8-hr Ozone Simulation: Further Work

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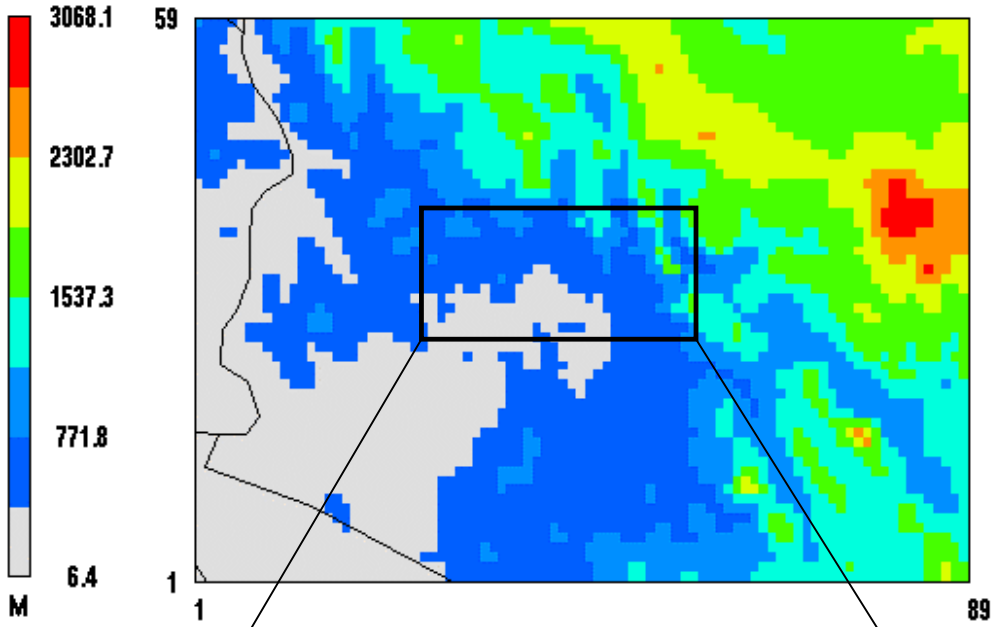
Summary of March 3, 2003 Presentation

- MM5 simulation for meteorology
- Validation of MM5
- Preparation of pollutant inventory
  - ✓ MAG domain
  - ✓ Outer domain
- Models-3/CMAQ
- Model Validation
- 8-hr Ozone boundaries
- Socio-Economic analysis
- Projected ‘2018 inventory

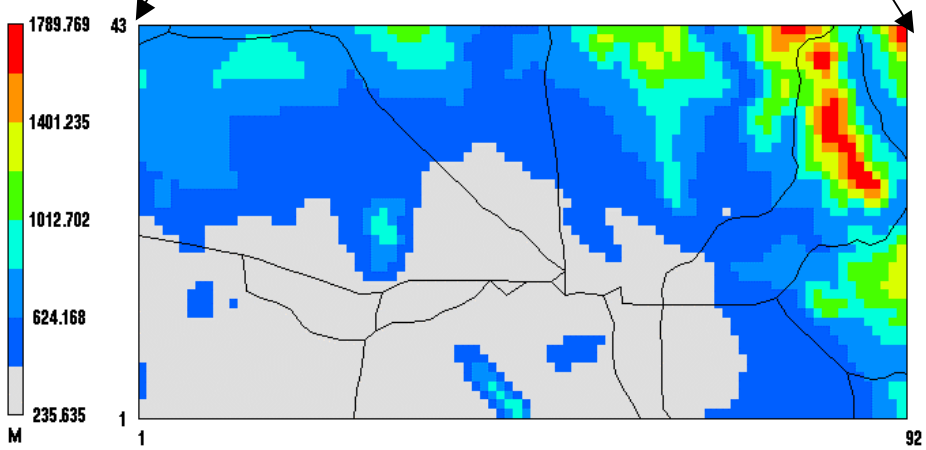
Topography

Extended domain with 6 km resolution

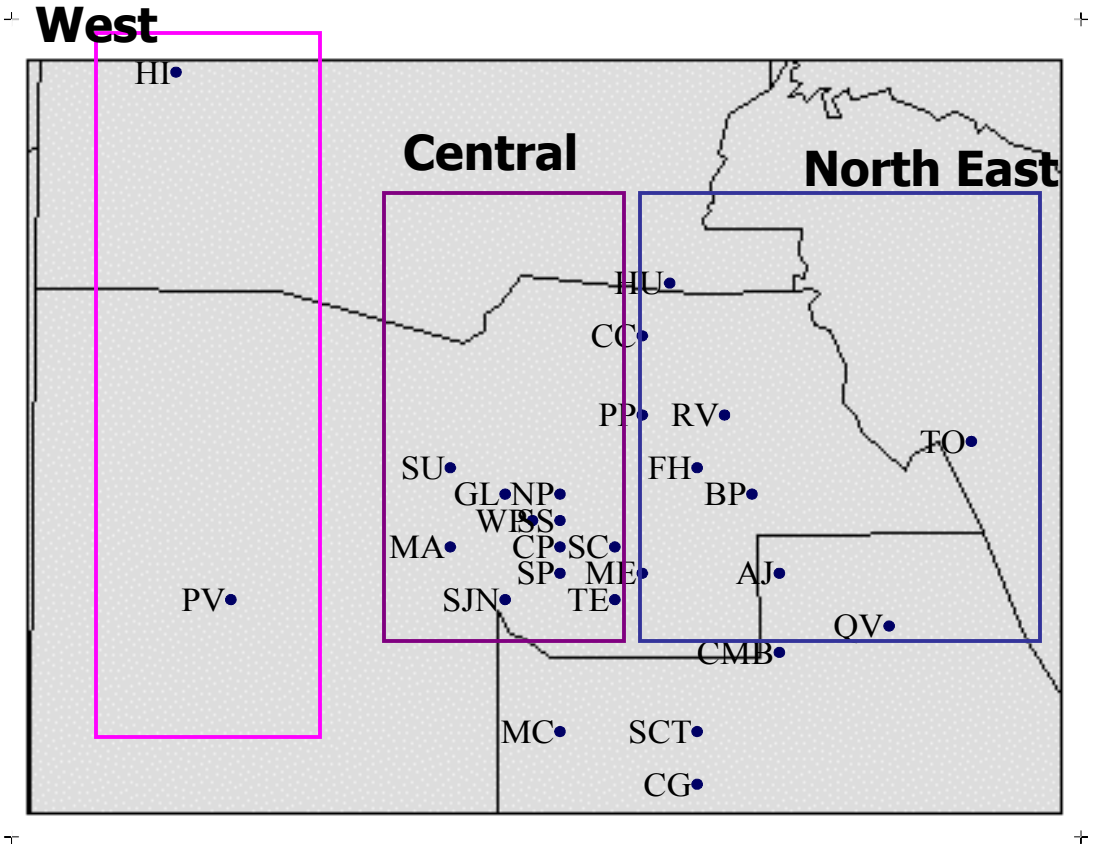


Terrain Height

MAG Domain



Monitor Areas



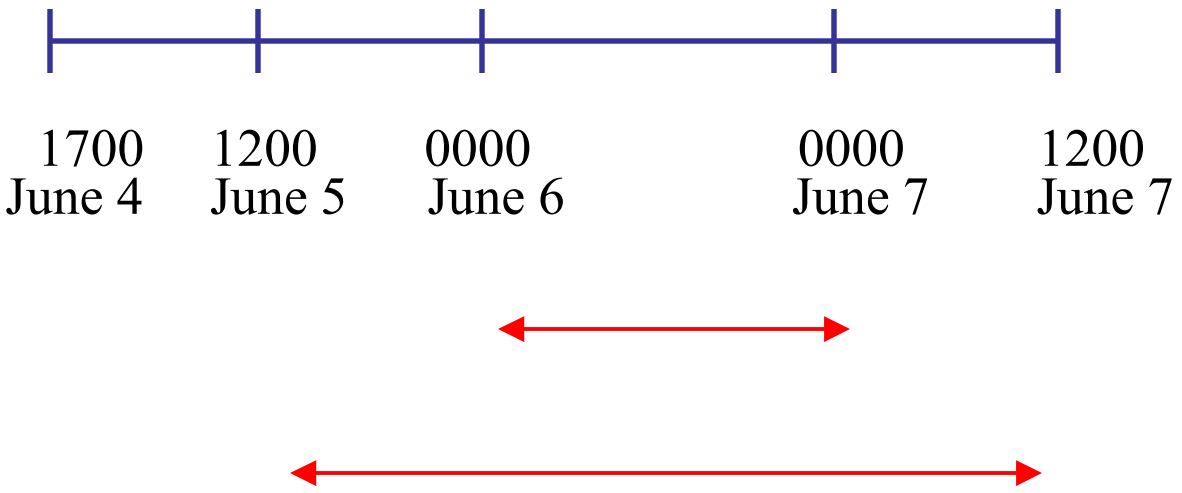
Design Days

- June 6th
  - High ozone in the Northeast Area (Fountain Hills, Blue Point Bridge, Rio Verde, Tonto)

- July 12th
  - High ozone at Humboldt Mt.
  - Elevated values in the Central Area

Design of Numerical Simulation

- **Study Case: 19 hrs of spin-up for MM5**
  - →1700 LST June 4 – 1700 LST June 7, 2002
  - →1700 LST July 10 – 1700 LST July 13, 2002



Models-3/CMAQ (Community Multi-scale Air Quality)

Meteorology

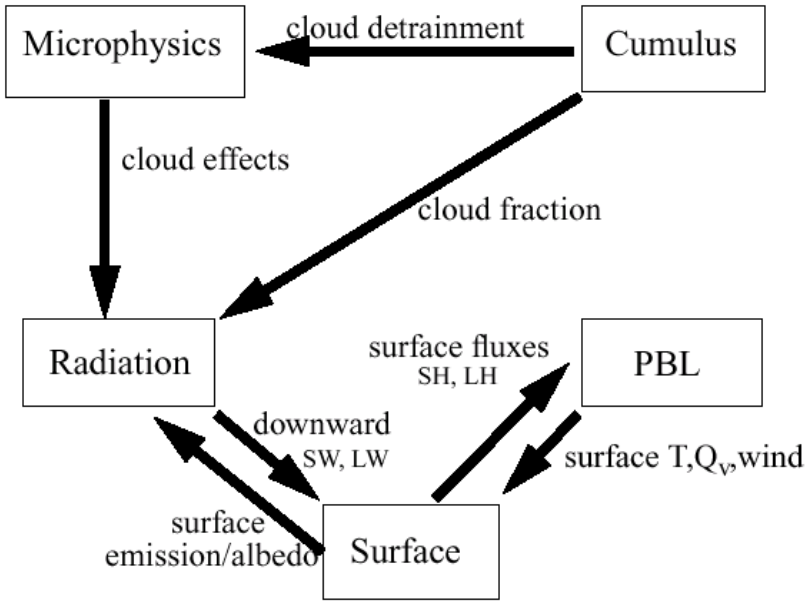
Emission

One-Atmosphere
(from Regional to Urban scale)

- Chemical reactions
- Advection & Diffusion
- Aerosol dynamics & chemistries
- Clouds effects
- Plume-in-Grid
- Dry/Wet depositions

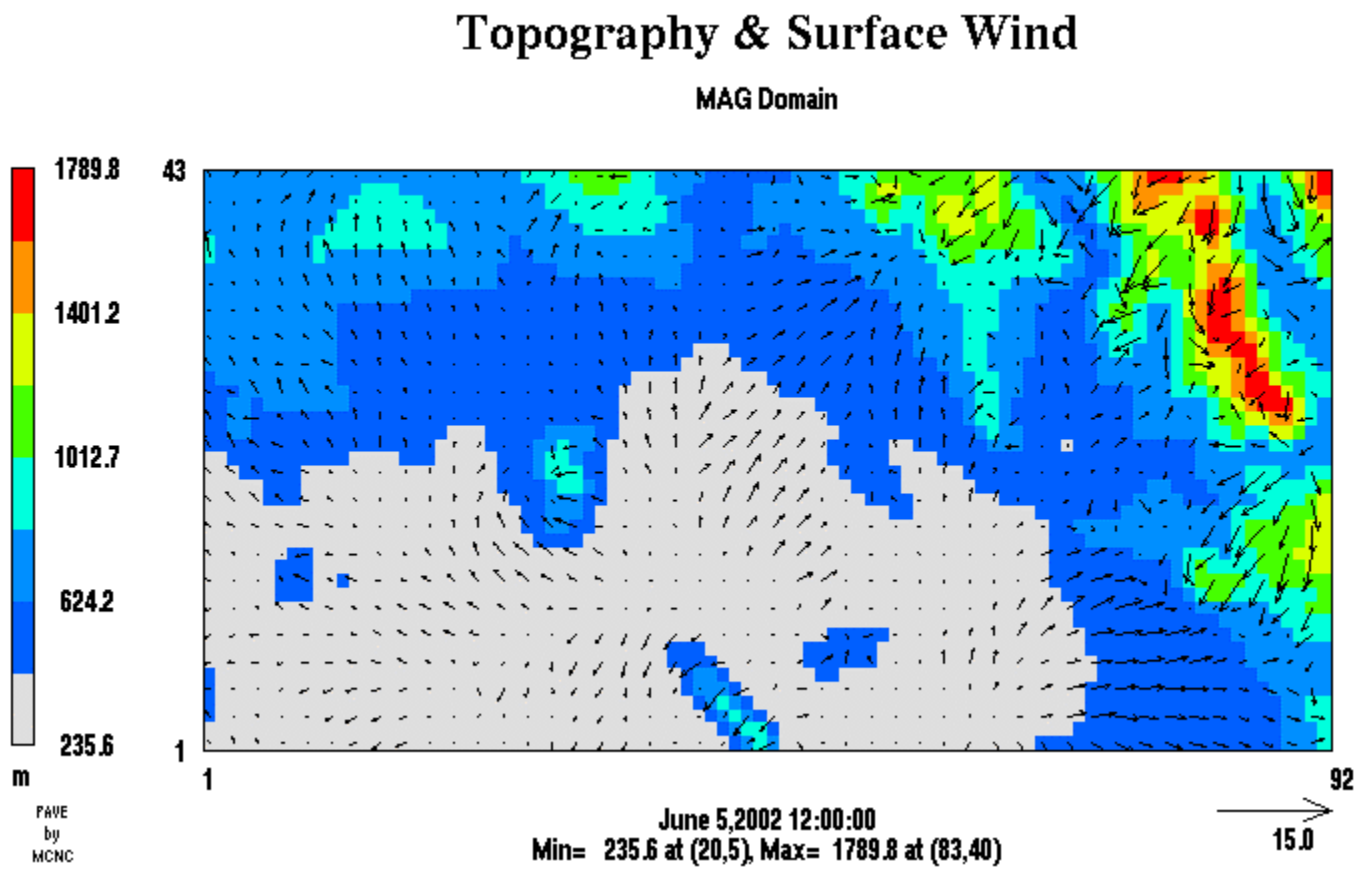
The Fifth-generation Penn State/NCAR Mesoscale Model (MM5)

- Terrain following σ - coordinate
- Non-hydrostatic dynamics
- Four-dimensional data assimilation
- Multiple nest capability
- Physics



Ground Level Wind Field

1200 LST June 5th – 1200 LST June 7st



SMOKE

Sparse Matrix Kernel Emissions Modeling System

SMOKE

- Emissions processing system for area, mobile and point sources.
- Biogenic emissions modeling.
- Provides specialized emission inputs for air quality models: gridded hourly 3-dimensional.

