The Impacts of Biogenic Emissions Estimates from BEIS-3 on Ozone Modeling in the Southeastern US

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Outline

- **Introduction**
  - **Background**
  - **Objectives**
- **Modeling Systems**
- **Results**
- **Discussion**
- **Future Work**

Background

- **Emissions of NO_x and VOCs from anthropogenic (man-made) and biogenic (natural) sources contribute to form ozone**
- **Grid-based photochemical air quality models used to study ozone formation**
  - **used for regulatory as well as scientific purposes**
  - **use emissions processing systems to estimate emissions from various sources**
- **Large uncertainties remain in these emissions estimates**
  - **A factor of three for total VOCs nationwide is quoted in literature**
- **Understanding contribution of natural sources to ozone formation has significant implications towards choice and extent of controls needed on anthropogenic sources to demonstrate attainment of ozone standards**

Objectives

- **To evaluate the impacts of using biogenic emissions estimates from a prototype version of BEIS-3 on ozone predictions**
  - **Perform sensitivity simulations of MAQSIP and compare model predictions when using BEIS-2 versus BEIS-3 emissions estimates in a nested domain in the Southeastern United States**

Modeling Systems

- **Fifth-Generation Penn State/NCAR Mesoscale Model Version 2 (MM5 V2.12)**
- **Sparse Matrix Operator Kernel Emissions (SMOKE) for generating emissions inputs**
- **Biogenic Emissions Inventory System**
  - **(BEIS-2 and BEIS-3)**
- **Multiscale Air Quality SImulation Platform (MAQSIP)**
- **Platform Independent I/O API format for all inputs and outputs**
- **June 19-30, 1996 episode in North Carolina**

Biogenic Emissions Inventory System

- **BEIS-2**
  - Five CB-4 Species (NO, ALD2, ISOP, OLE, PAR)
- **BEIS-3**
  - Prototype version with explicit speciation
  - 1-km resolution landuse data from BELD3
  - 230 different landuse types
  - 34 BEIS-3 species mapped to 12 CB-4 Species (CO, NO, ALD2, ETH, ETOH, FORM, ISOP, MEOH, OLE, PAR, TOL, XYL)
  - Treats CO, NO production from soils, and biomass burning

The Multiscale Air Quality SImulation Platform

A comprehensive urban to intercontinental atmospheric chemistry/transport model

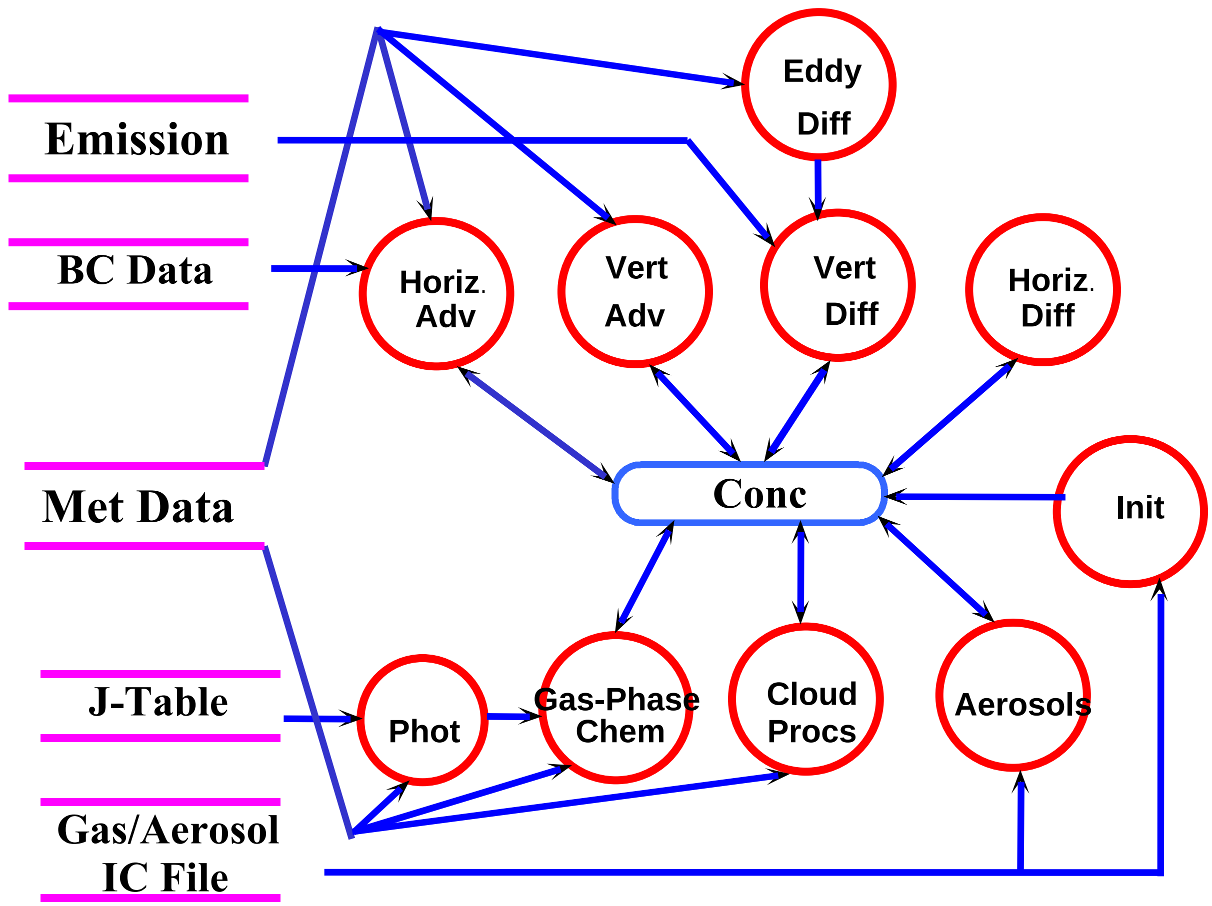
- **Developed at MCNC in collaboration with EPA**
  - Served as a prototype for EPA's Models-3/CMAQ modeling system
- **Has been used at various scales to study problems related to tropospheric O_3, acidic substances, and aerosol formation**
  - Seasonal simulation for 1995 over Eastern US
  - Regulatory episodic applications in NC, VA
  - Other studies to analyze
    - Relationship between pollutant transport and distribution over western Europe
    - CO transport and distribution over the North Atlantic region and the Asia Monsoon Region
    - Transport and chemical evolution of Asian outflow over the Pacific Ocean
  - Real-time Ozone forecasting system over the Eastern United States
    - Fine grids around Houston, Boston, Birmingham in summers of 1999-2001

MAQSIP (..contd.)

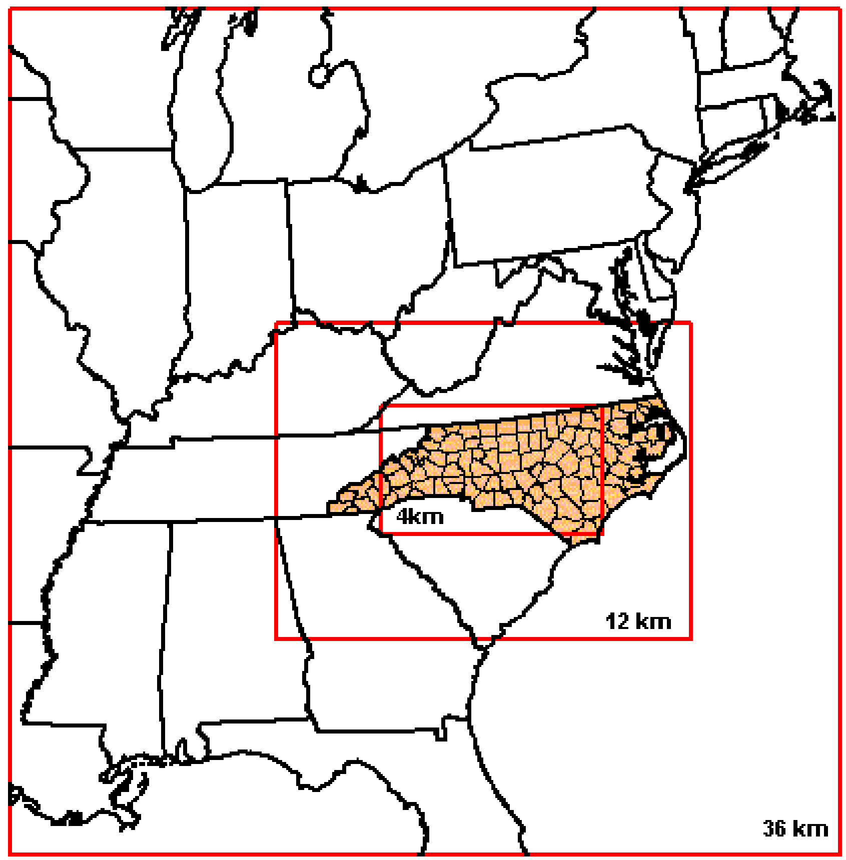
- **Modular**
  - Physical/chemical processes cast as modules; each process module operates on a common concentration field
- **Flexible**
  - Alternate process representations and algorithms
  - Provides a test-bed to compare different process representations/schemes
- **Expandable**
  - New modules can be added to the system
- **Multiscale**
  - Multiple multi-level nested grids
  - One-way and two-way
- **Generalized Coordinates facilitates**
  - Use of different map projections – applications of various geographic regions around the globe
  - Interfacing with meteorological models

