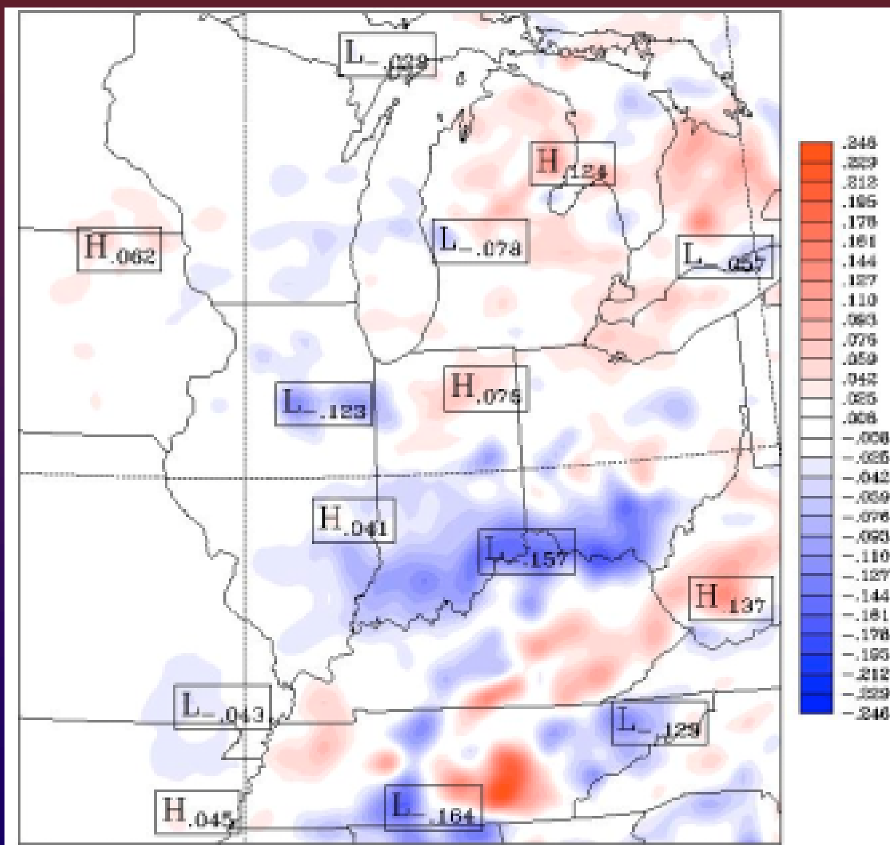


Domain average= 4.73×10^{-3} K

Domain average= -1.82×10^{-5} kg/kg

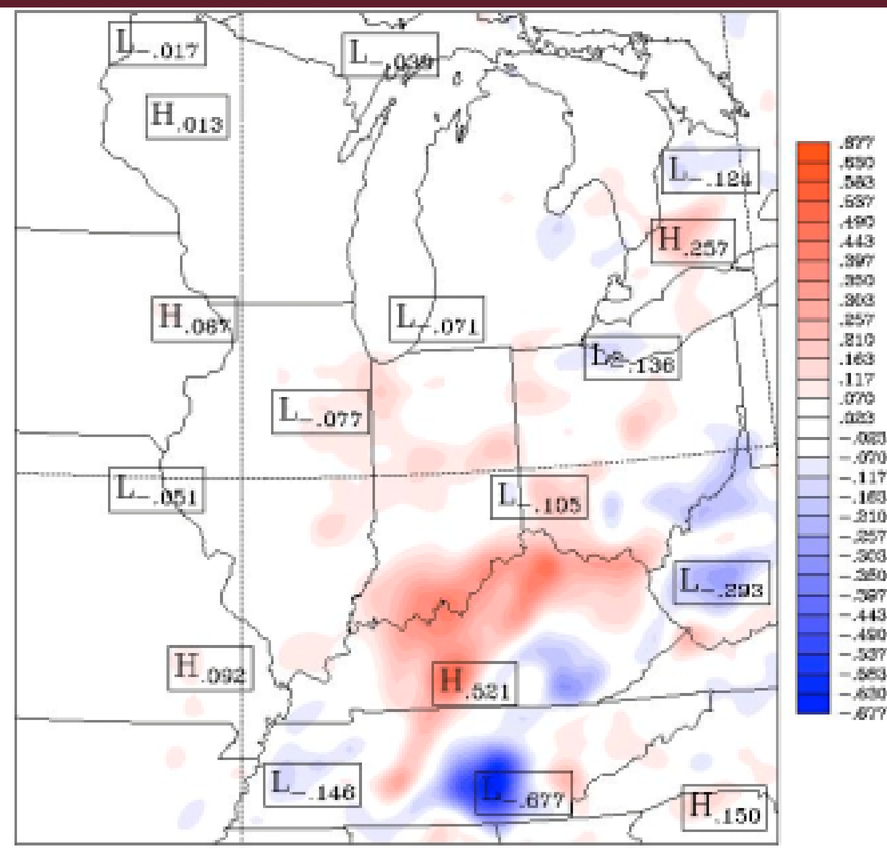
Air temperature and Q_v at 700 mb

(PRCCM run- PRCM control run)
mean Air temperature (k)