SMOKE Input Data

Emissions Inventory

Western Regional Air Partnership (WRAP)
1996 Base Case Scenario
County data for area, mobile and point source emissions
Inventory species: NO_x CO NH_3 SO_2 VOC

Meteorological Data

MM5 simulation results for episode days June 4-7, 2002 & July 10-13, 2002

SMOKE Input Data

Land Use Data

U.S. EPA's Biogenic Emissions Landcover Database (BELD3),1 km x 1km resolution, 230 land use types

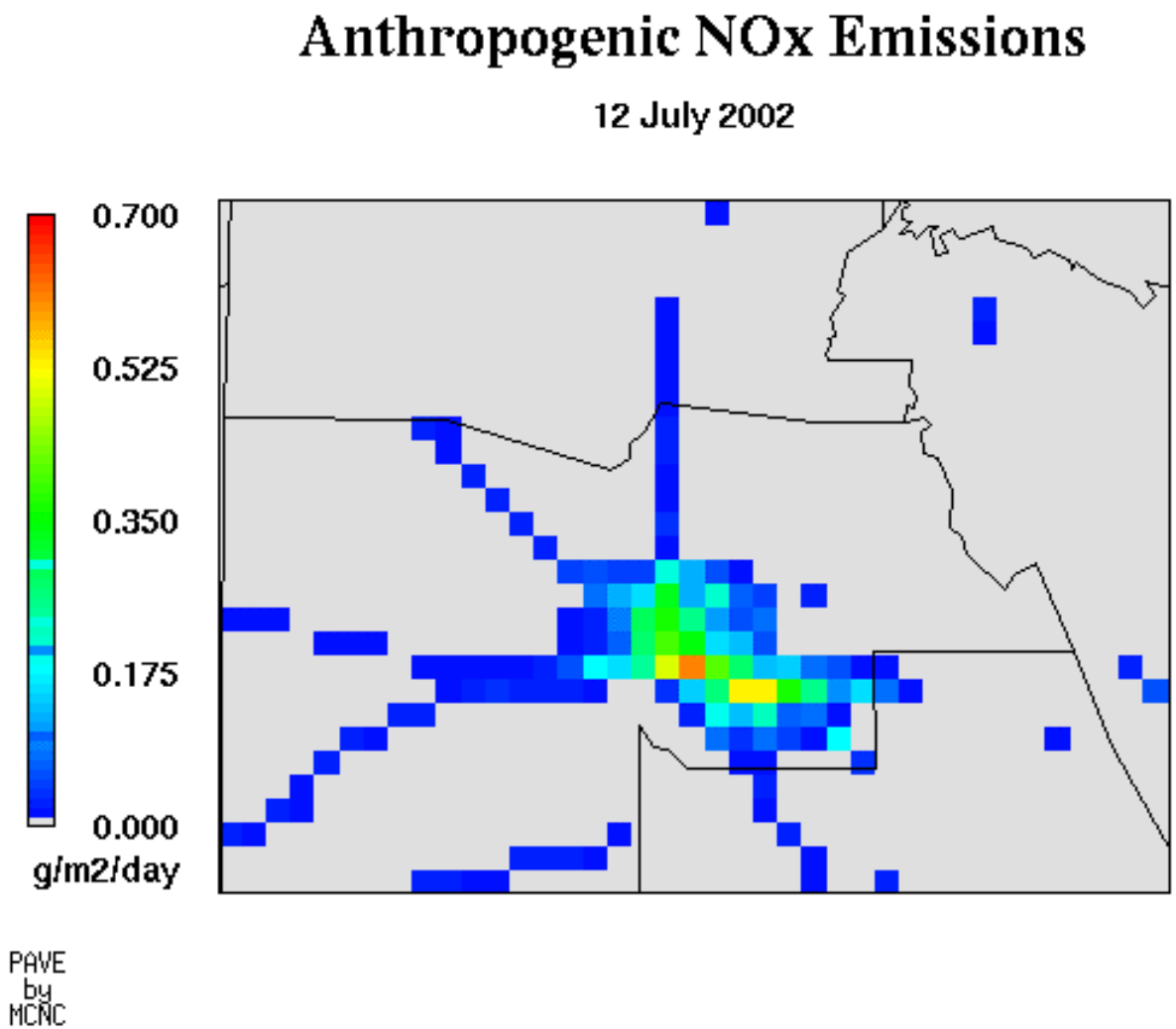
ftp://ftp.epa.gov/amd/asmd/beld3

Spatial Surrogate Data

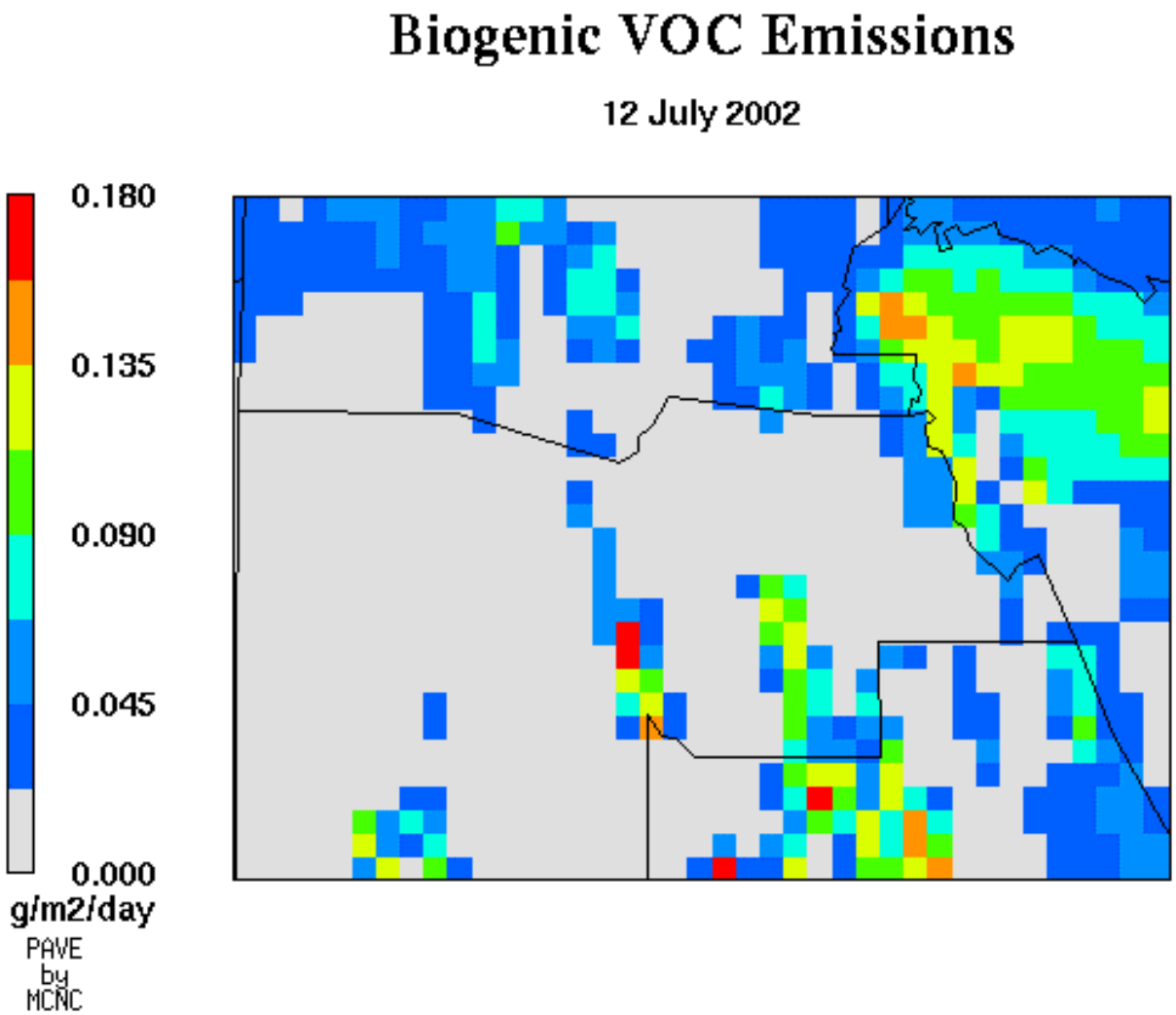
U.S. EPA's 4km Spatial Surrogate Data covering the United States