MAQSIP

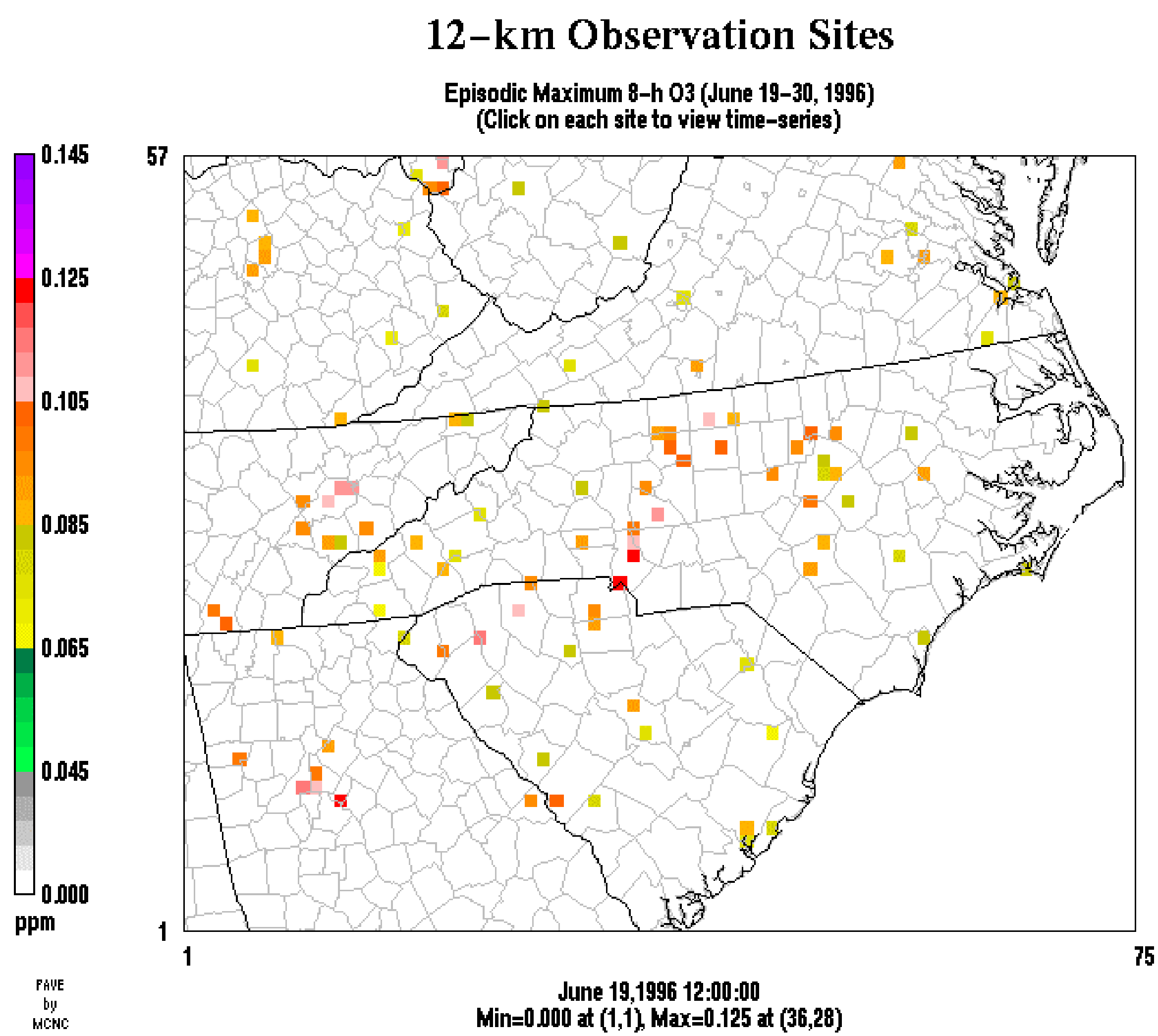
Processes Represented & Interrelationships



Nested Modeling Domain
[36/12/4-km Grids]



AQ Monitors in the 12-km Grid



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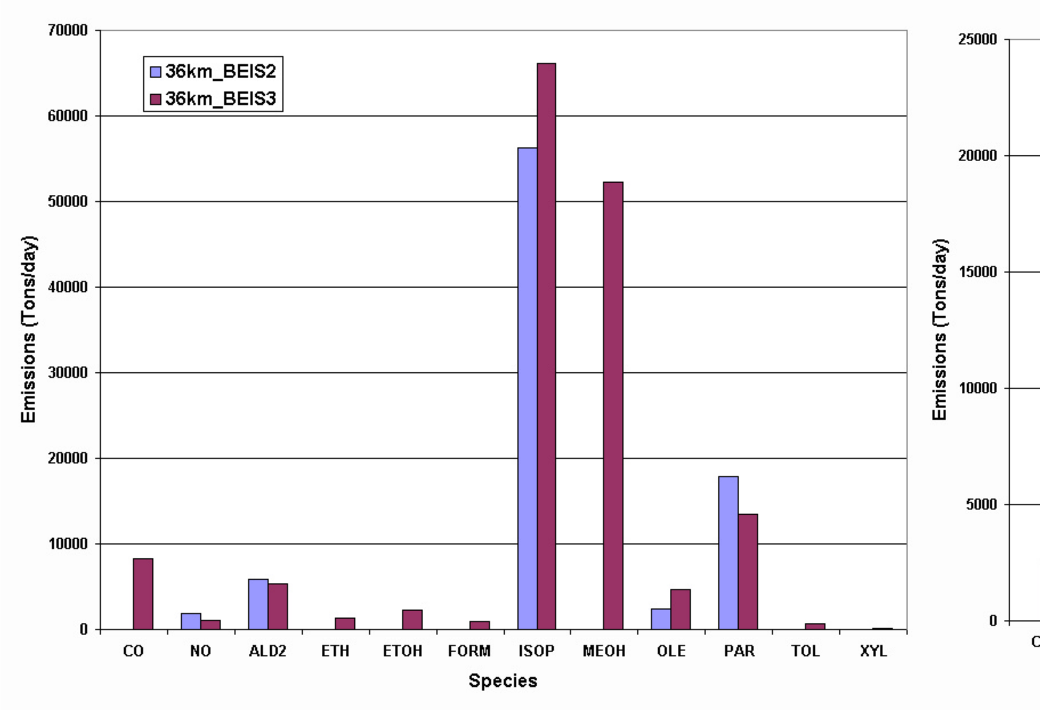
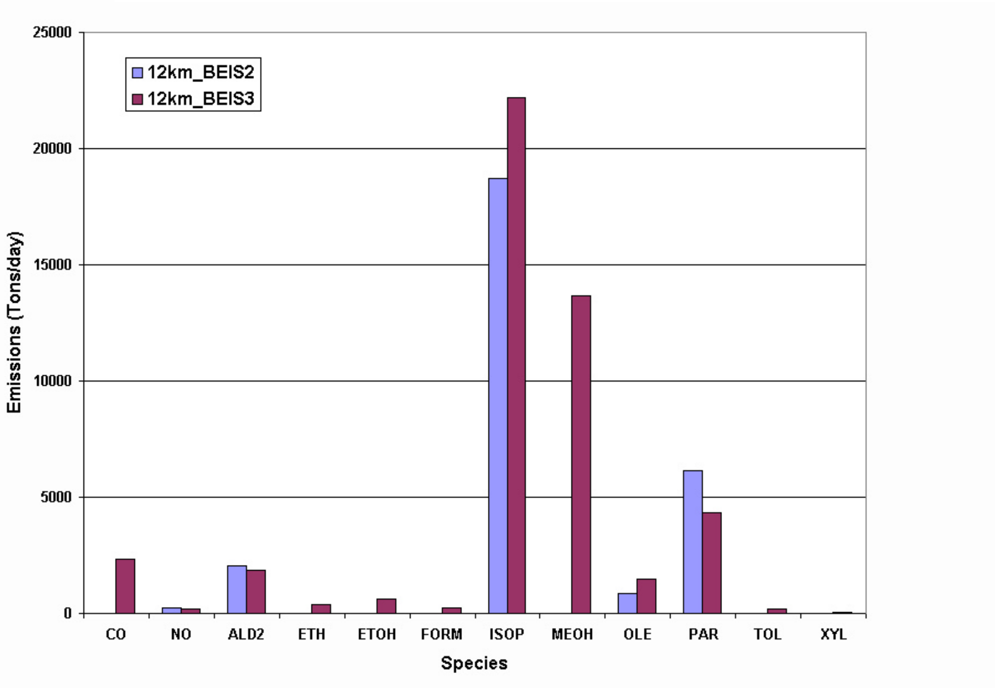
Biogenic Emissions Estimates
[Jun 24, 1996]