Domain average= -2.25×10^{-3} K

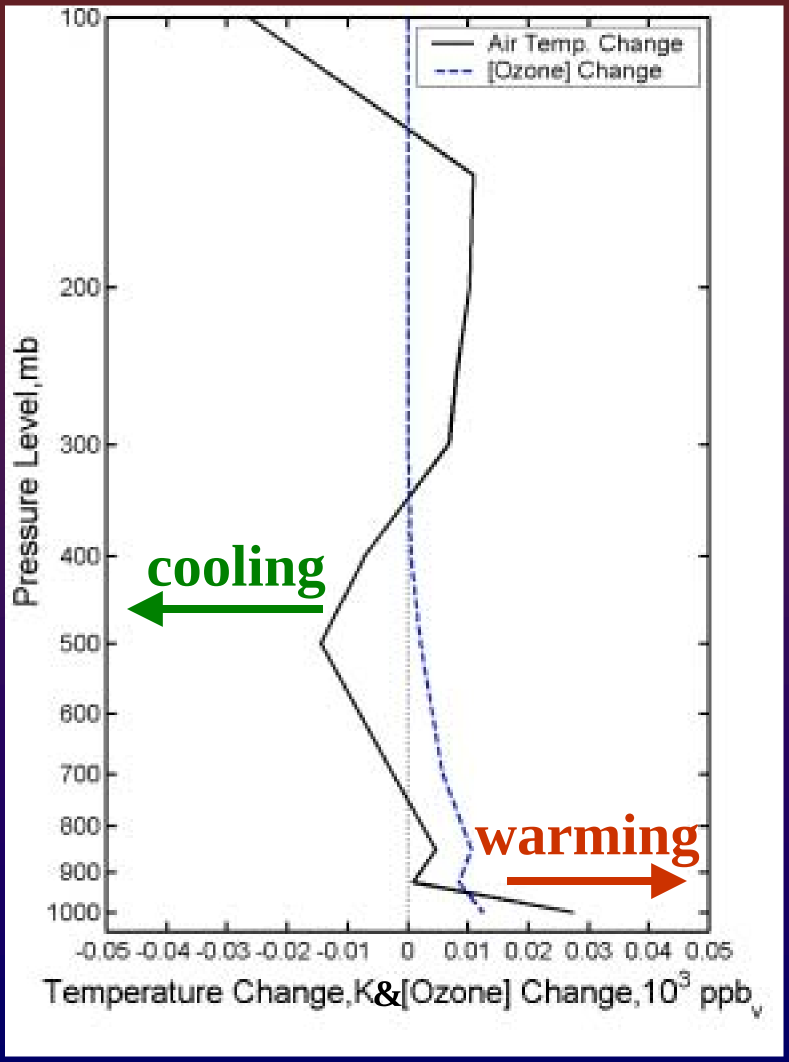
(PRCCM run- PRCM control run)
mean water vapor mixing ratio (kg/kg)