http://www.epa.gov/ttn/chief/emch/spatial/

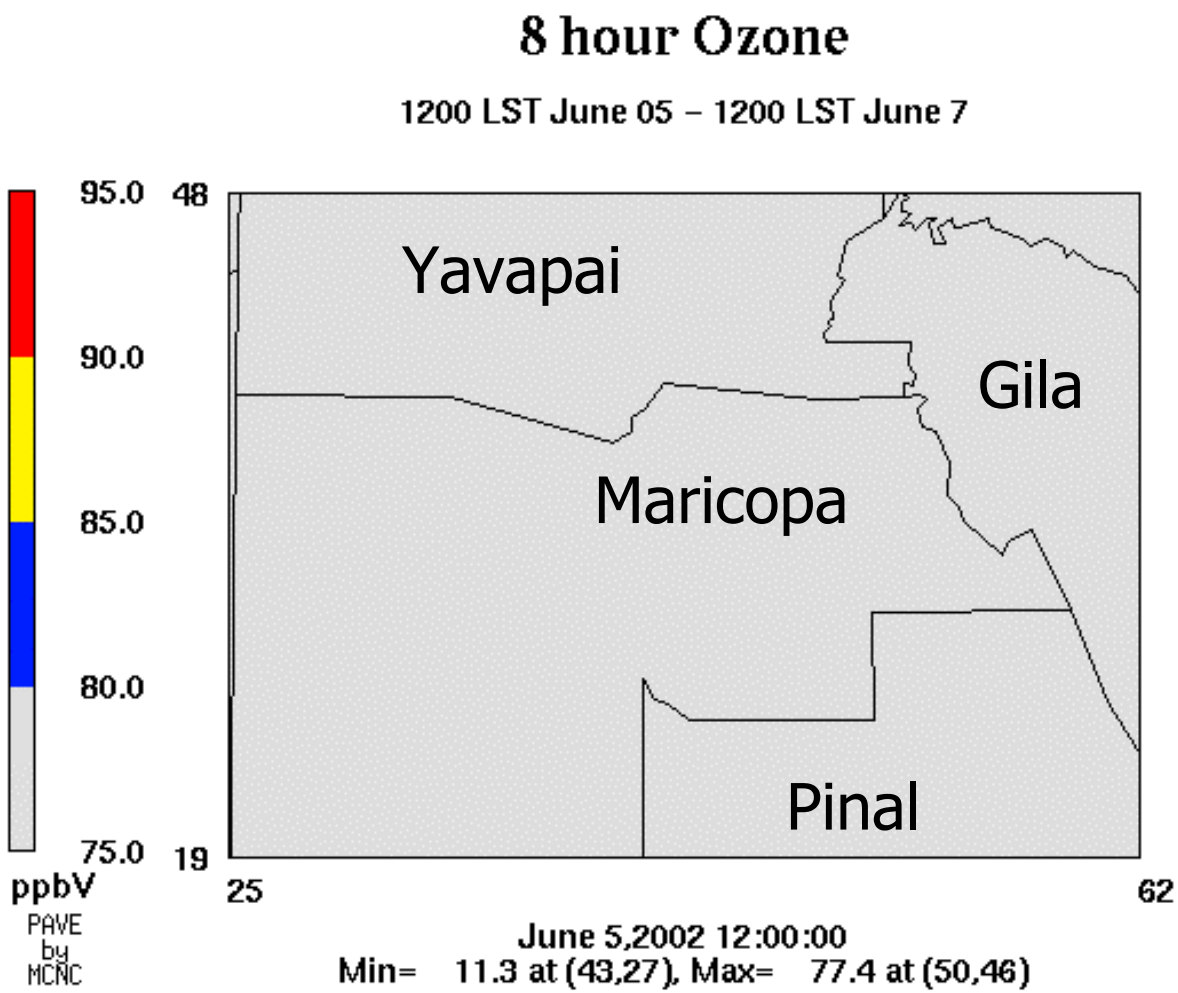
Smoke Results



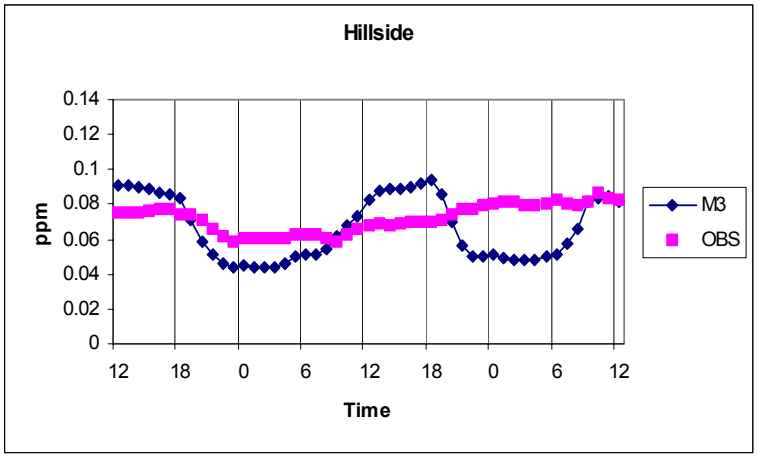
Smoke Results

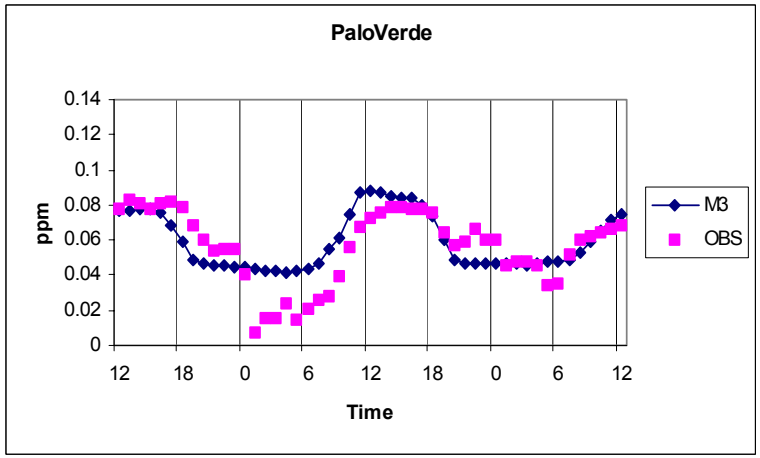


8hr Averaged Ozone: June 6th

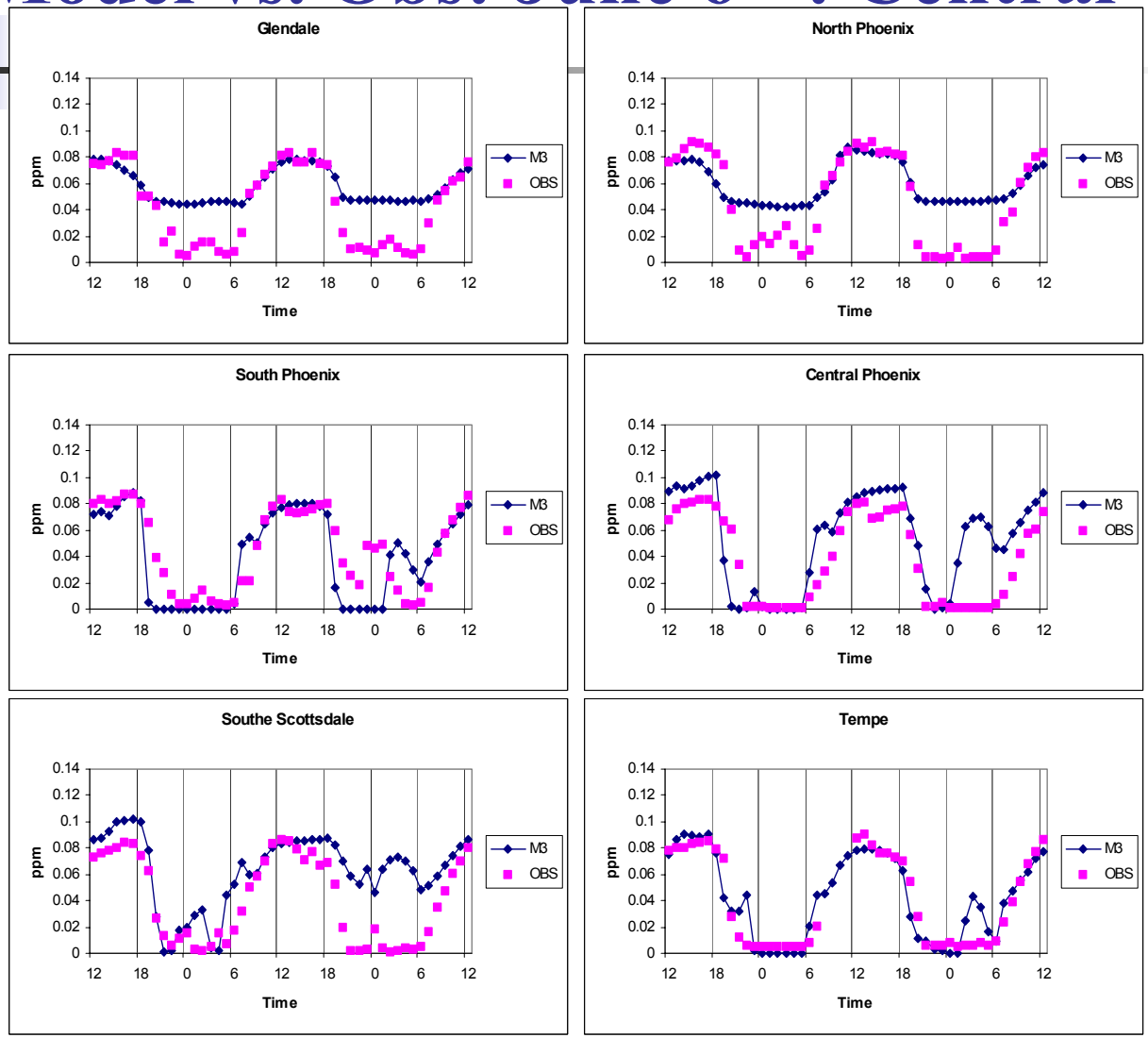


Model vs. Obs: June 6th : West

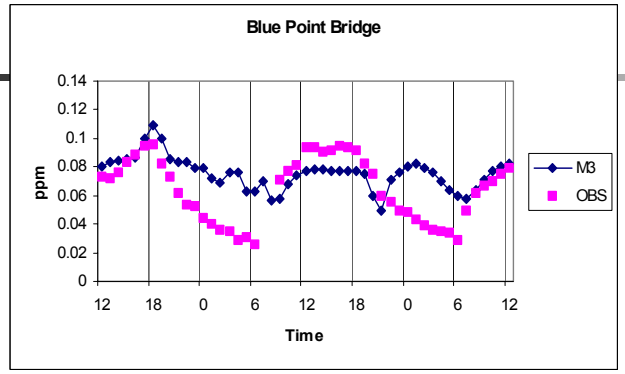


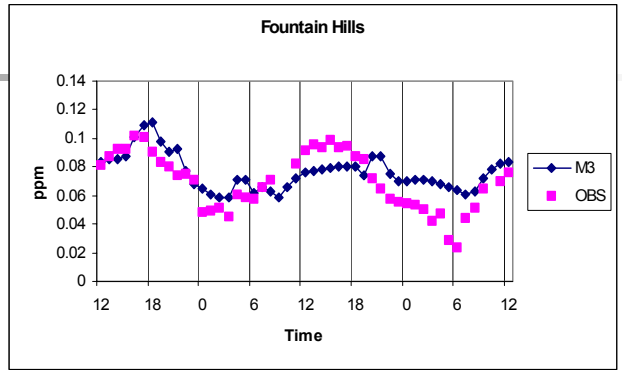


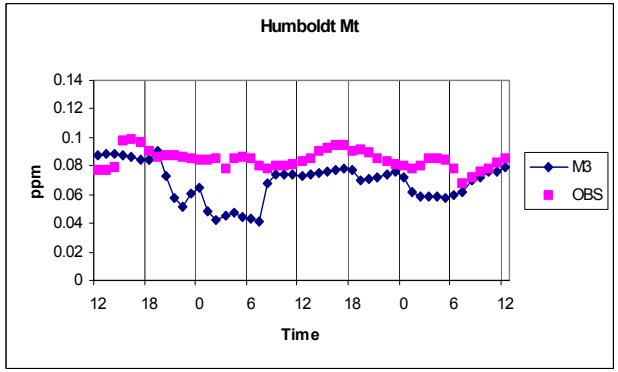
Model vs. Obs: June 6th : Central

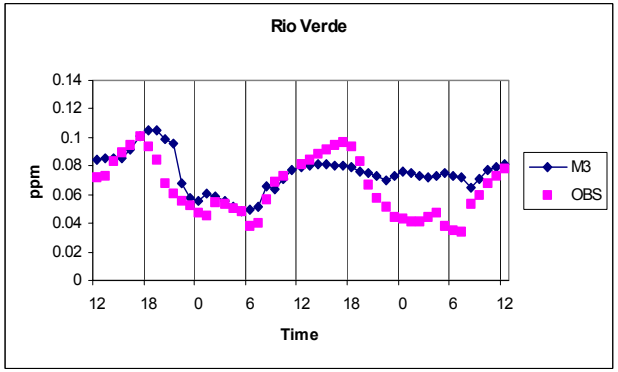


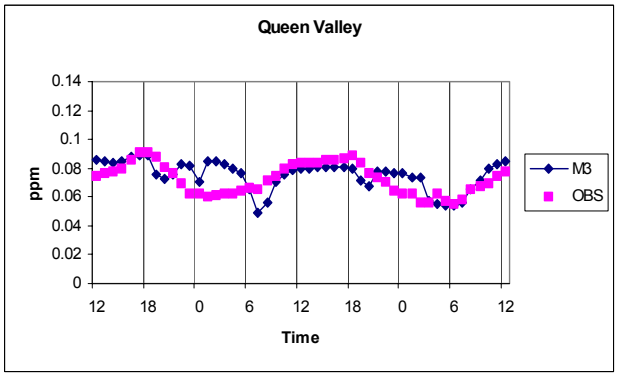
Model vs. Obs: June 6th : Northeast

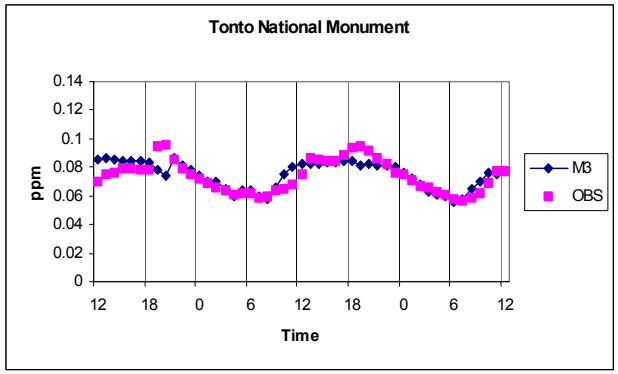




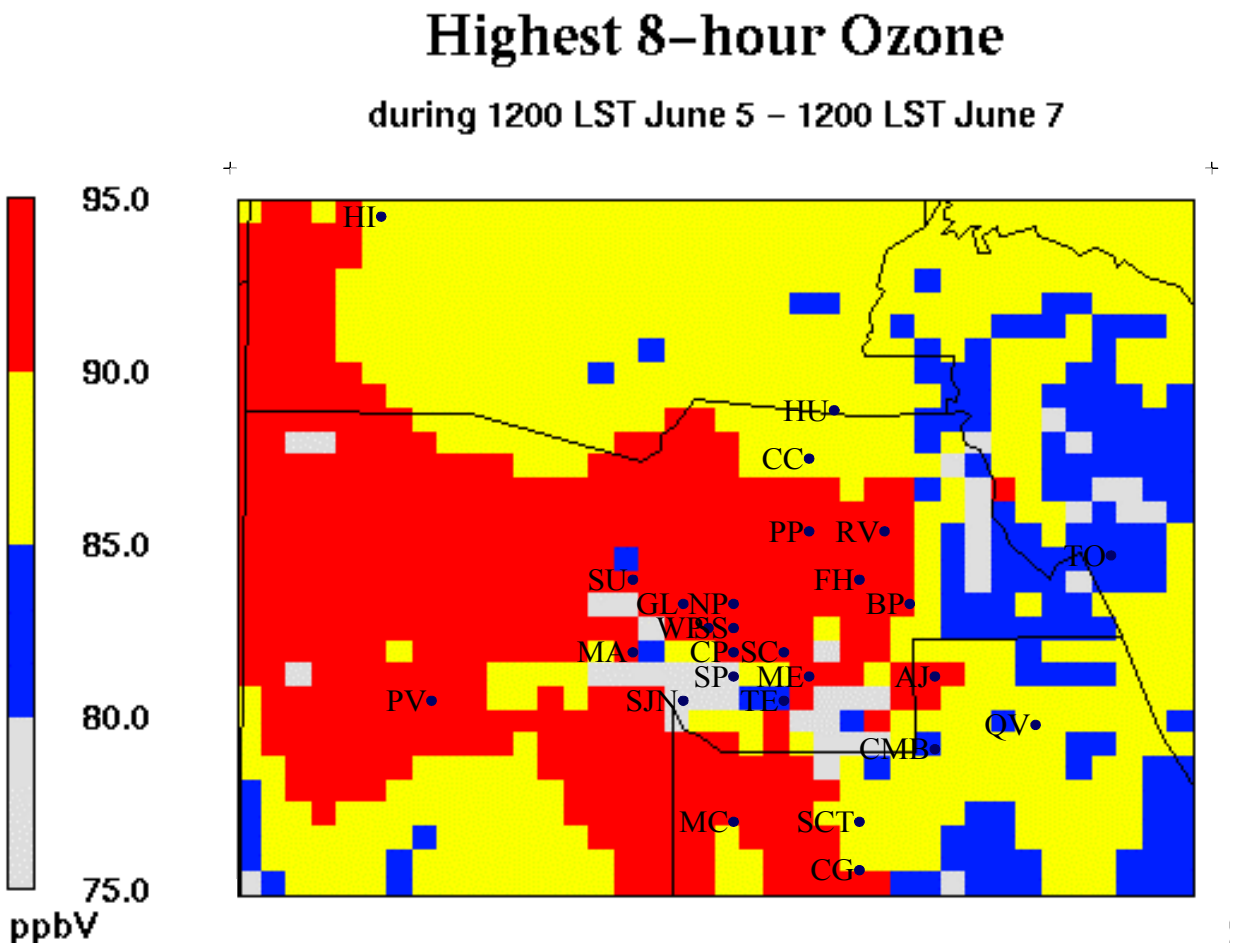




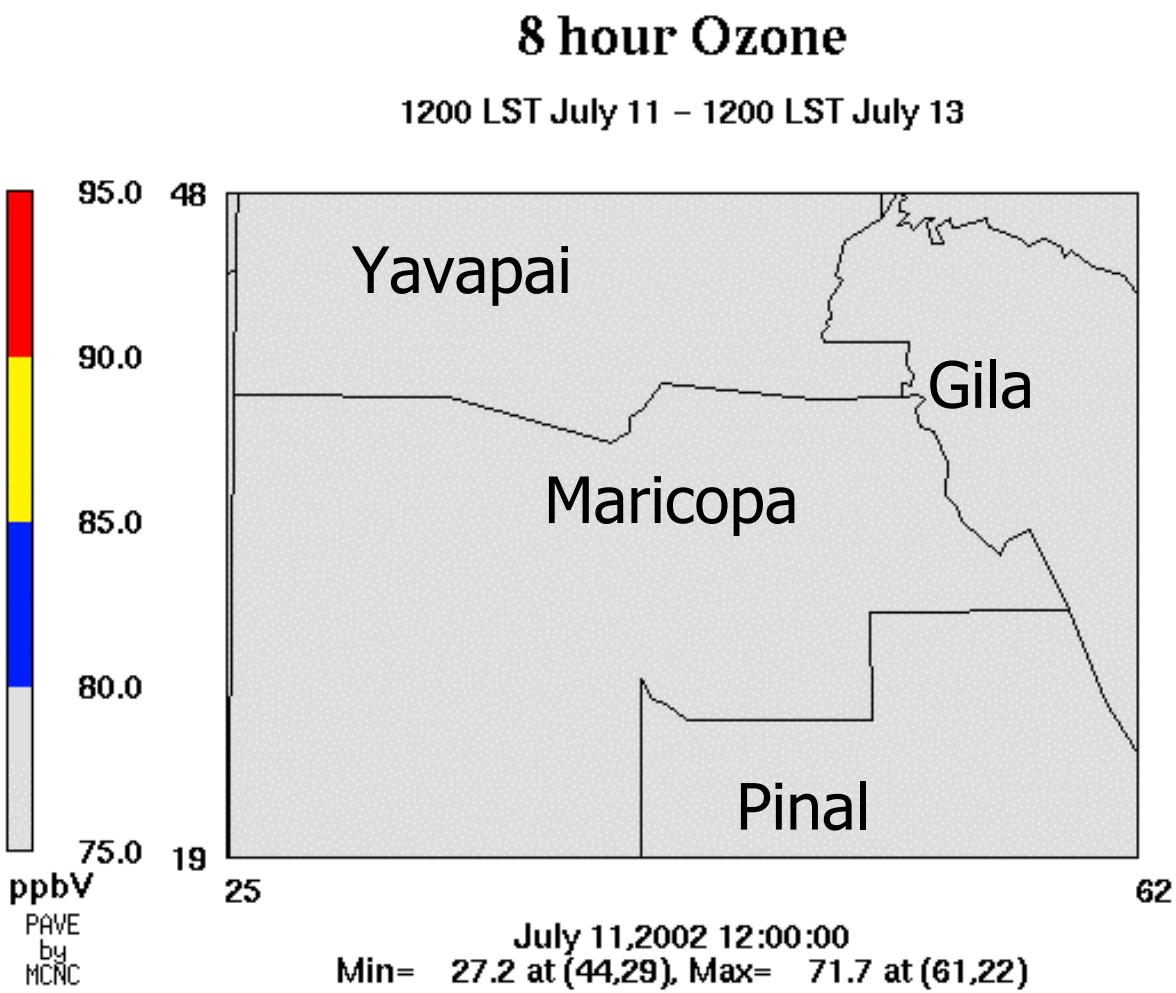




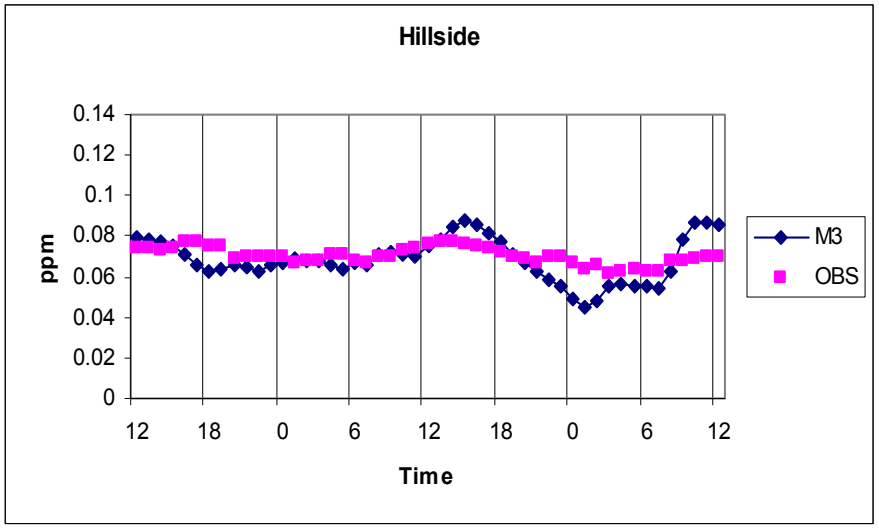
Highest 8hr Ozone: June 6th

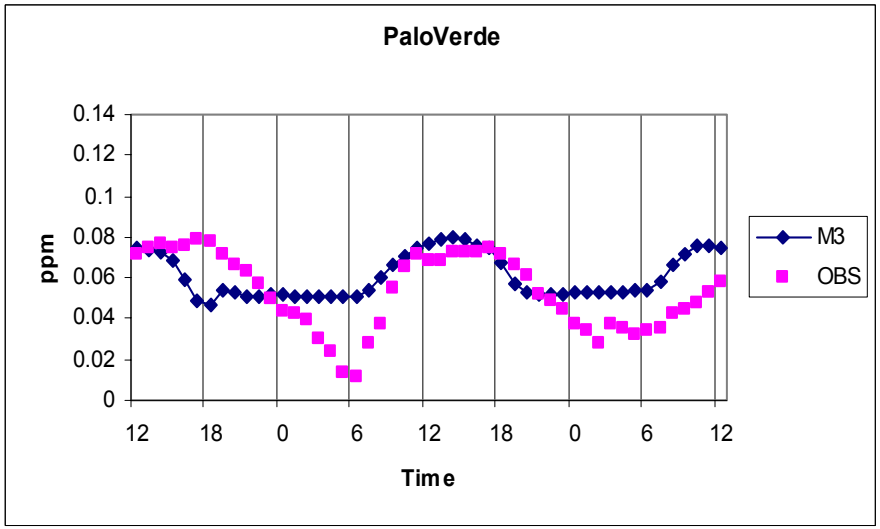