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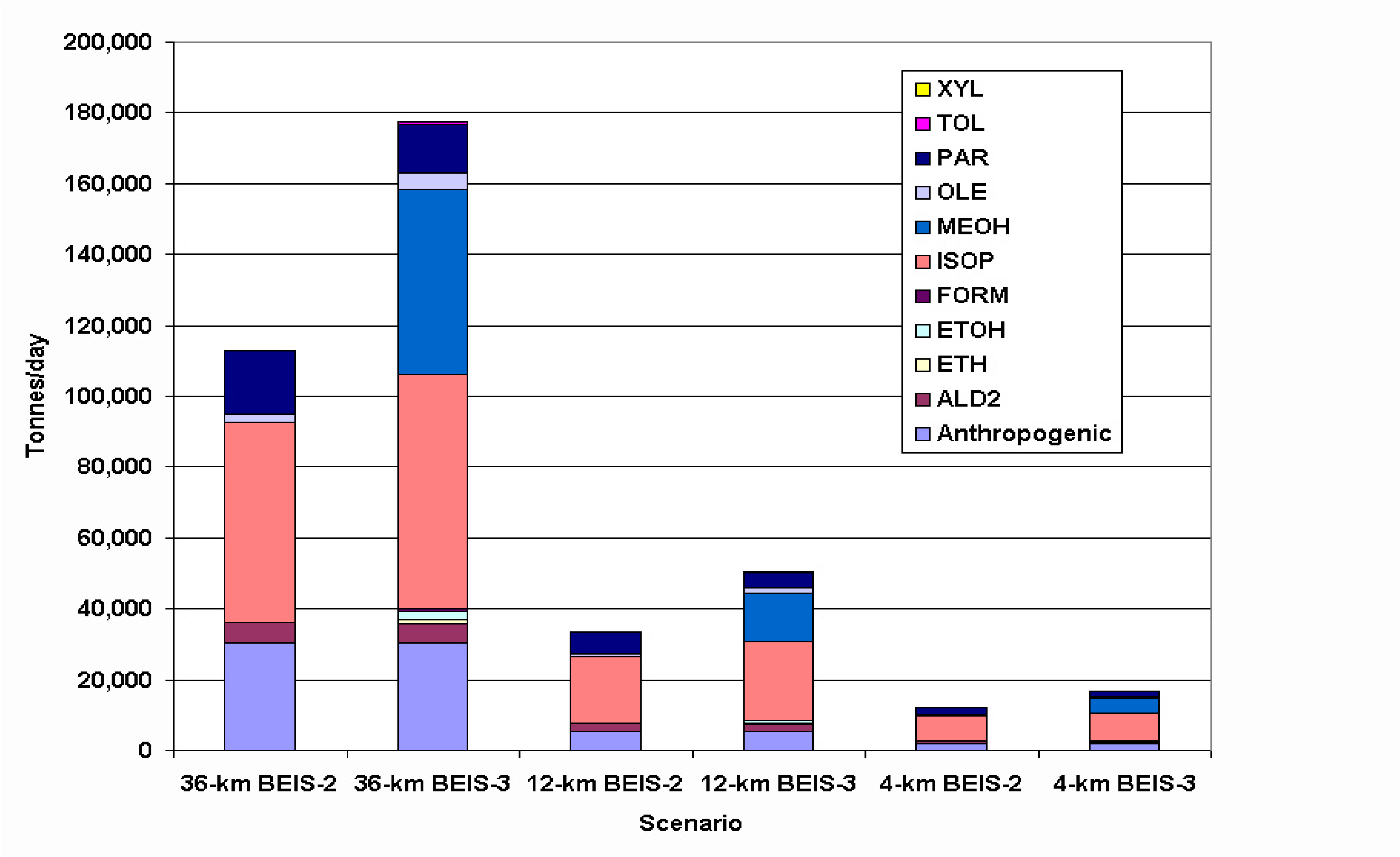
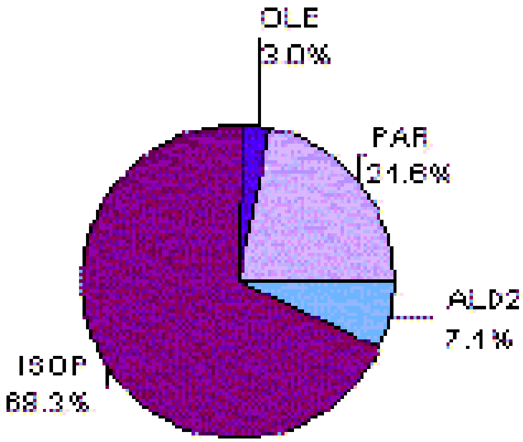
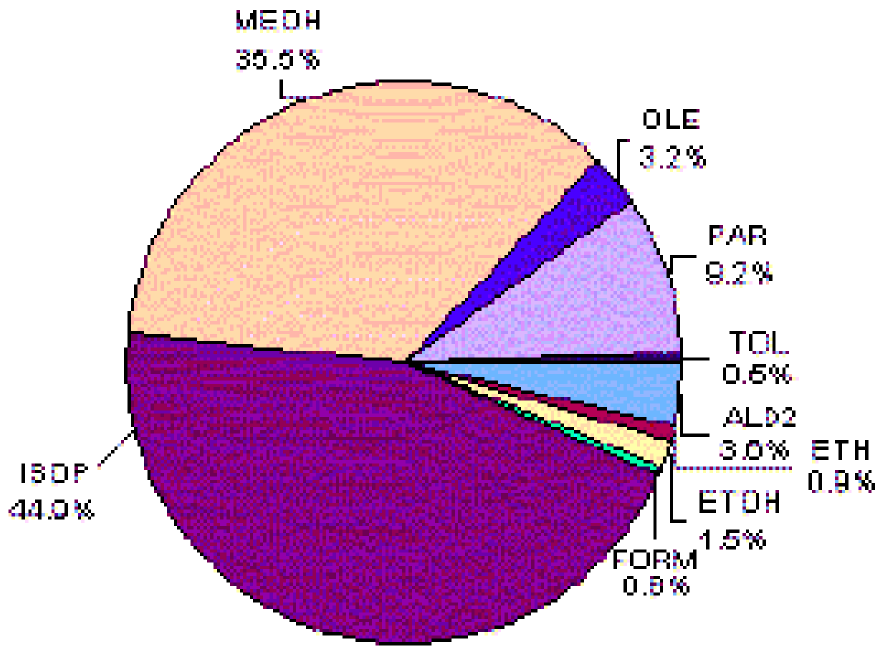
Total (Anth+Biog) Emissions Estimates
[Jun 24, 1996]



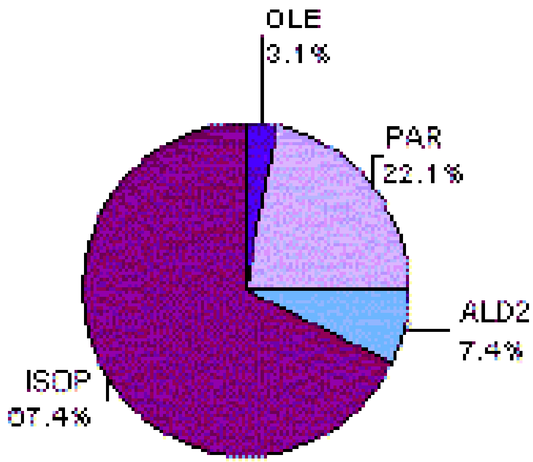
Biogenic Emissions Estimates

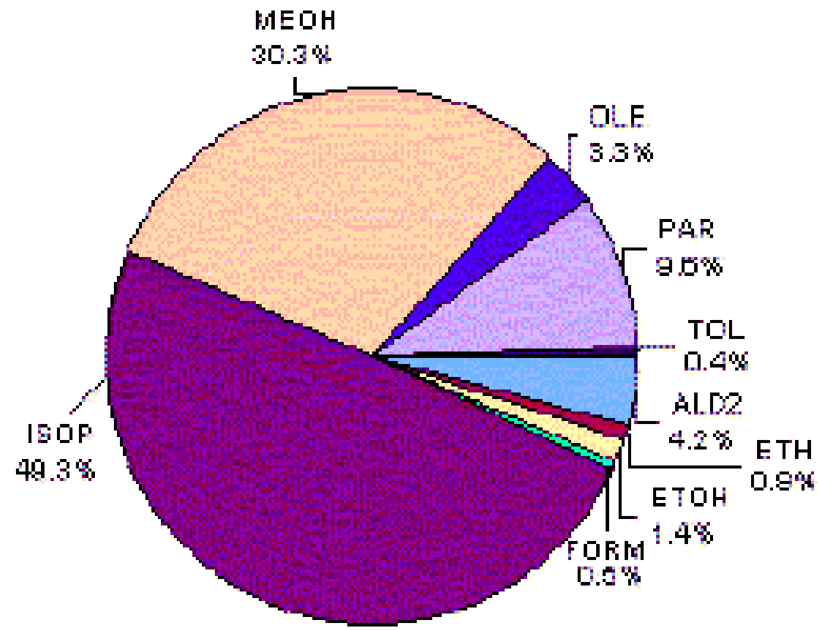
[36-km Grid: Jun 24, 1996]



