## Regional Photochemical Modeling for the Ozark Isoprene Experiment (OZIE)

Thomas Pierce NOAA/EPA Atmospheric Modeling Division

Jim Greenberg and Alex Guenther National Center for Atmospheric Research

Michael Koerber Lake Michigan Air Directors Consortium

Jay Turner Washington University (St. Louis)

Chris Geron EPA National Risk Management Research Lab.

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**Motivation for OZIE...** 

...biogenic hydrocarbons are important for ozone attainment modeling (National Academy of Sciences, 1991);

...abnormally high (>250 ppbC) isoprene concentrations are being modeled over the Ozark Plateau; and,

...southern Missouri has the highest density of oaks (high isoprene emitters) in the United States.



## Urban Airshed Model (UAM) Layer 1 (~50 m deep), 4 km Grid

### Peak 1-Hour Isoprene



### Urban Airshed Model (UAM) Layer 1, 4 km Grid

#### Peak 1-Hour Formaldehyde





## **Ft. Leonard Wood measurement sites**









## **Summary of Surface Isoprene**

Site	n	Mean	Range
Giant City, IL (7% oak, 8-24Jul)	41	32 ppbC	3-77 ppbC
Morgan-Monroe, IL (8% oak, 8-24Jul)	23	32 ppbC	12-76 ppbC
Ft. Leonard Wood, MO (34% oak, 9-20Jul)	69	54 ppbC	9-179 ppbC
Willow Springs, MO (36% oak, 21Jul)	16	75 ppbC	41-136 ppbC
Sinkin Creek, MO (53% oak, 22Jul)	17	75 ppbC	33-121 ppbC



## Photochemical Model used to Compare to OZIE Measurements

Model:	Models-3/Community Multiscale Air Quality Modeling (CMAQ) System
Domain:	Eastern North America 36 km horizontal resolution 21 vertical layers (layer 1 = ~38 m)
Chemistry:	CBIV w/ Carter isoprene
Meteorology:	MM5v2.10 <sup>+</sup>
<b>Biogenic Emissions:</b>	BEIS2.2
Simulation date:	12 July 1995* *similar to 18-21 July 1998



## CMAQ Prediction of Isoprene in Layer 1. Grid = 36 km, Layer 1 =0-35 m. Layer 1 ISOPe

e=CCTM\_s1kCONC.s2j



#### Comparison of Near Surface Observed and Modeled Isoprene at FLW, Missouri



Obs: Average of 5 surface sites, 18-21Jul98 Model: Layer 1, 36-km grid centered over FLWood, 12Jul95,

#### **Comparison of Observed and Modeled Aloft Isoprene Concentrations at FLW**



Aircraft obs: 450-900 m (agl), July 18-21, 18-20 GMT.
Balloon obs: 15/5 flights, 400-1000/400 m (agl).
CMAQ: model layers 8-11, 18-19 GMT, 12 July 1995, 36-km grid cell centered on Ft. Leonard Wood.

### Comparison of Tethersonde Measurements and CMAQ Predictions of Isoprene (ppbv) for Willow Springs and Sinkin Creek

Willow Springs	Obs (n=9)	CMAQ (18-22 GMT)	Sinkin Creek	Obs (n=7)	CMAQ (16-20 GMT)
Isop (ppbv)	2.4	8.5	Isop (ppbv)	3.2	12.6
Temp. (°C)	33.8	34.3	Temp (°C)	31.9	33.0
PAR (µmol m <sup>-2</sup> s <sup>-1</sup> )	1150	1683	PAR (µmol m <sup>-2</sup> s <sup>-1</sup> )	1300	1873

Tethersonde: ~200 m agl CMAQ: model layer 5 (150-220 m, 12 July 1995)

#### **Tethersonde Measurements and CMAQ Predictions for Oak Ridge, TN**





CMAQ: 36-km grid

#### Comparison of Observed and Modeled Meteorology





## Summary

 $\Rightarrow$  Relatively high isoprene concentrations (~75 ppbC) were measured at the surface sites in Missouri. CMAQ results are comparable, but UAM (4 km) results are more than x2 higher than observations.

 $\Rightarrow$  Above Willow Springs and Sinkin Creek, CMAQ overestimated by >x3. This may be due partially to poor treatment of meteorology.

 $\Rightarrow$  Above Ft. Leonard Wood, CMAQ and observed isoprene compared favorably (w/in the range observed by the aircraft and the balloon). UAM (4 km) is ~x2 higher.





⇒CMAQ comparisons have neither disproved nor confirmed abnormally high isoprene predictions. However, preliminary UAM comparisons clearly show overestimates. Possible model problems include meteorology, vertical diffusion, and chemistry.

⇒Caveats:

- (1) July 1995 simulation v. July 1998 obs.
- (2) Coarse grid resolution in the CMAQ model.
- (3) Representativeness of measurement footprint.



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