8hr Averaged Ozone: July 12th

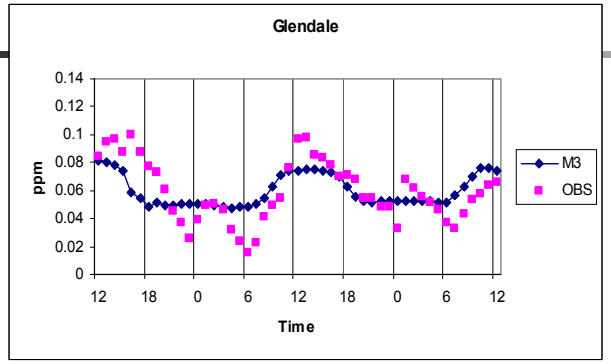


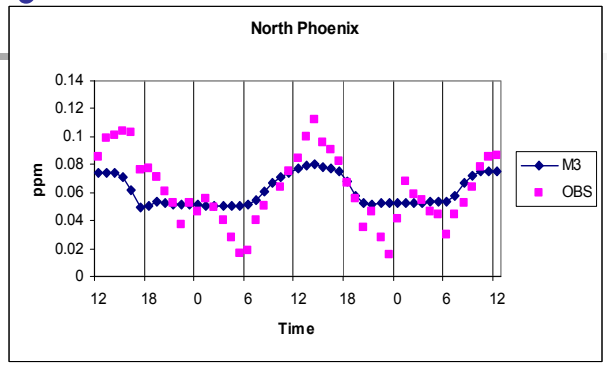
Model vs. Obs: July 12th : West

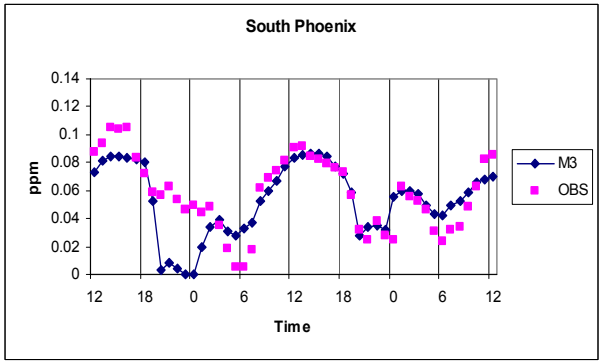


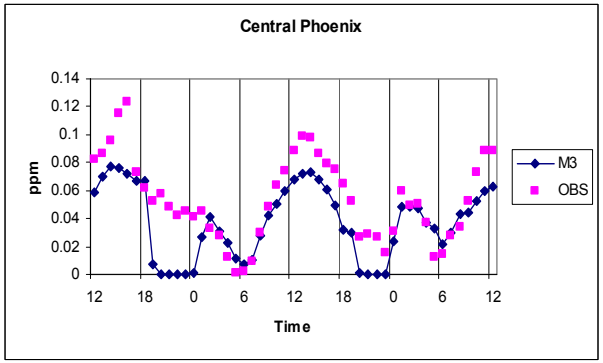


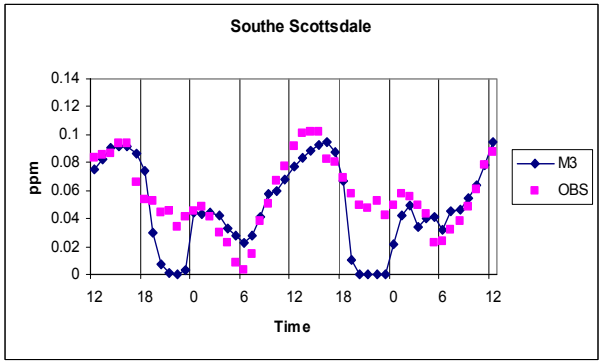
Model vs. Obs: July 12th : Central

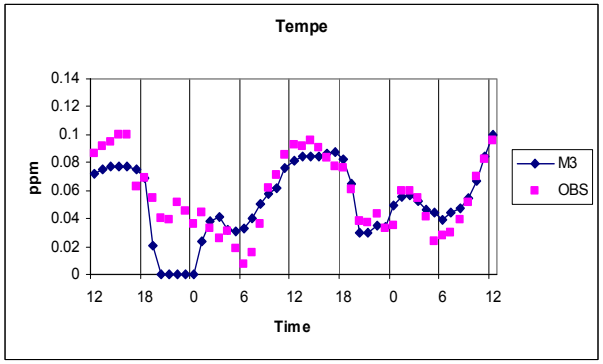




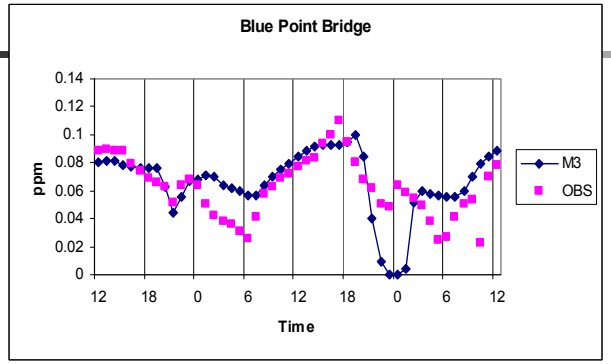


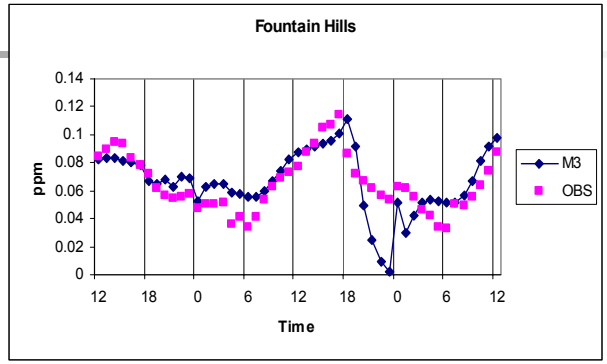


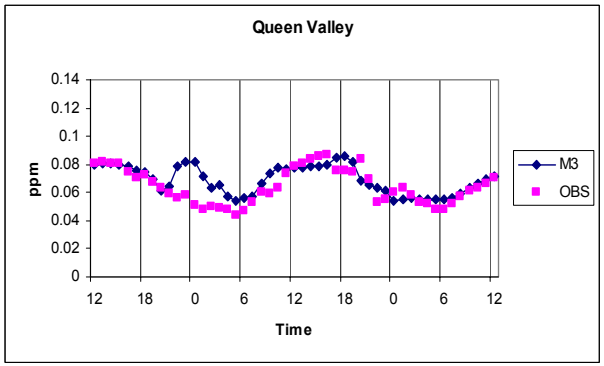


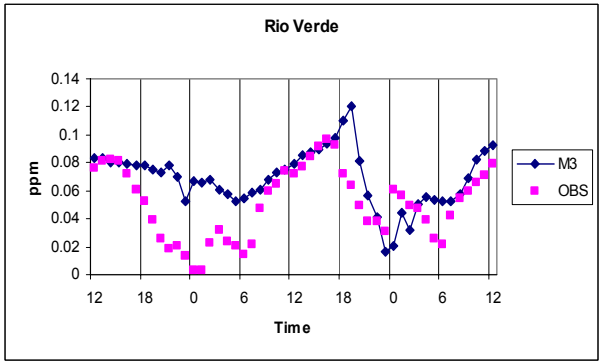


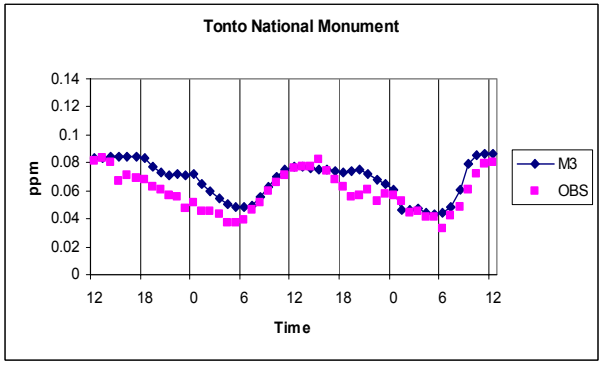
Model vs. Obs: July 12th : Northeast

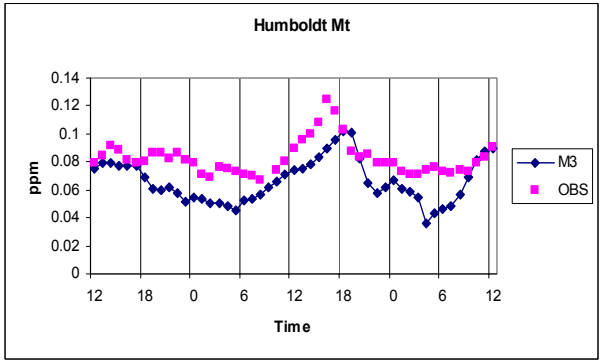




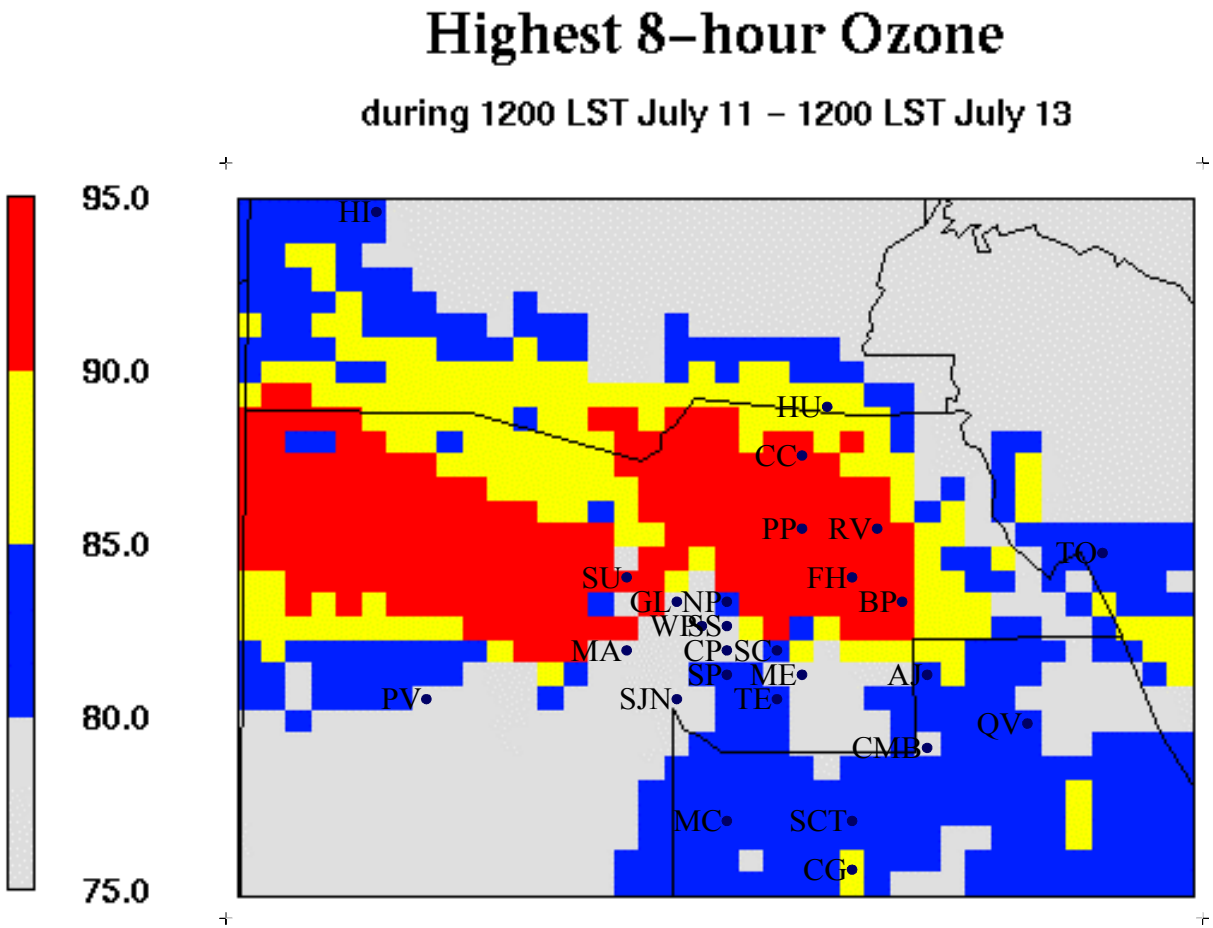








Highest 8hr Ozone: July 12th

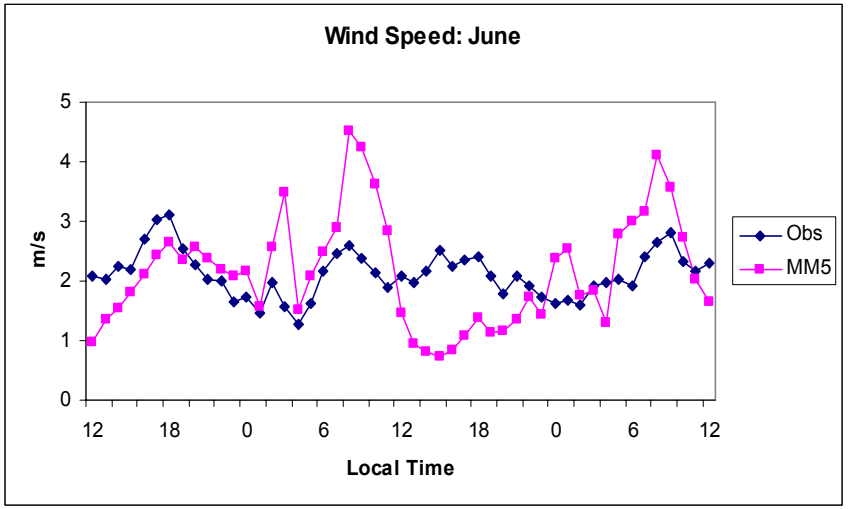


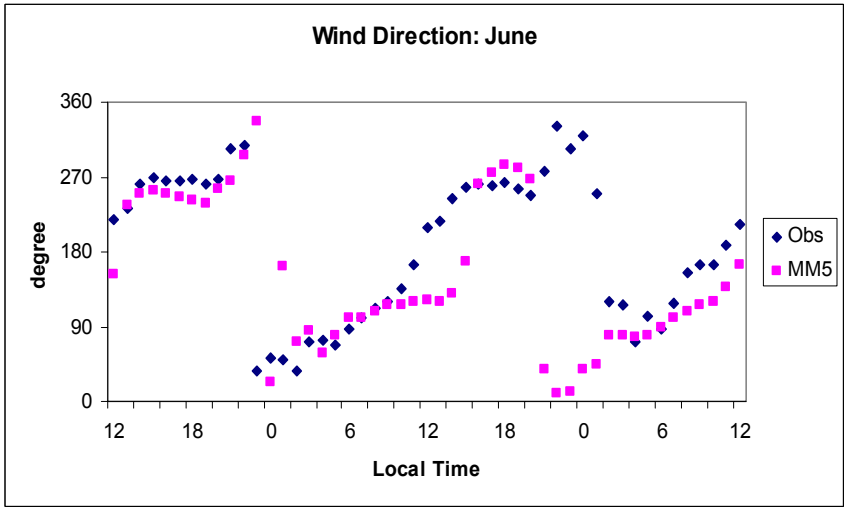
New Work:

Phoenix 8hr ozone simulation:

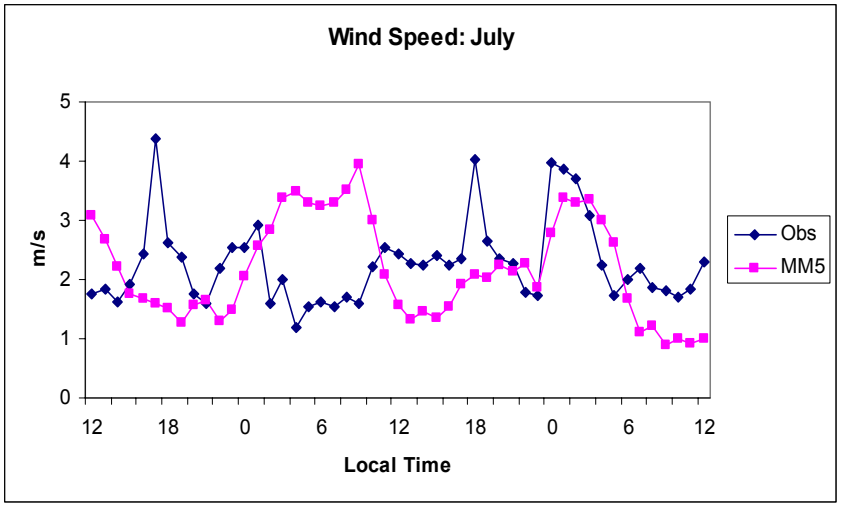
MM5 Validation

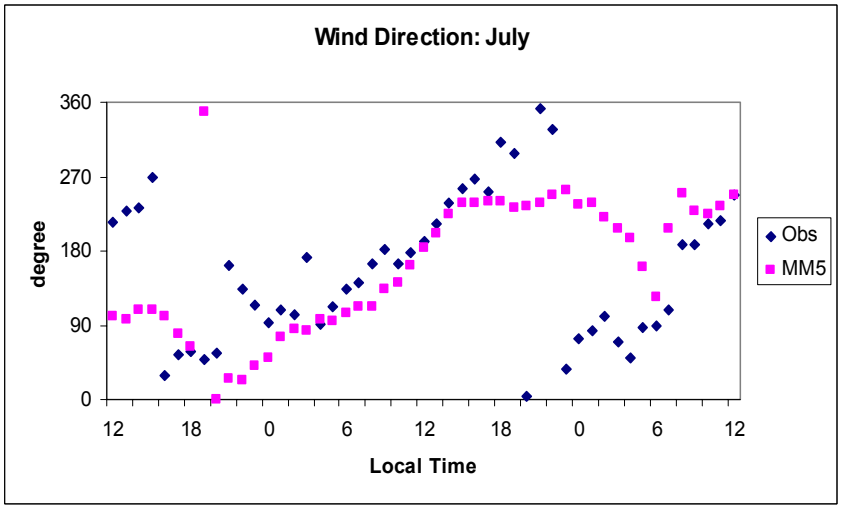
Surface Wind Measurements





Surface Wind Measurements





Performance Measures

- Relative Mean Bias $$\frac{\overline{x_o} - \overline{x_p}}{0.5\left(\overline{x_o} + \overline{x_p}\right)}$$

- Mean Difference $$\overline{x_o - x_p}$$

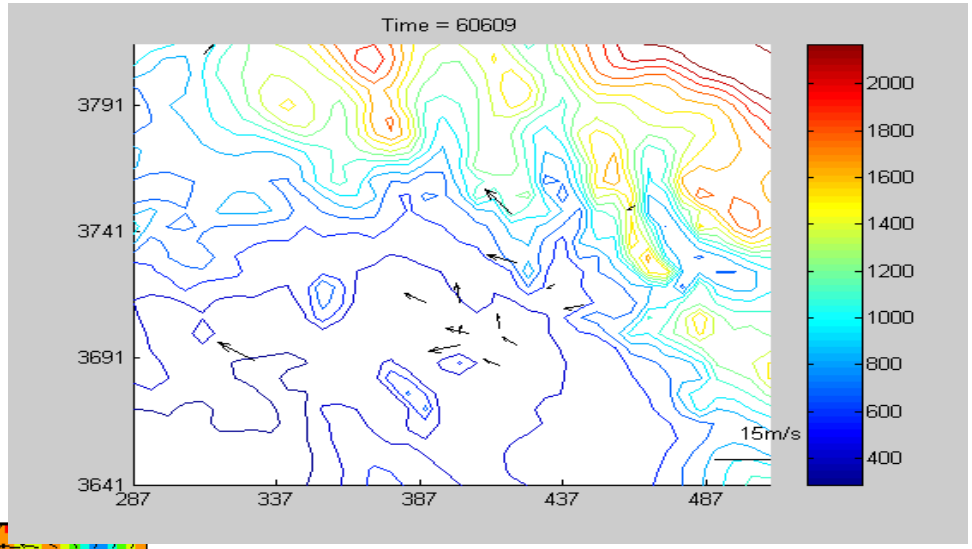
- Index of Agreement $$1 - \frac{\sum\left(x_o - x_p\right)^2}{\sum\left(x_o - \overline{x_o} + x_p - \overline{x_o}\right)^2}$$

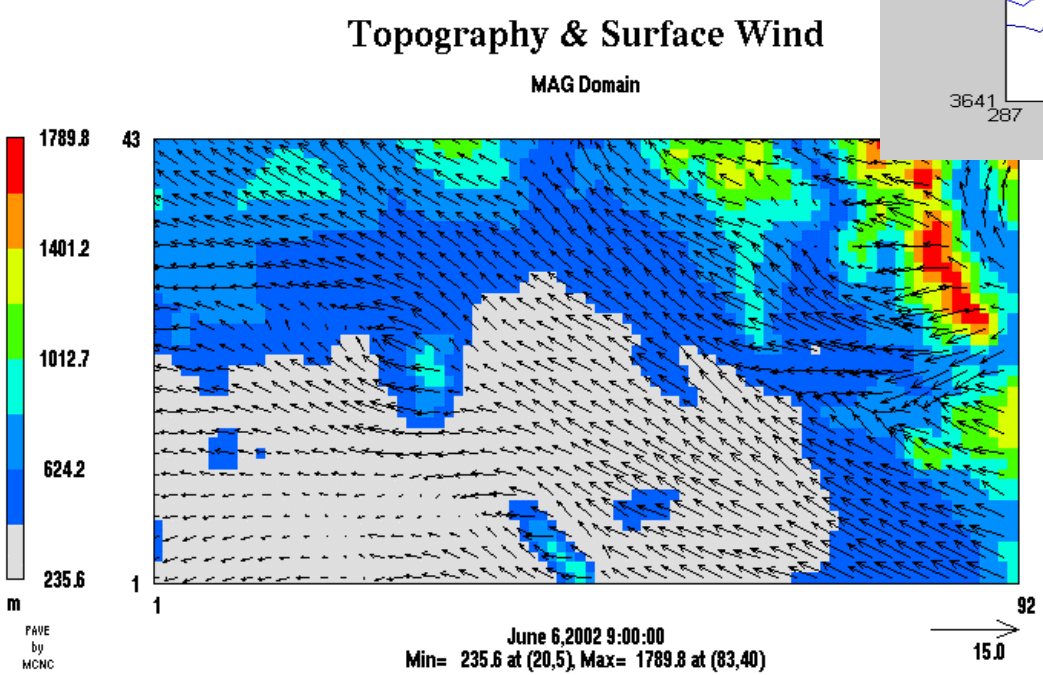
- RMS Vector Error $$\left\{\frac{1}{N}\sum(u_p - u_o)^2 + (v_p - v_o)^2\right\}^{1/2}$$

Model Performance

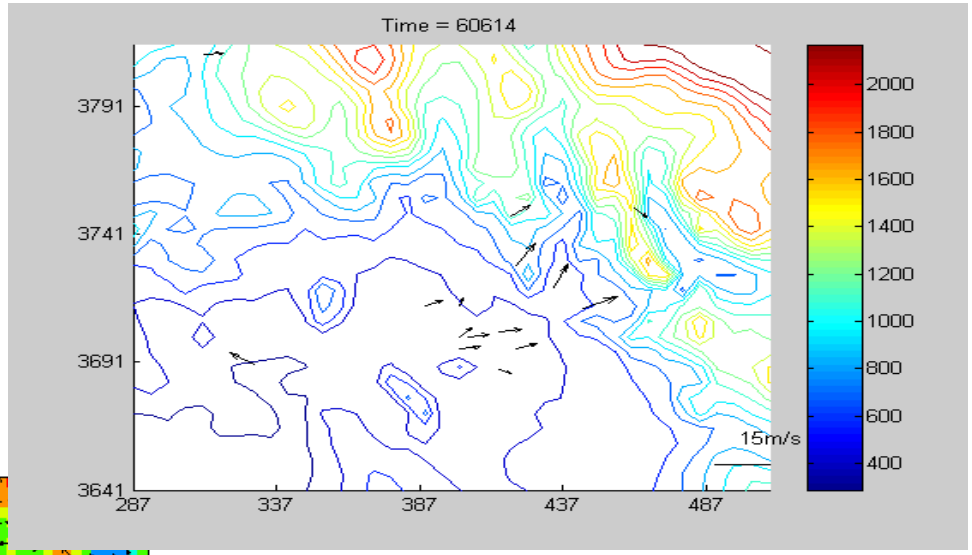
	June WS	June WD	July WS	July WD
Mean of Obs	2.2	192.4	2.4	171.0
STD of Obs	0.9	83.1	1.3	93.8
Mean	2.1	180.3	2.1	146.6
STD of Obs	1.4	109.5	1.2	123.6
Relative Mean Bias	0.0	0.1	0.1	0.2
Mean Difference	0.1	12.1	0.3	24.3
Index of Agreement	0.5	0.9	0.4	0.8
RMSE	1.5	71.5	1.7	92.7
RMS Vector Error	2.3		3.3	