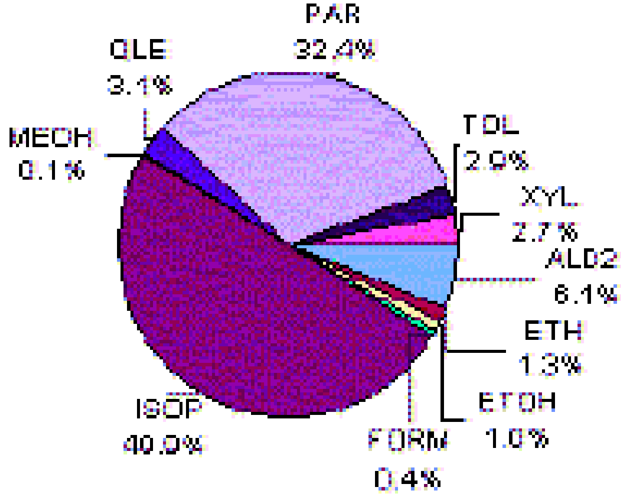


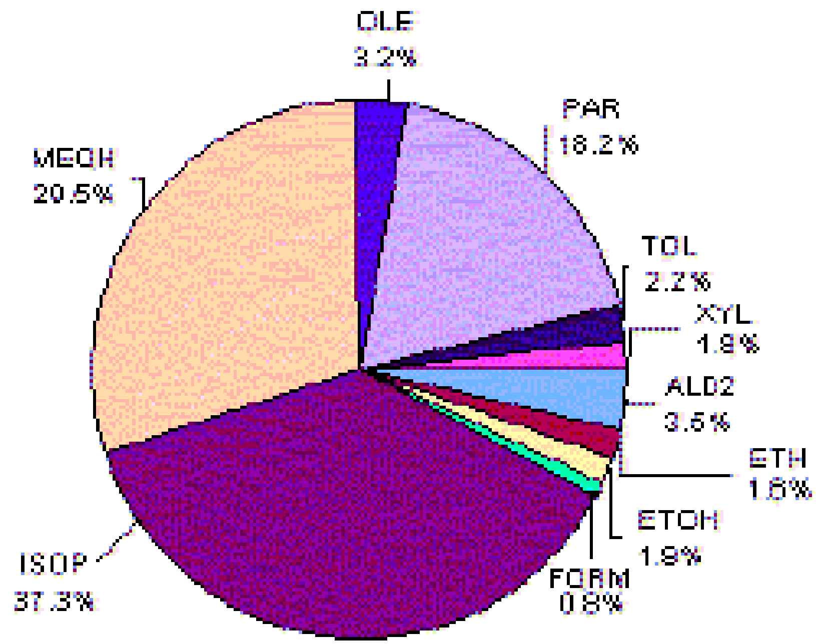
Biogenic Emissions Estimates
[12-km Grid: Jun 24, 1996]





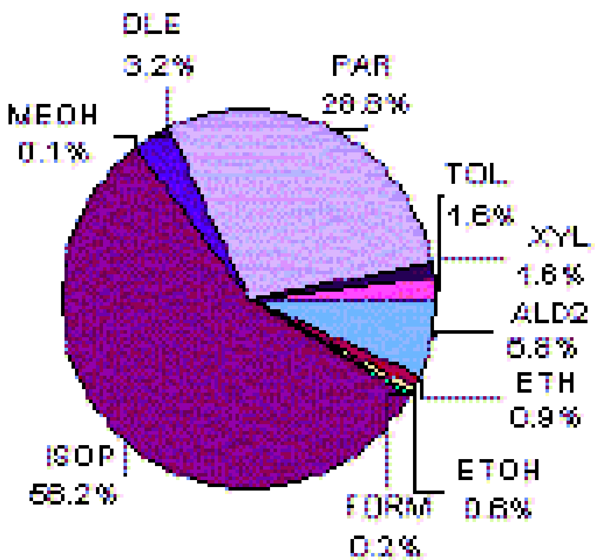
Total (Anth+Biog) Emissions Estimates
[36-km Grid: Jun 24, 1996]

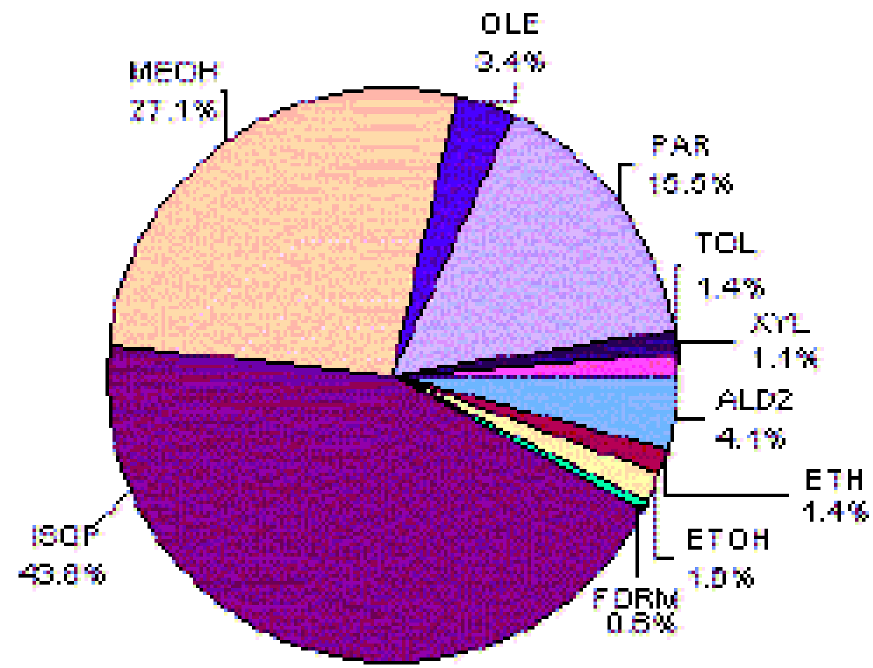




Total (Anth+Biog) Emissions Estimates

[12-km Grid: Jun 24, 1996]





Discussion

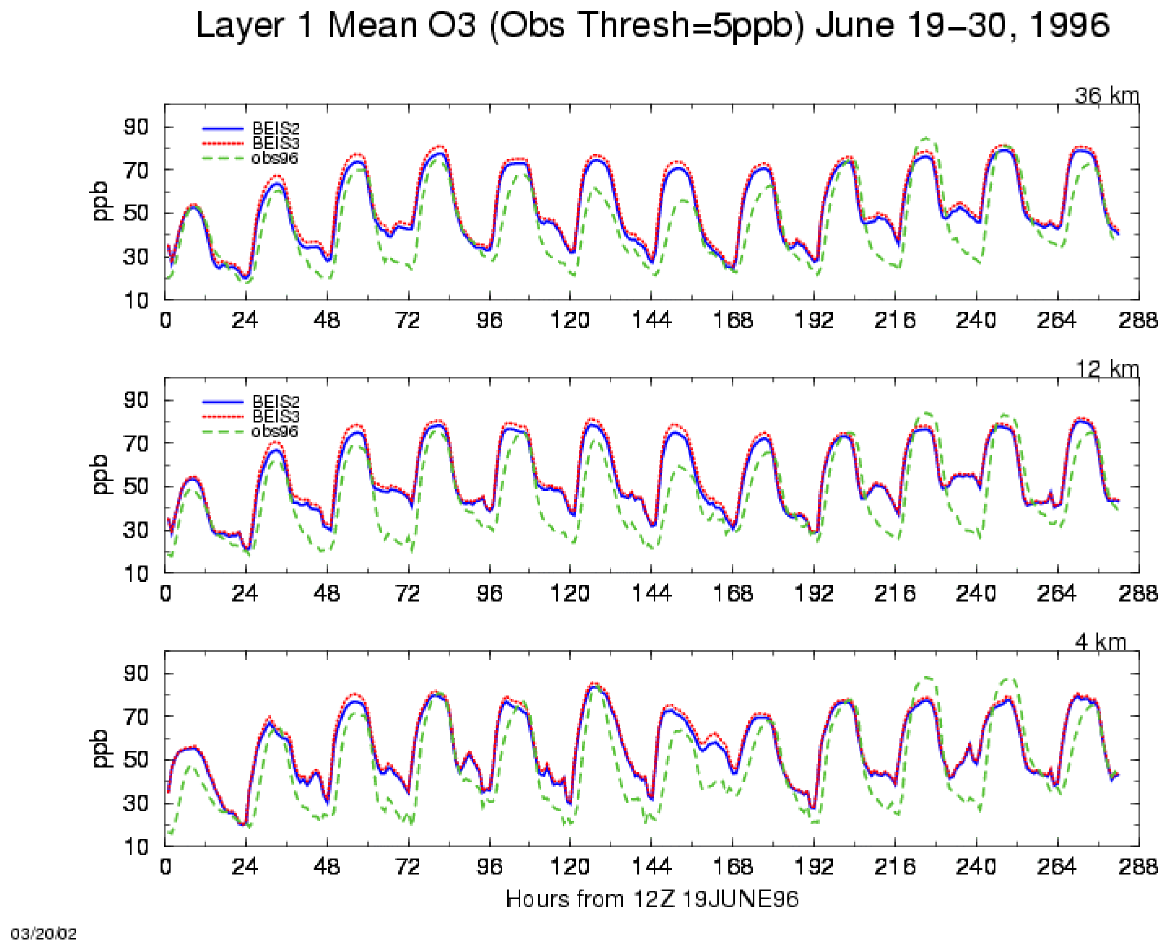
- Biogenic VOCs using BEIS-3 (compared to BEIS-2) increased by 79%, 62%, and 47% in the 36,12, and 4-km grids
- Total (Anth+Biog) VOCs using BEIS-3 (compared to BEIS-2) increased by 58%, 52%, 40% in the 36,12, and 4-km grids
- Corresponding increase in ISOP by 17%, 18% and 4%
- Large increases in MEOH, ETOH, and FORM
- ALD2, PAR, and NO emissions decrease
  - Total decrease in NO budget range from 1-3% in the 3 grids