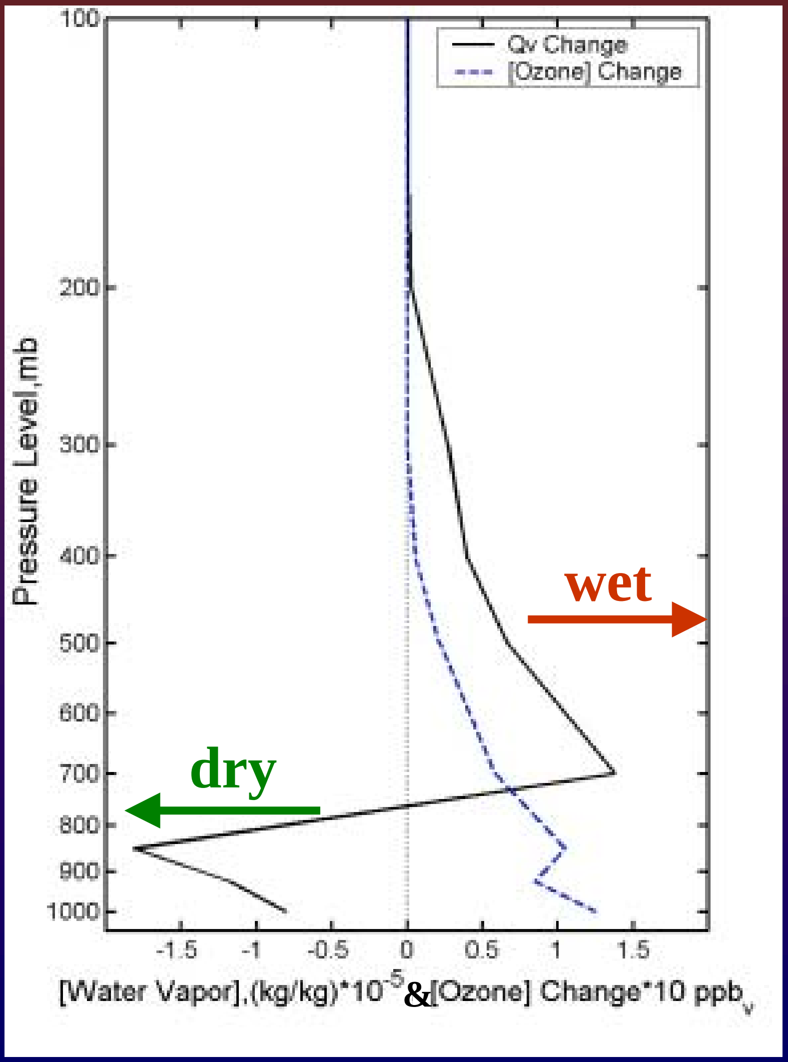
Domain average= 1.38×10^{-5} kg/kg

Vertical Profiles of Temperature and Water Vapor Changes

Air Temperature Change vs. [Ozone] Change



Water Vapor Mixing Ratios Change Vs. [Ozone] Change



Sensitivities to Tropospheric Ozone Changes

	Air temperature change (k) per ppb ozone	Water vapor change (kg kg $^{-1}$) per ppb ozone
400 MB	-1.31E-02	7.21E-06
500 MB	-6.76E-03	3.09E-06
700 MB	-3.88E-04	2.38E-06
850 MB	4.51E-04	-1.73E-06
925 MB	9.70E-05	-1.39E-06
1000 MB	2.20E-03	-6.44E-07

Outline

- *Background*
- *Research Objectives and Approach*
- *Model Descriptions: Purdue Regional Climate and Chemistry Model (PRCCM)*
- *Case Study*
- *Model Results*
- *Summary & Conclusions*

Summary and Conclusions

- **A regional coupled climate-chemistry model PRCCM has been developed.**
  - On-line tropospheric ozone modeling is carried out with quality-assured meteorology directly from the atmospheric model including the radiation to drive photochemistry.
  - The feedback of ozone in lower troposphere is considered in climate modeling processes through its radiative properties.
  - A truly interactive climate-chemistry model.
- **Model validation and evaluation**
  - The atmospheric model successfully reproduced the meteorological fields.
  - Tropospheric ozone predictions are reasonable accurate compared with surface-level and airborne measurements.

Summary and Conclusions

- **Improvements of climate modeling with chemistry**
  - That implies the necessity to include atmospheric chemistry in weather/climate modeling processes.
- **Strong climatic impacts due to tropospheric ozone**
  - PRCCM results show the uneven climatic impacts at the regional scale due to a photochemical episode. Strong warming effects were observed near pollutant areas.
  - Regional moisture redistribution and modification of atmospheric stratification may further influence regional dynamics.
- **This coupled mode can be the future generation of air quality model as well as climate model that accounts for dynamical, physical and chemical processes in the atmosphere**

Acknowledgements

- Dr. Robert B. Jacko
- Dr. Jiun-dar Chern and Dr. Ming-dah Chou (NASA/GSFC)
- Lake Michigan Air Directors Consortium (LADCO)
- Purdue Research Computing Center
- NCAR Scientific Computing Division

Support from NSF

Future Considerations

- Aerosols and their interactions with other atmospheric constituents in atmospheric processes should be included in future development.
- Many uncertainties remain in the modeling processes. To name a few, emissions and photolysis as well as chemistry mechanism to represent atmospheric chemistry.
- Computational efficient chemical model to present atmospheric chemistry is needed.
- Future regional/global climate change studies can benefit from this kind of coupled climate-chemistry model.