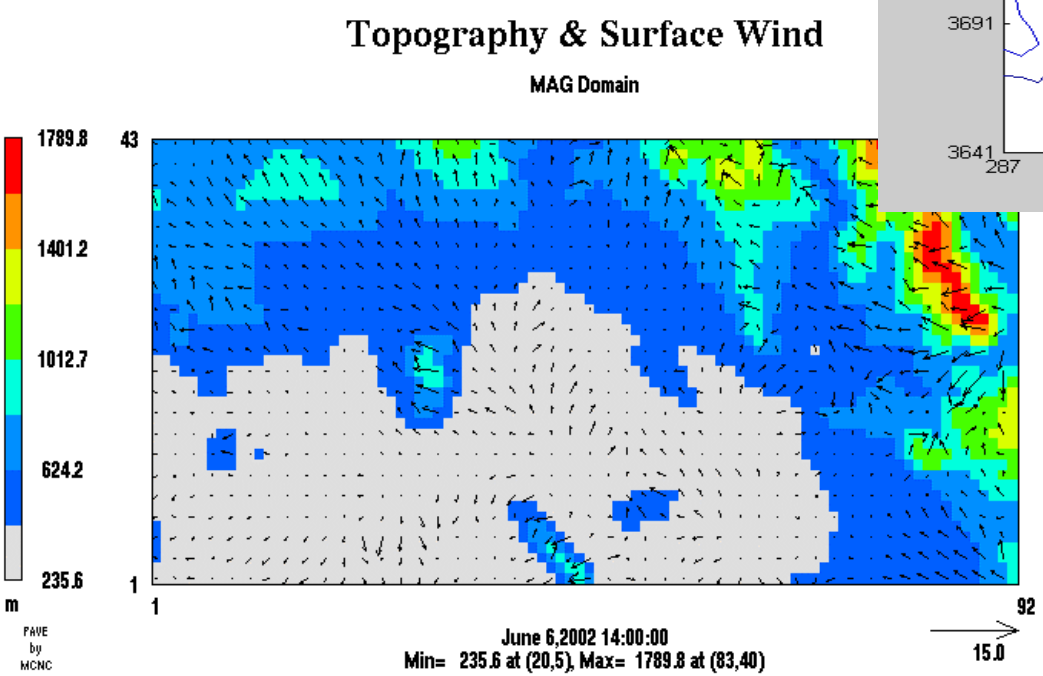
High O3 in the W & NW: 0900 LST, June 6



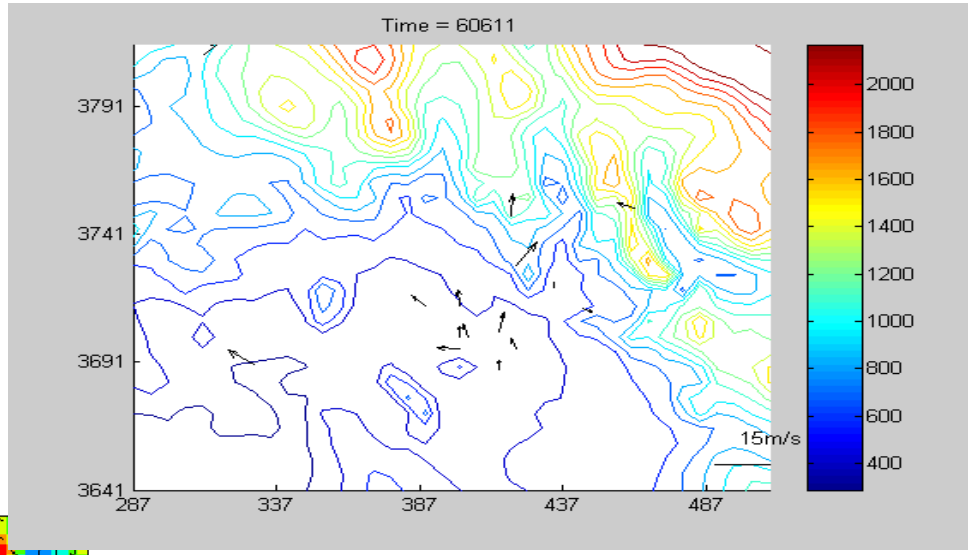


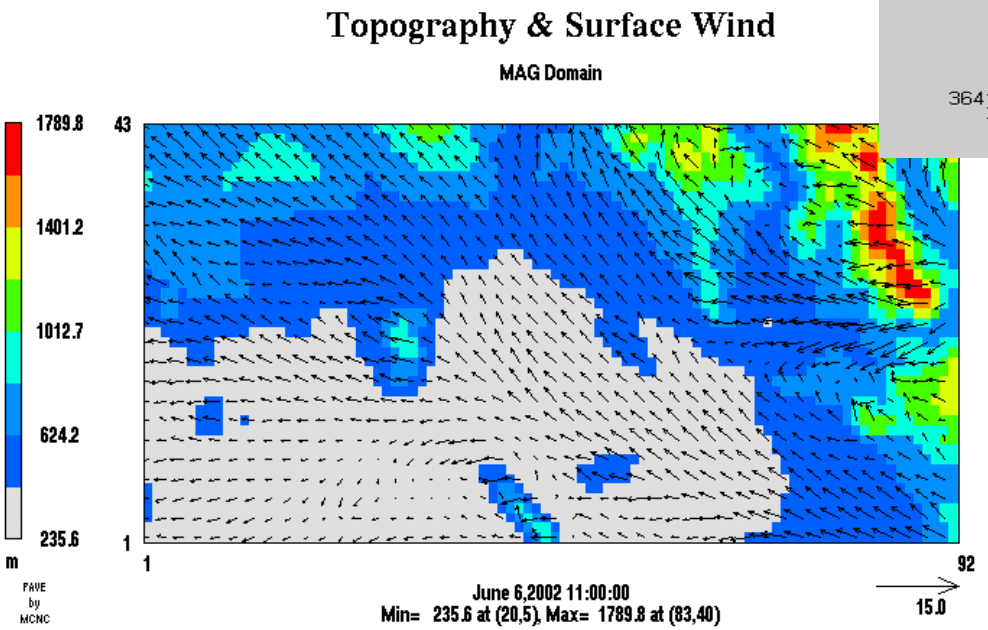
High O3 in the W & NW: 1400 LST, June 6



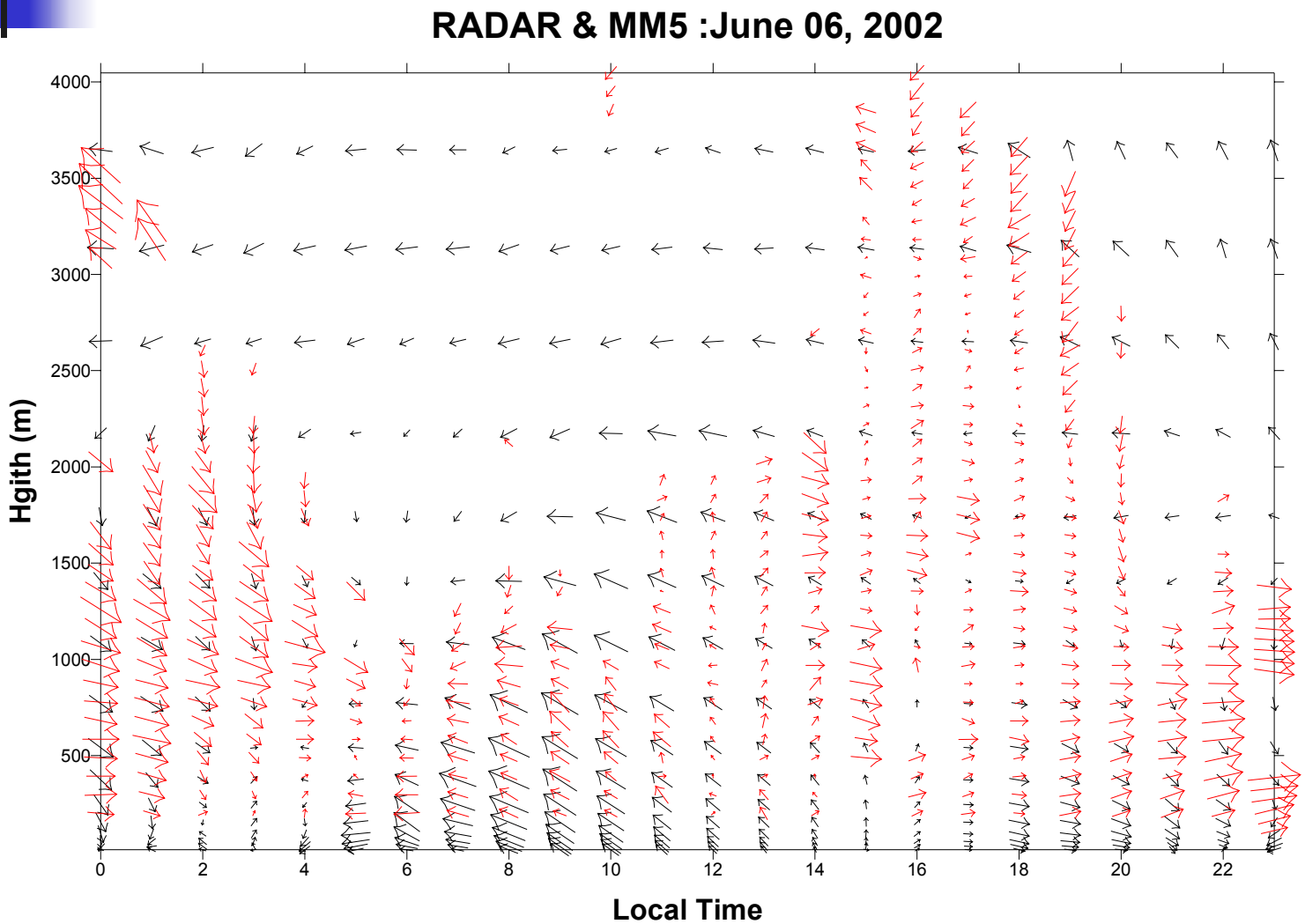


High O3 in the W & NW: 1100 LST, June 6



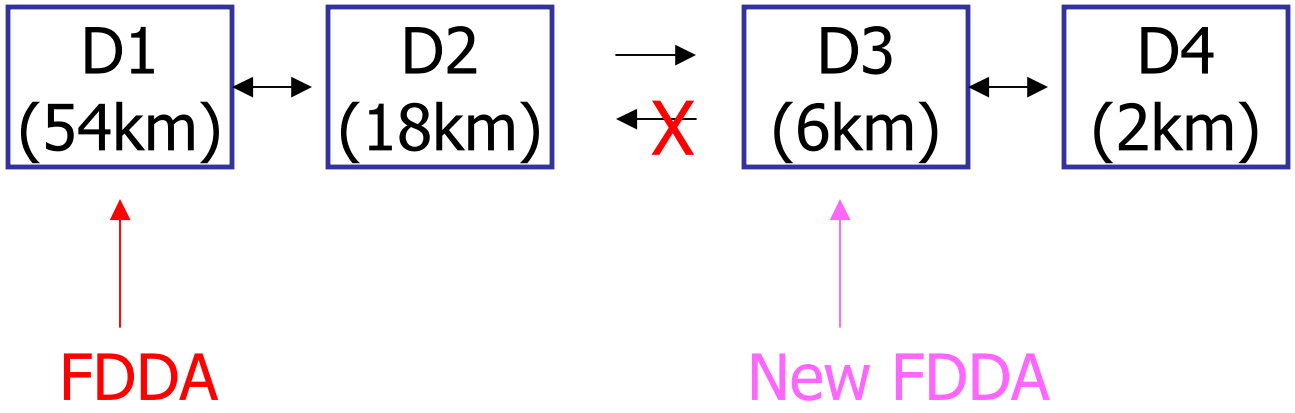


MM5 vs RADAR: June 06

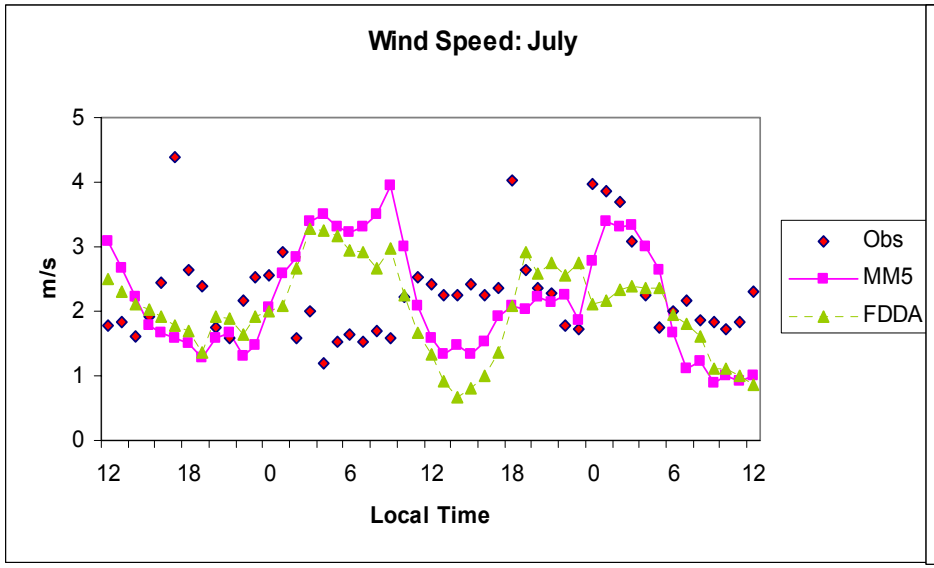


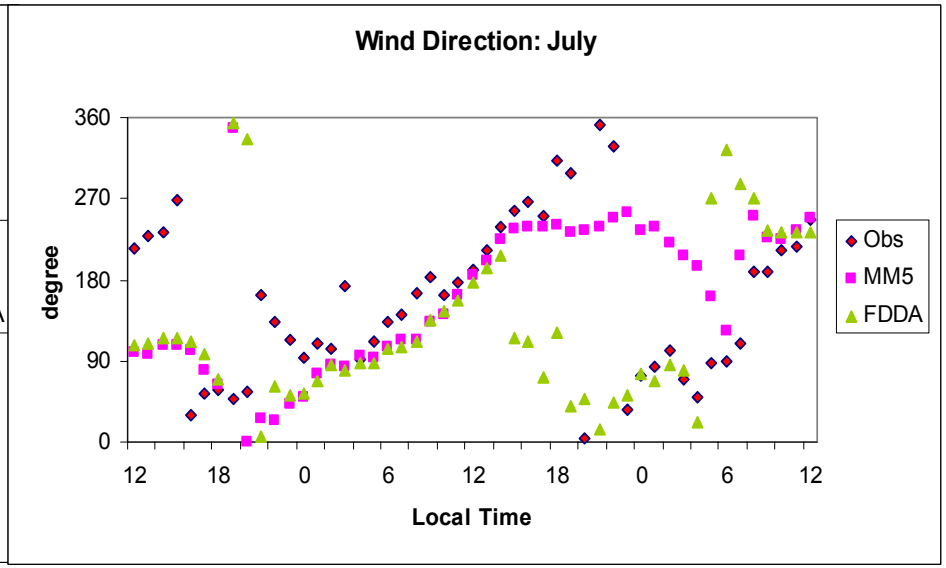
MM5 FDDA
(Four Dimensional Data Assimilation)

July Case



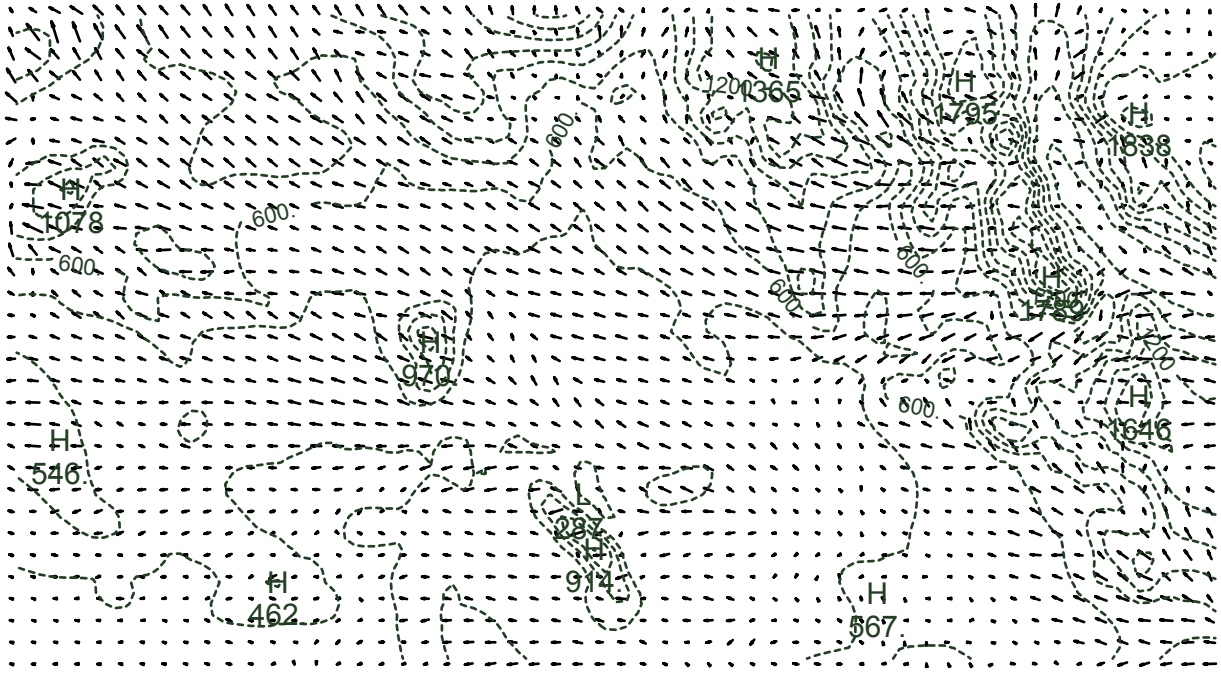
MM5 w/o vs w/ FDDA





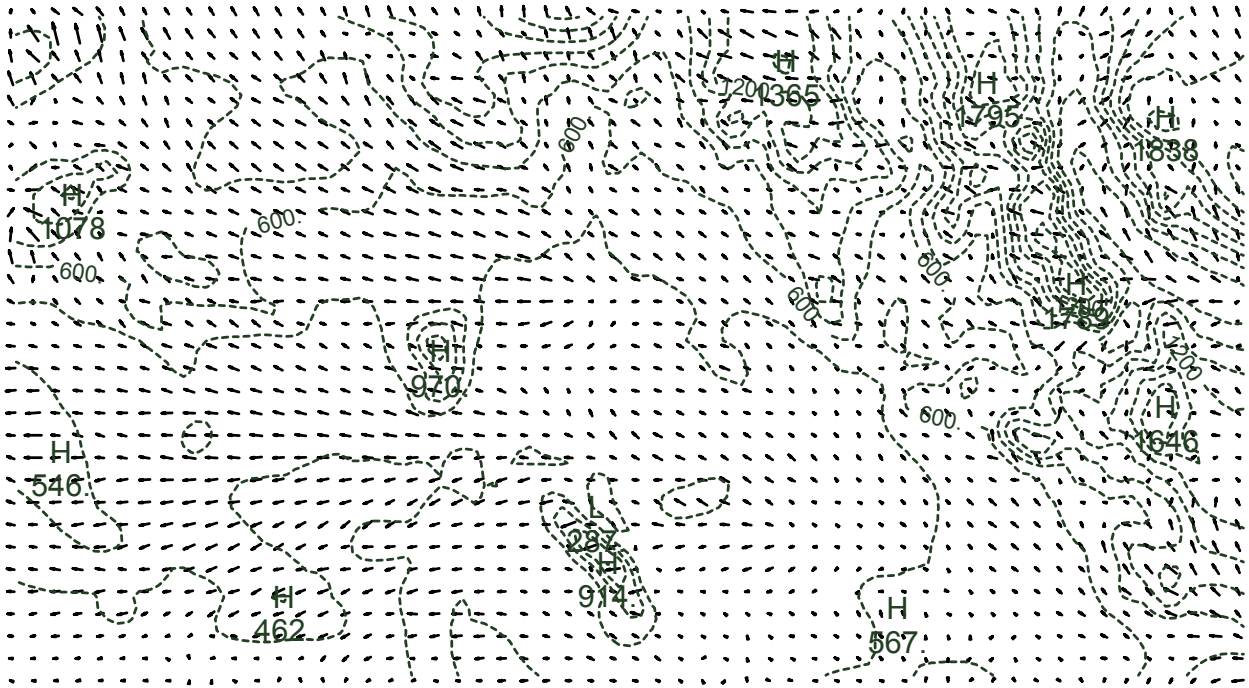
SIGMA =0.999 BARB UV (m/s) 2002-07-11_19:00:00 = 2002-07-10_12 + 31.00H SMOOTH= 0
SIGMA =1.000 TERRAIN (m) 2002-07-11_19:00:00 = 2002-07-10_12 + 31.00H SMOOTH= 0