Modifications to MAQSIP

- **Added two reactions to explicitly treat MEOH and ETOH oxidation within MAQSIP**
  - **MeOH + OH → HO_2 + HCHO**
    EtOH + OH → HO_2 + ALD_2
  - **Reaction Rate Constants from DeMore et al. *Chemical Kinetics and Photochemical Data for Use in Stratospheric Modeling*, Jet Propulsion Laboratory, California Institute of Technology, 1997**
- **Dry deposition velocities for paraffins (PAR) were used as approximations for MEOH and ETOH**

Model Performance Evaluation

[O3 Obs Threshold = 5ppb]



Statistical Measures

[Layer 1 O_3 in the 36-km Grid: Jun 19-30, 1996]

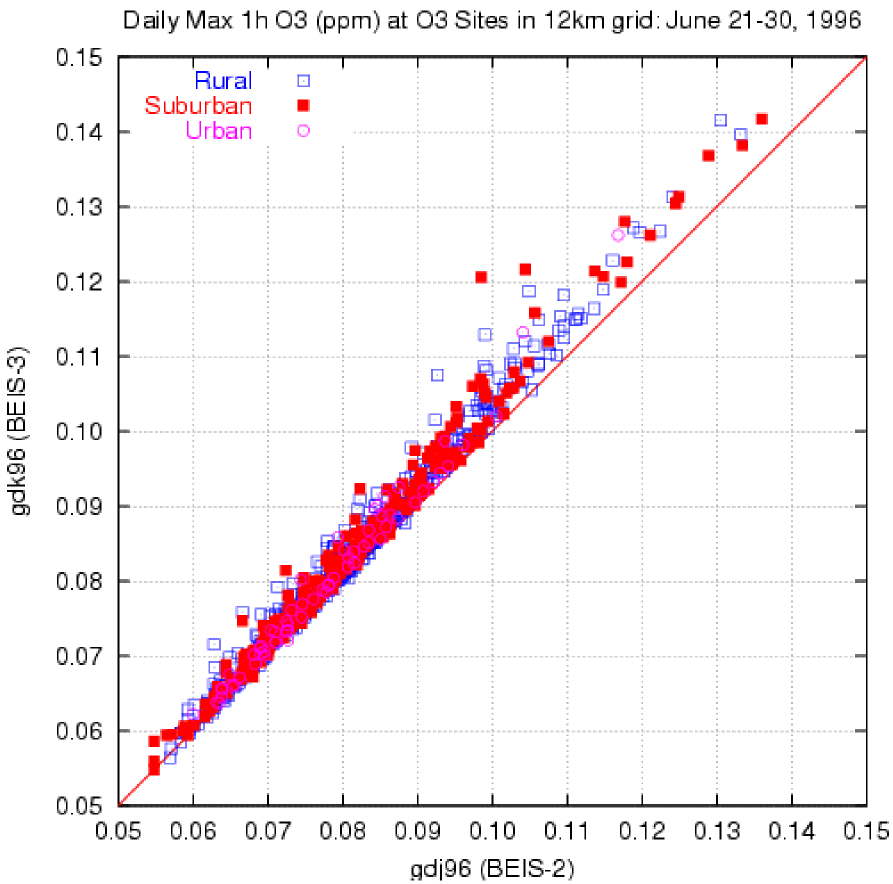
AQM	Thres (ppb)	Avg Mod	Avg Obs	Bias	R^2	NBias	GrEr
BEIS-2	60	69.6	74.8	-5.2	0.13	0.061	0.184
BEIS-3	60	72.7	74.8	-2.1	0.14	0.020	0.181
BEIS-2	40	62.0	62.7	-0.7	0.22	-0.010	0.244
BEIS-3	40	64.8	62.7	2.1	0.23	-0.056	0.249
BEIS-2	5	53.2	46.5	6.8	0.33	-0.483	0.683
BEIS-3	5	55.6	46.5	9.2	0.35	-0.549	0.714

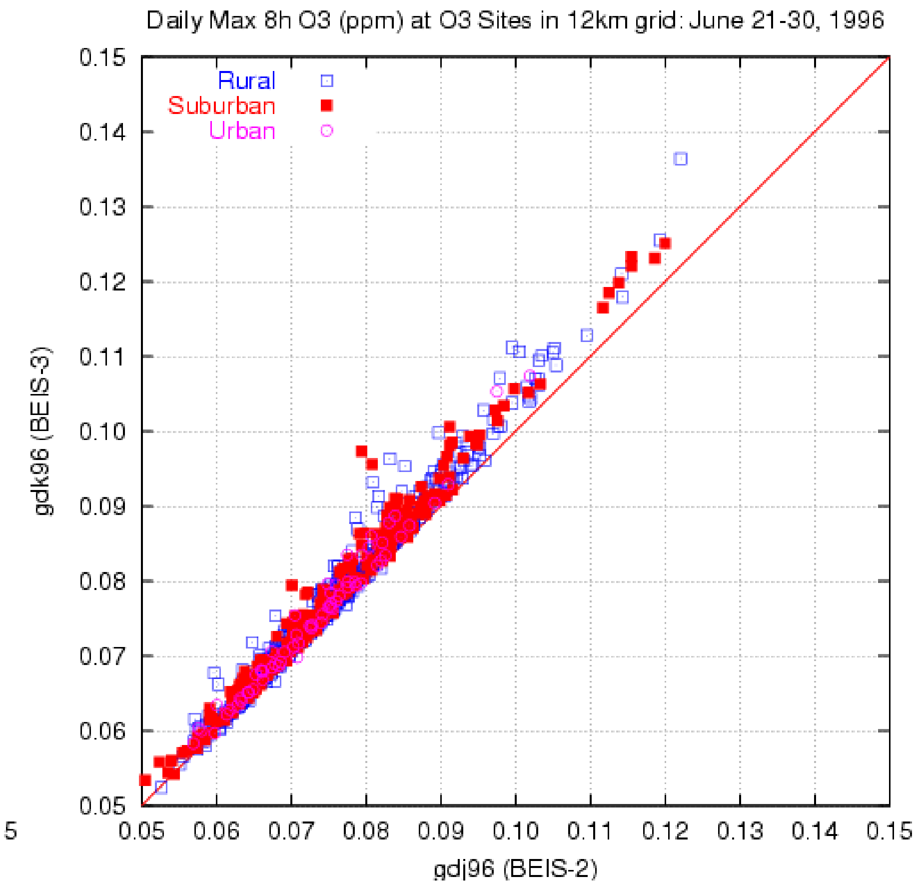
Statistical Measures

[Layer 1 O_3 in the 12-km Grid: Jun 19-30, 1996]

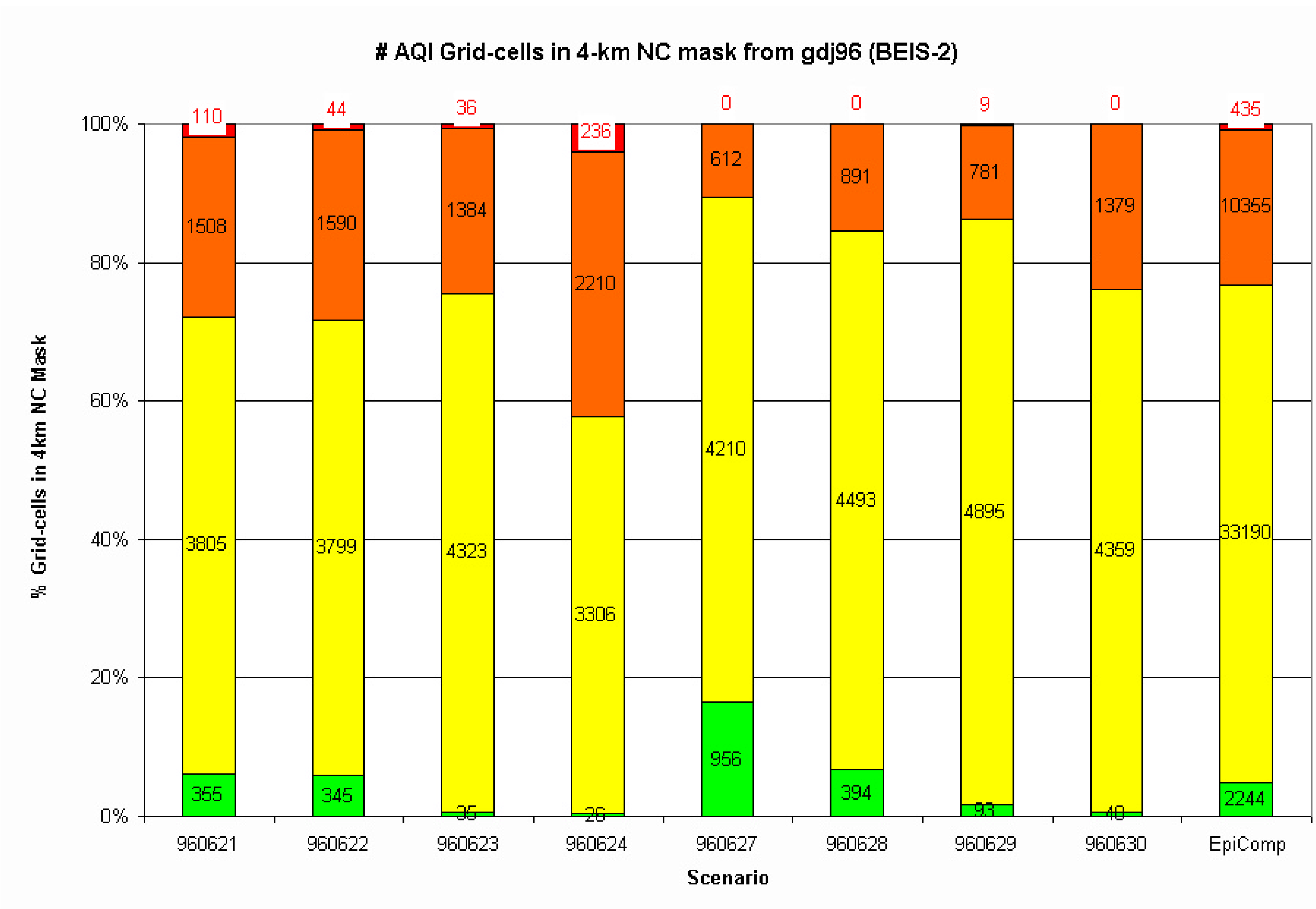
AQM	Thres (ppb)	Avg Mod	Avg Obs	Bias	R^2	NBias	GrEr
BEIS-2	60	70.6	75.6	-5.0	0.13	0.057	0.171
BEIS-3	60	73.0	75.6	-2.5	0.14	0.024	0.176
BEIS-2	40	63.6	63.8	-0.3	0.25	-0.020	0.224
BEIS-3	40	65.8	63.8	2.0	0.24	-0.056	0.236
BEIS-2	5	55.4	47.9	7.5	0.35	-0.525	0.700
BEIS-3	5	57.3	47.9	9.5	0.35	-0.577	0.732