MM5 w/o FDDA: 1200 LST July 11



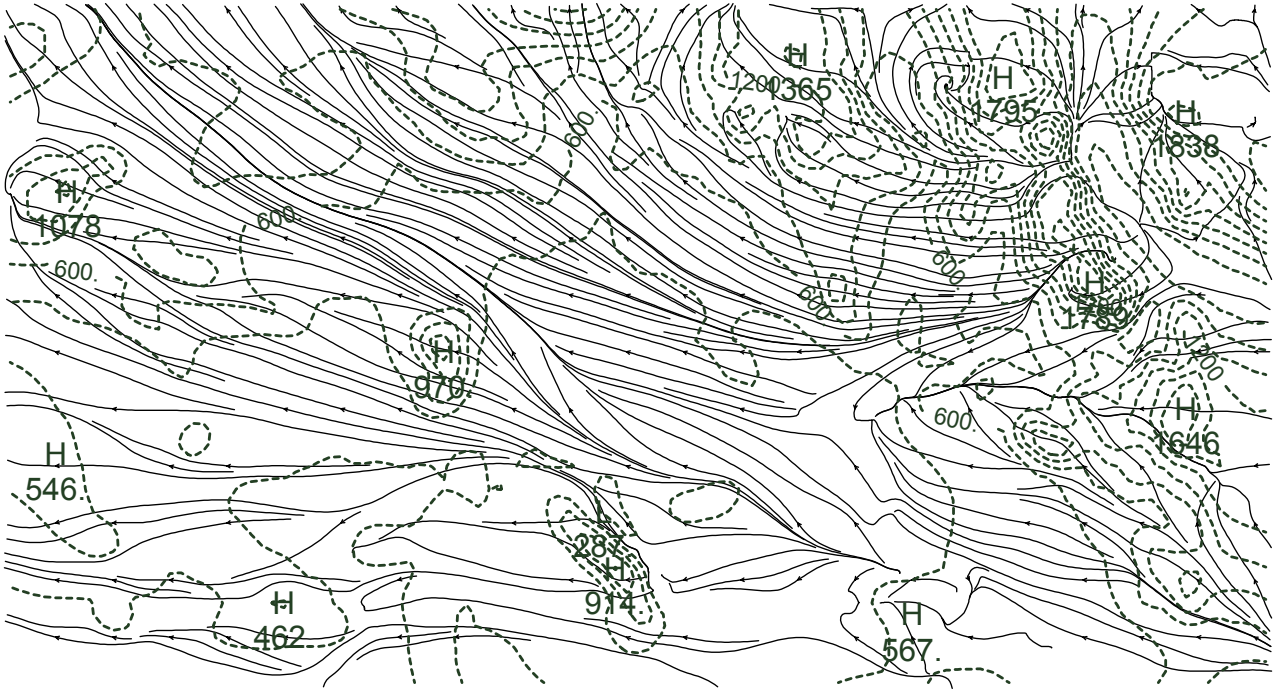
SIGMA =0.999 BARB UV (m/s) 2002-07-11_19:00:00 = 2002-07-11_00 + 19.00H SMOOTH= 0
SIGMA =1.000 TERRAIN (m) 2002-07-11_19:00:00 = 2002-07-11_00 + 19.00H SMOOTH= 0

MM5 w/ FDDA: 1200 LST July 11



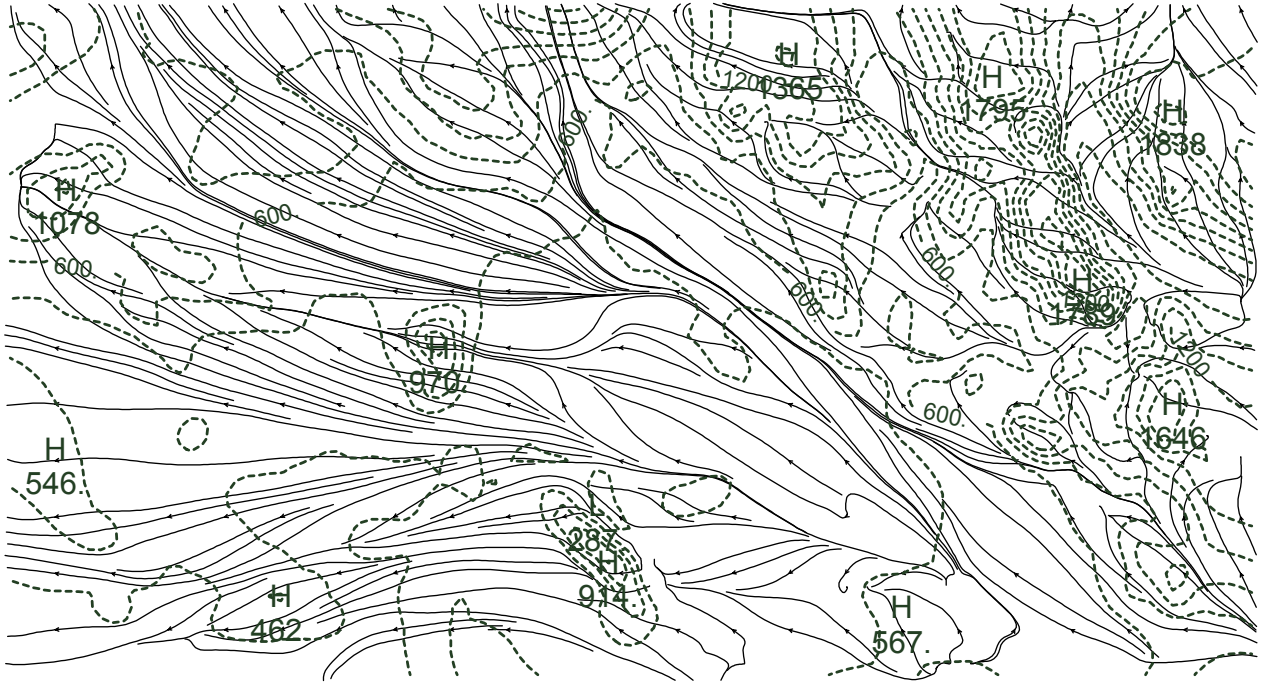
SIGMA =0.999 BARB UV (m/s) 2002-07-11_19:00:00 = 2002-07-10_12 + 31.00H SMOOTH= 0
SIGMA =1.000 TERRAIN (m) 2002-07-11_19:00:00 = 2002-07-10_12 + 31.00H SMOOTH= 0

MM5 w/o FDDA: Streamlines



SIGMA =0.999 BARB UV (m/s) 2002-07-11_19:00:00 = 2002-07-11_00 + 19.00H SMOOTH= 0
SIGMA =1.000 TERRAIN (m) 2002-07-11_19:00:00 = 2002-07-11_00 + 19.00H SMOOTH= 0

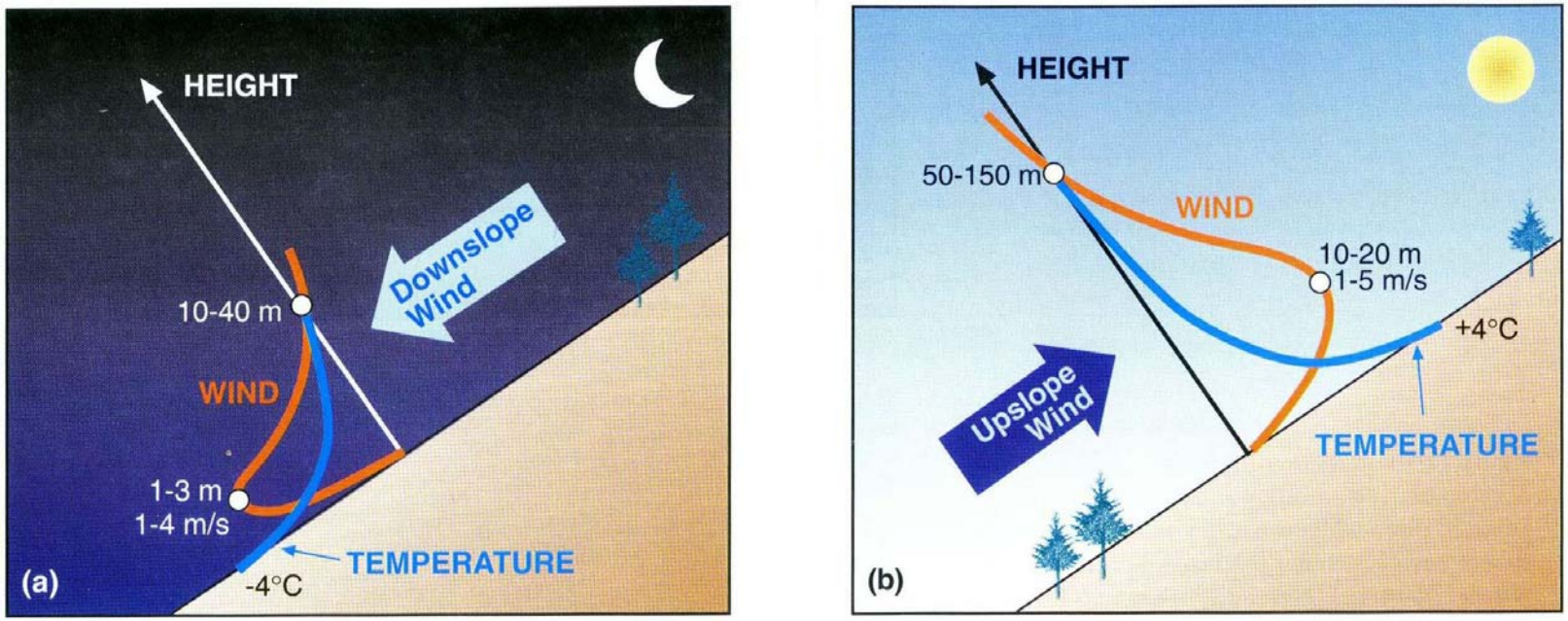
MM5 w/ FDDA: Streamlines



Transition Periods

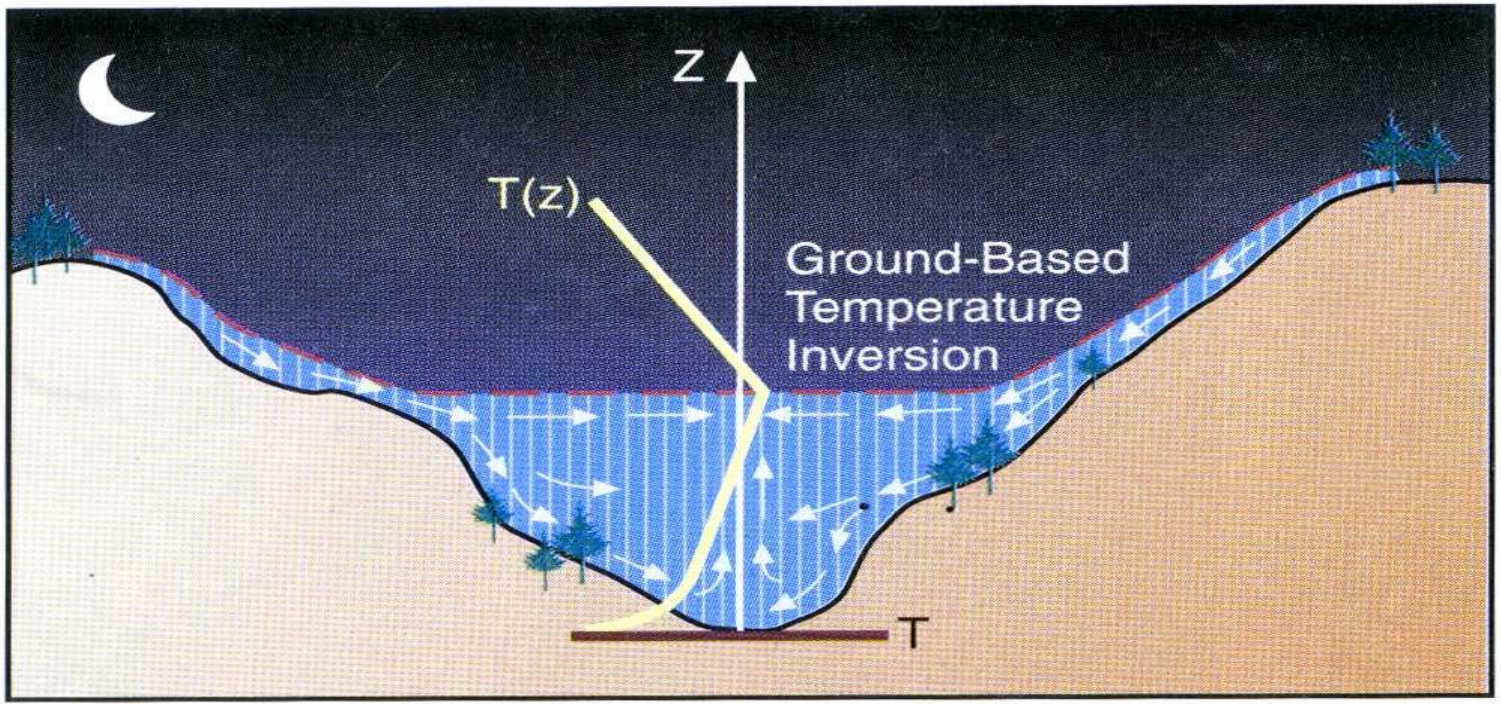
- Morning Transition
- Evening Transition

Thermally Driven Slope Flows



Reproduced from *Mountain Meteorology* (2000). Courtesy of Dr. Whiteman, PNNL.

Morning Transition



Reproduced from *Mountain Meteorology* (2000), and *Observations of thermally developed wind systems in mountainous terrain* (1990). Courtesy of Dr. Whiteman, PNNL.