Daily Max O_3 in 12-km grid
[Jun 21-30, 1996]

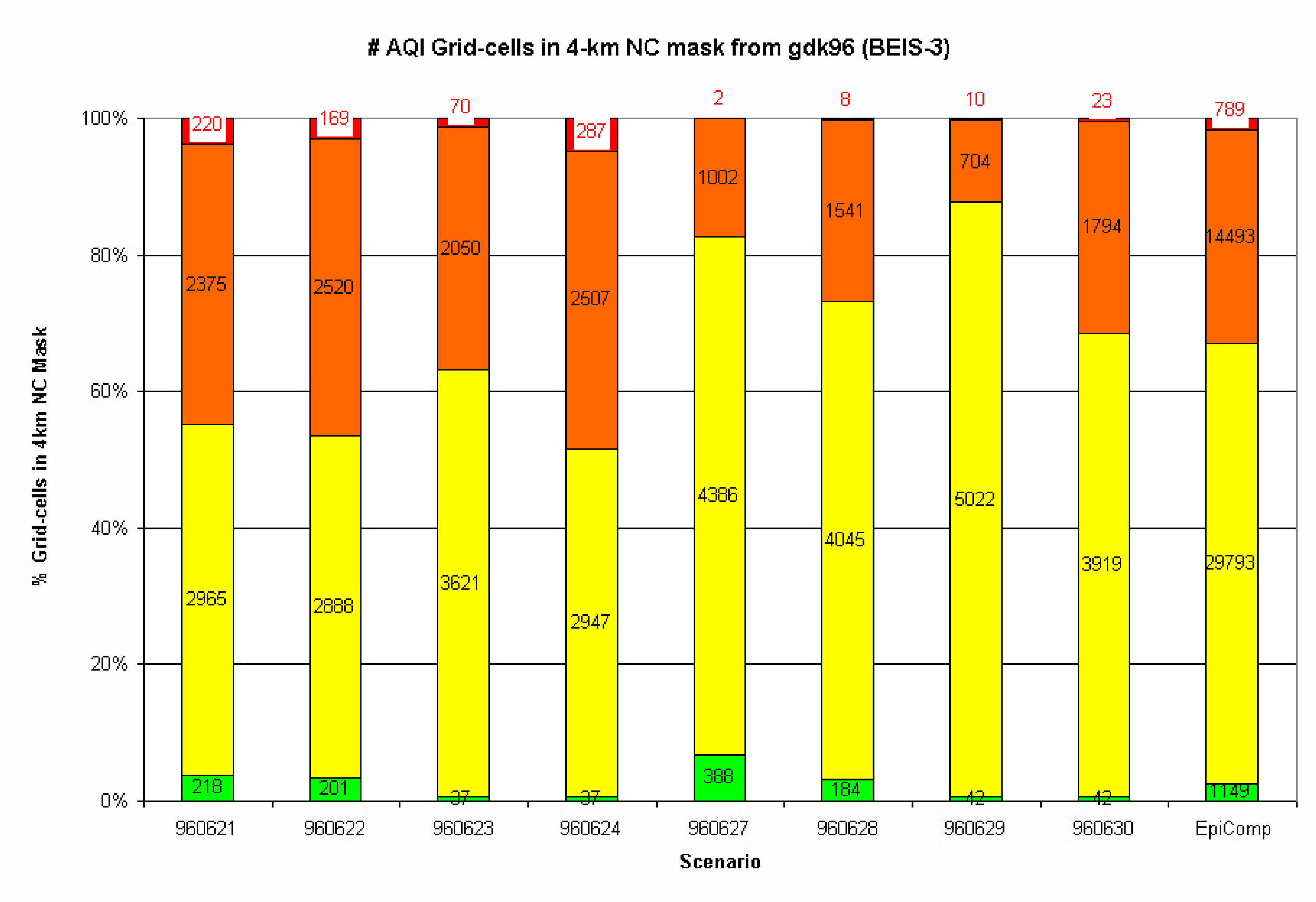




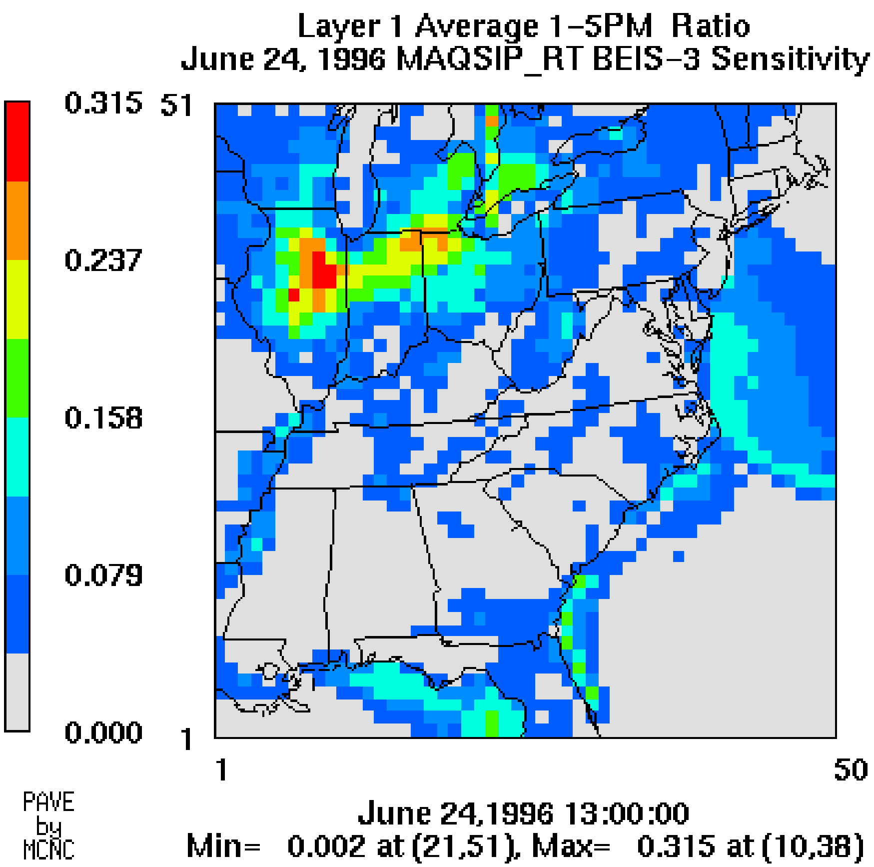
8-h AQI Counts from BEIS-2 Simulation



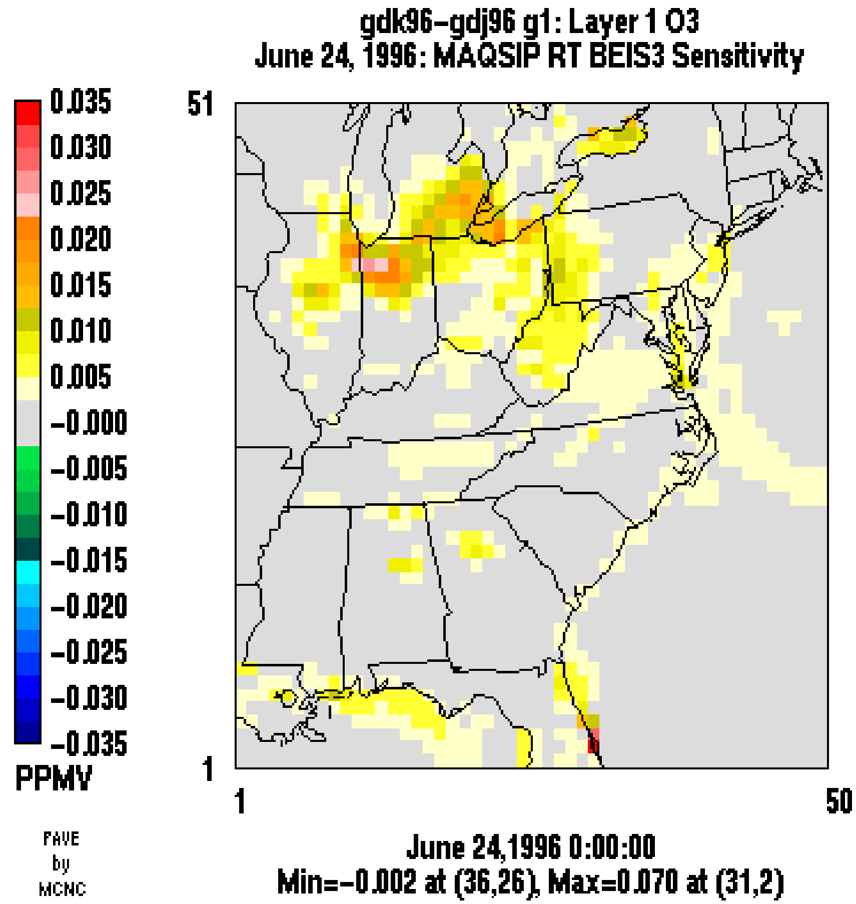
8-h AQI Counts from BEIS-3 Simulation



Loss of MEOH / Prod of FORM



Diff in Daily 8hr Max O3



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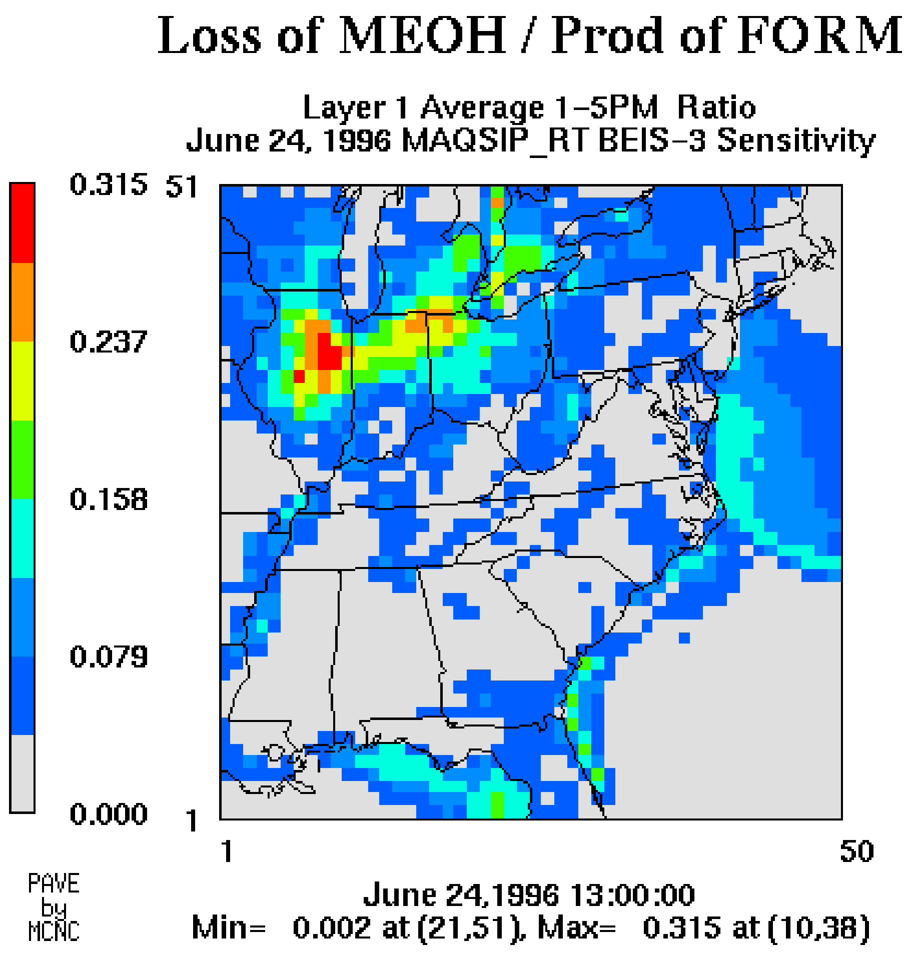
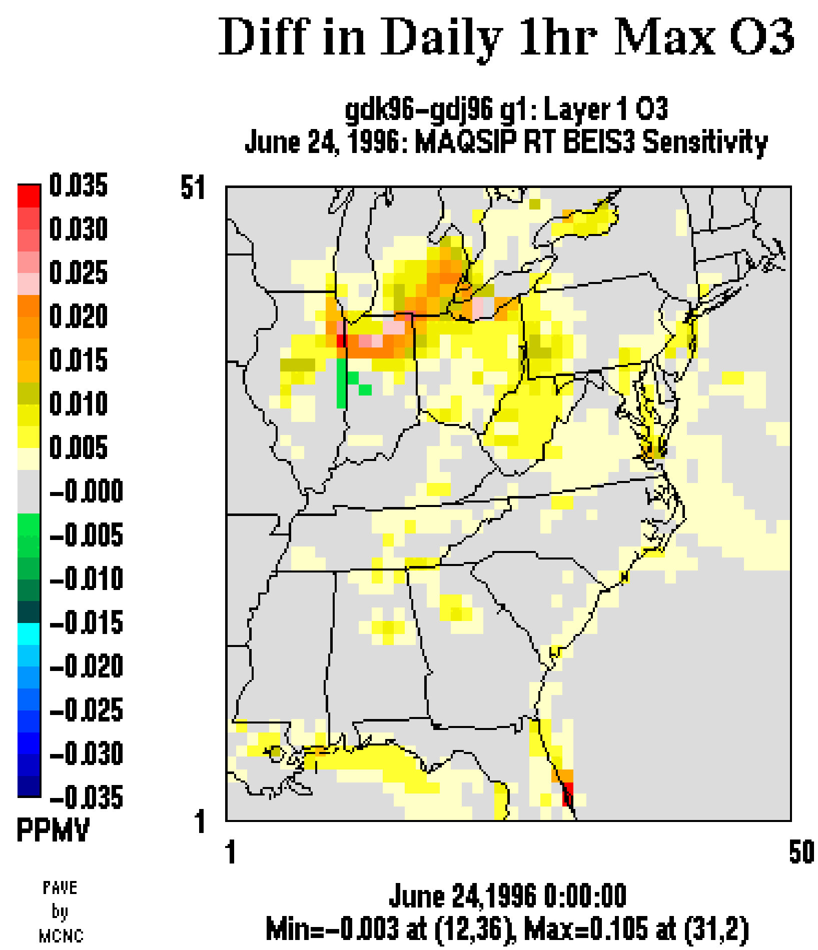
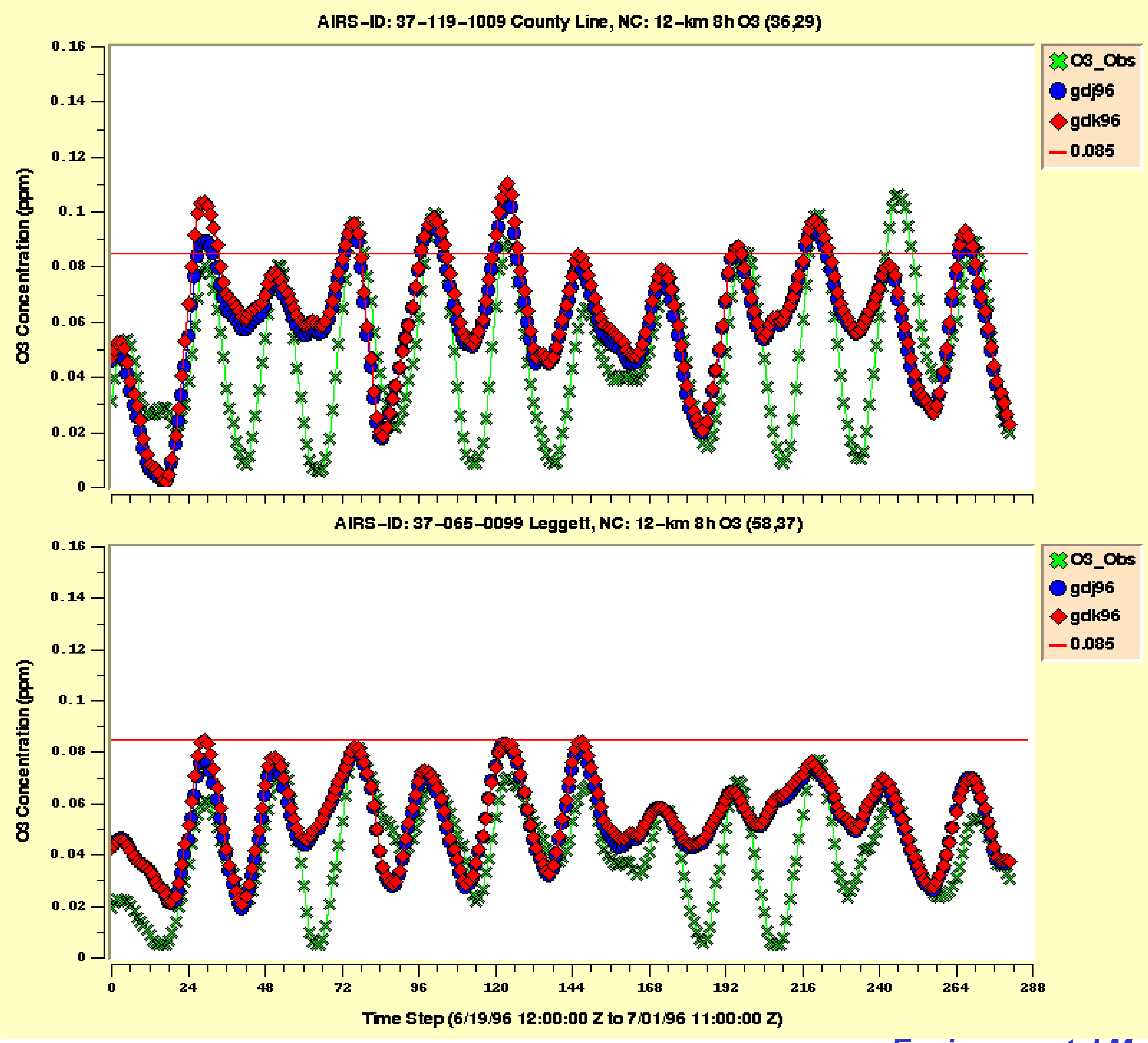