Cold Pool Breakup

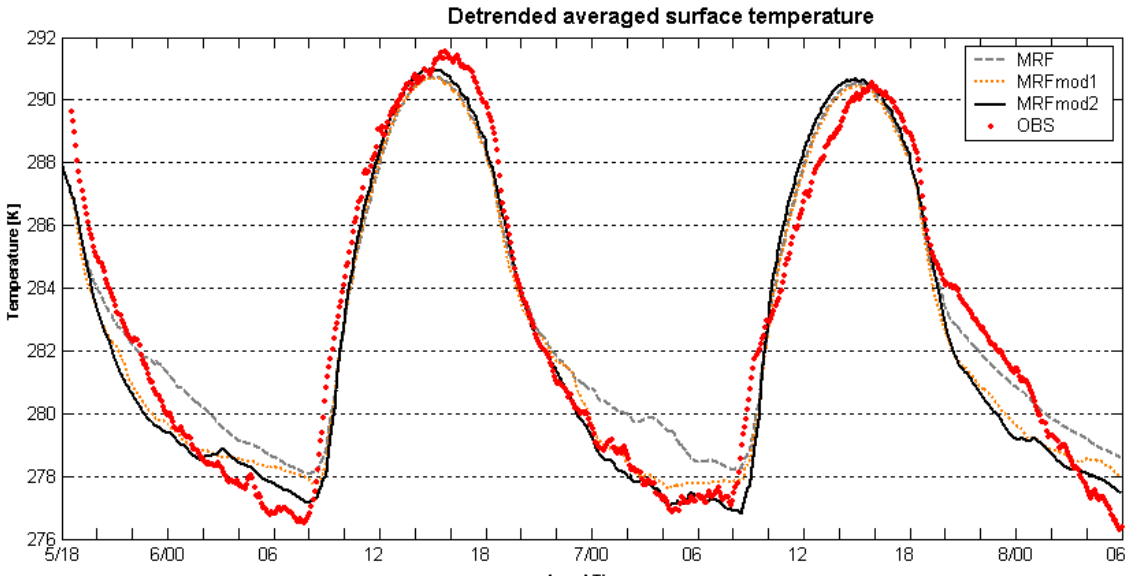
Low B

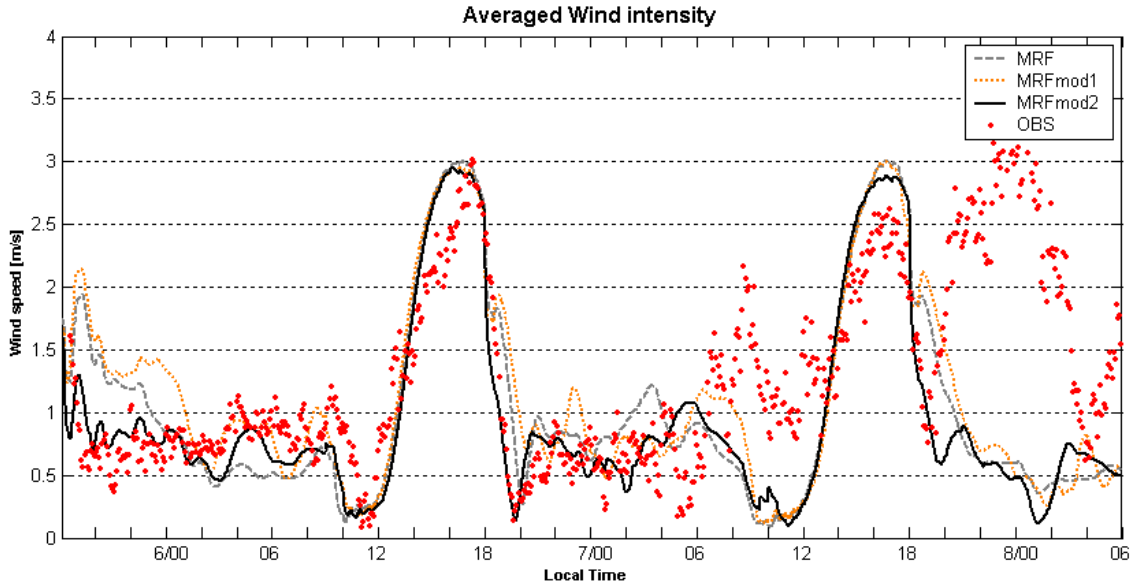
Run 11 - Thermally Stratified

Click in the window to play (will take a few seconds to load).

See Run11-temp.avi
for Temperature Profiles

Temperature & Wind comparison





Second modification to MRF (only below PBL and STABLE conditions.)

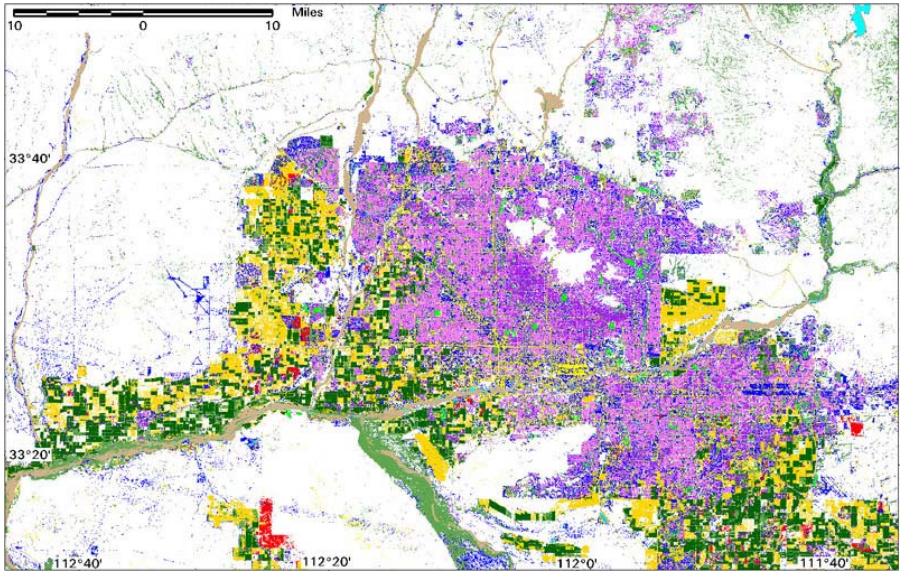
$$\frac{K_m}{\sigma_w^2 / \left| d\tilde{V}/dz \right|} = (0.34)\overline{Rig}^{-0.02} \approx 0.34$$

$$\frac{K_m}{\sigma_w^2 / \left| d\tilde{V}/dz \right|} = (0.08)\overline{Rig}^{-0.49} \approx (0.08)\overline{Rig}^{-0.5}$$

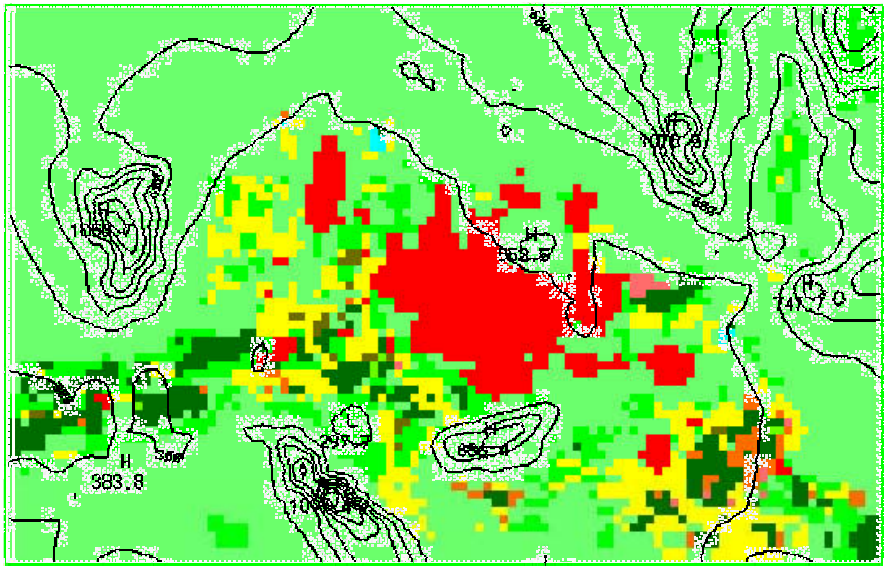
$$\begin{cases} K_m \approx 0.34\,\sigma_w^2 / \left| d\tilde{V} / dz \right| \\ K_h \approx 0.08\,\sigma_w^2 / N \\ \dfrac{\sigma_w^2}{u_*^2} = 2.5\left[1 - \left(\dfrac{z}{h}\right)^{0.6}\right] \end{cases}$$

Land Cover Comparison

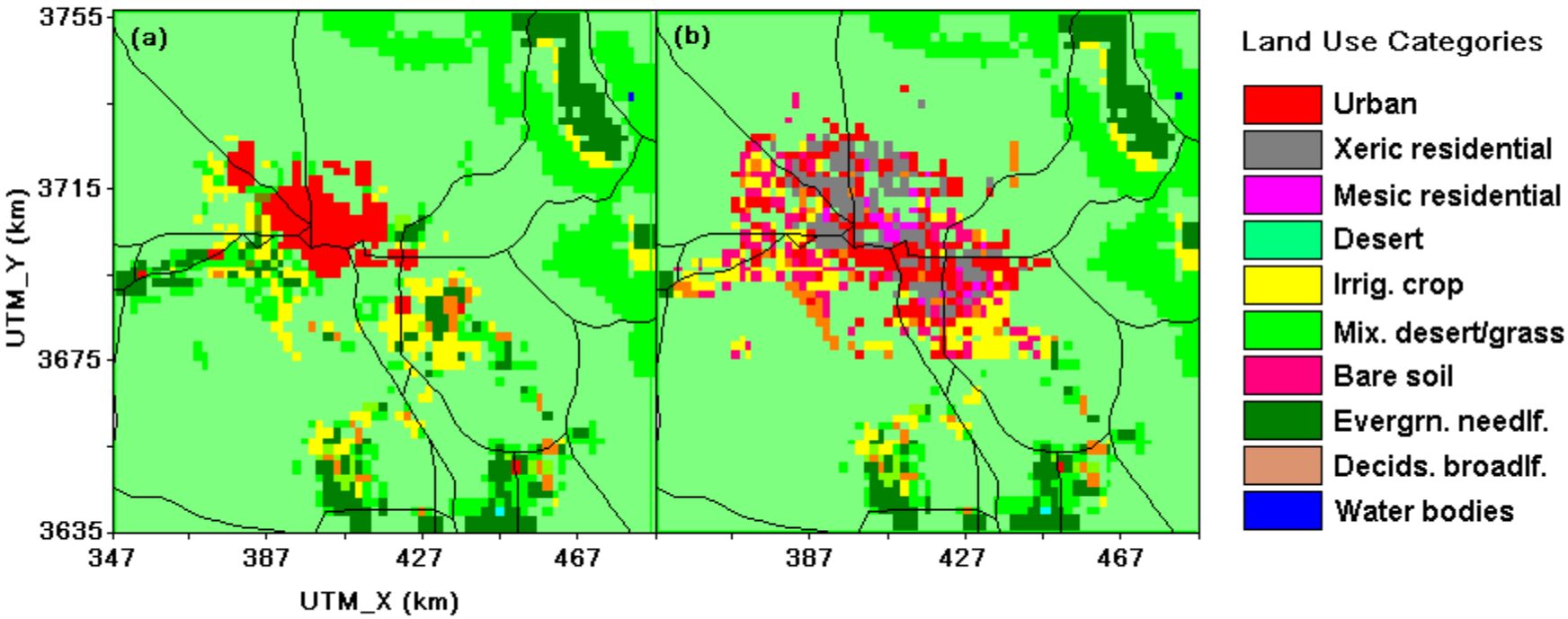
Actual (1998 AVHRR, Will Stefanov, ASU)



MM5 (1976 USGS 25 category)



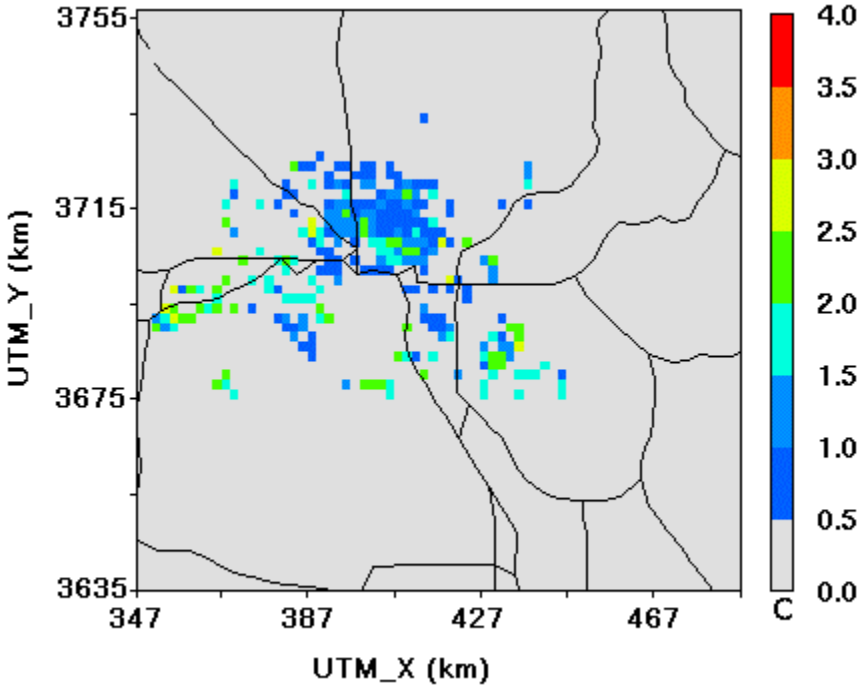
Large portions of urban area missing
Active agricultural areas misclassified
Large effect on surface energy budget and regional scale circulation


(a)
(b)
3755
3715
3675
3635
UTM_Y (km)
347
387
427
467
387
427
467
UTM_X (km)
Land Use Categories
Urban
Xeric residential
Mesic residential
Desert
Irrig. crop
Mix. desert/grass
Bare soil
Evergrn. needlf.
Decids. broadlf.
Water bodies

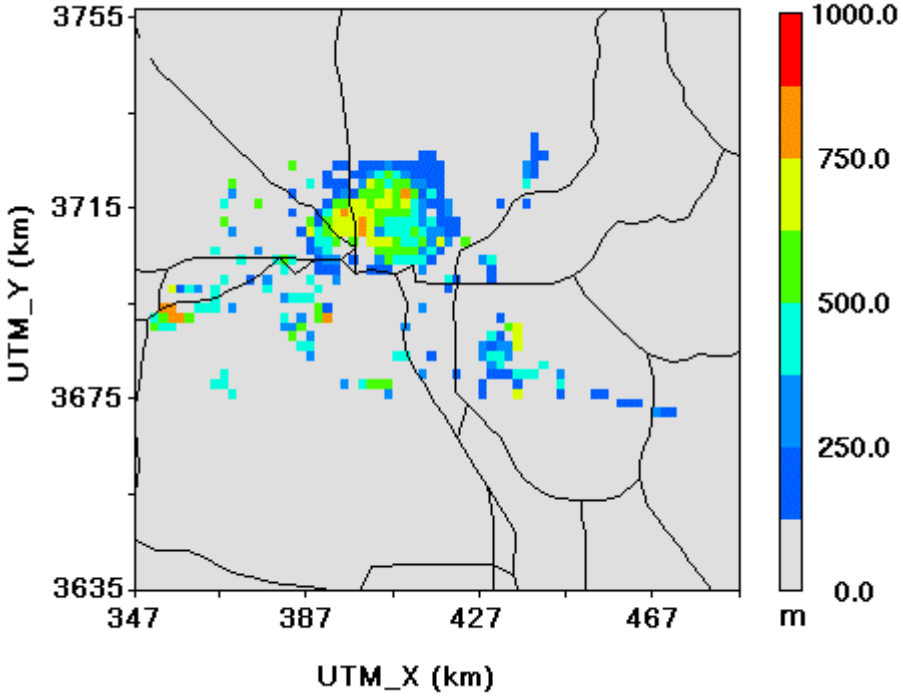
USGS less 1998 Land Use Classification

Simulated differences at 2 pm in:

2m Air Temperature



Boundary Layer Height



END