Loss of MEOH / Prod of FORM
Layer 1 Average 1-5PM Ratio
June 24, 1996 MAQSIP_RT BEIS-3 Sensitivity
0.315
0.237
0.158
0.079
0.000
51
1
1
50
PAVE by MCNC
June 24,1996 13:00:00
Min= 0.002 at (21,51), Max= 0.315 at (10,38)


Diff in Daily 1hr Max O3
gdk96-gdj96 g1: Layer 1 O3
June 24, 1996: MAQSIP RT BEIS3 Sensitivity
0.035
0.030
0.025
0.020
0.015
0.010
0.005
-0.000
-0.005
-0.010
-0.015
-0.020
-0.025
-0.030
-0.035
PPMV
PAVE by MCNC
51
1
1
50
June 24,1996 0:00:00
Min=-0.003 at (12,36), Max=0.105 at (31,2)

Impacts of Biogenic Emissions Estimates from BEIS-3



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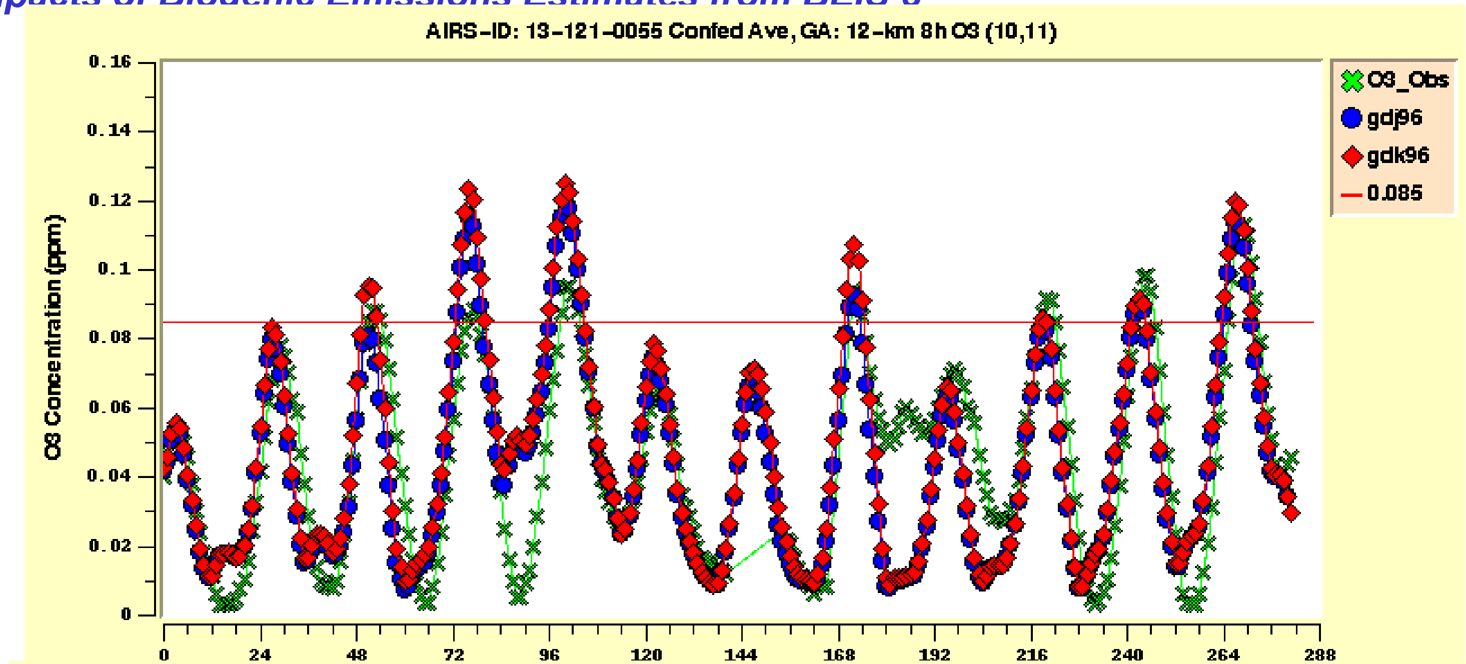
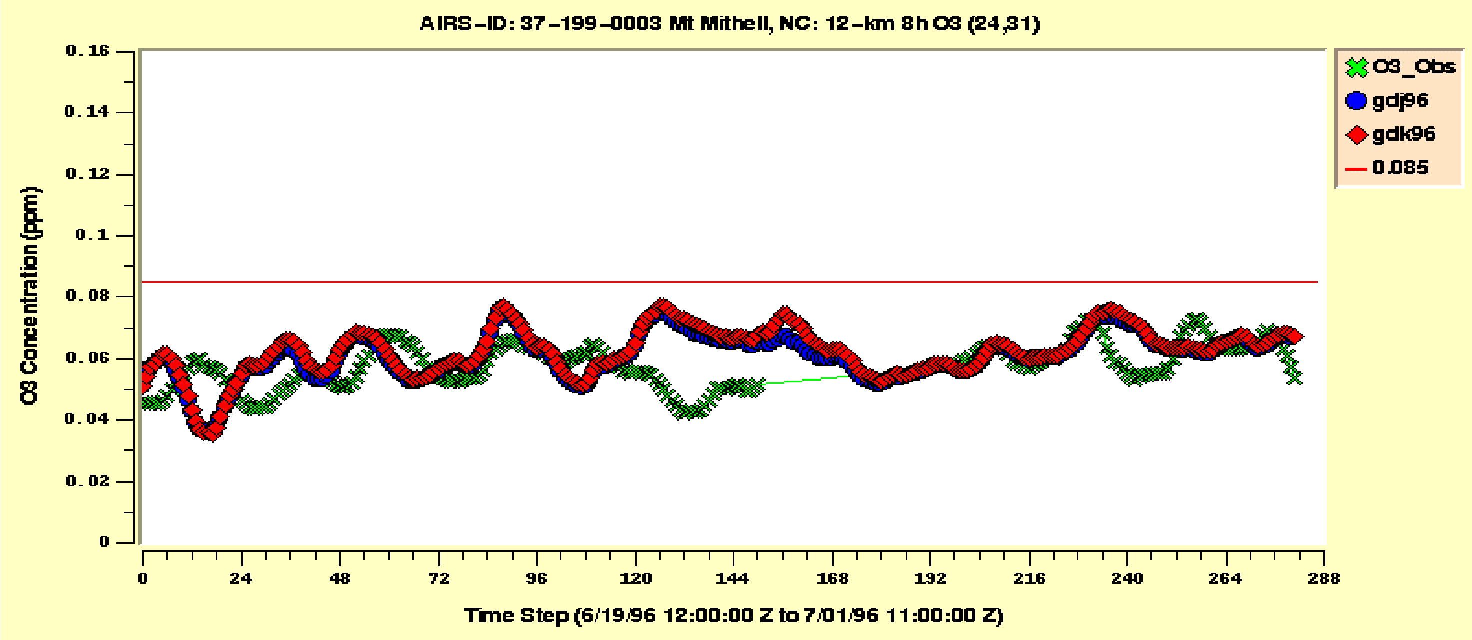
Impacts of Biogenic Emissions Estimates from BEIS-3





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Discussion

- **Sensitivity study performed to compare BEIS-2 vs. BEIS-3 emissions estimates in MAQSIP**
  - **Biogenic VOCs increase due to large amounts of MEOH from BEIS-3**
  - **MAQSIP CB-4 chemistry updated to treat explicit alcohol oxidation**
  - **Average 1-h O_3 increases by 1-3 ppb in all grids**
  - **Leads to better model performance at a 60ppb threshold**
  - **Some correlation seen in predicted ozone increases due to addition of radical sources from alcohol oxidation products**
  - **Comparison of daily maxima of 1-h and 8-h O_3 shows a consistent positive bias using BEIS-3 at all observed locations**
    - **However, not much bias seen based upon monitor location type (Urban/Rural/Suburban)**

Future Work

- **Continue IRR-type analyses**
- **Use actual deposition velocities for MEOH/ETOH in MAQSIP instead of PAR surrogates**
- **Continue evaluation using further updates to BEIS-3**
- **Perform sensitivities in other episodes/domains**

Acknowledgments

- **North Carolina Department of Air Quality**

Website for Results

- **http://www.emc.mcnc.org/projects/NCDAQ/PGM/results/basecase96/gdk96/index.html**