







#### Air Chemistry 101.01

- Ozone in the troposphere:
- NOx and hydrocarbons react in sunlight to produce ozone
- NOx comes from high temperature processes
  - power plants, diesels and gasoline engines
- Natural process
  - Lightning, soils,
- Hydrocarbons from vegetation, autos, paint, evaporation...

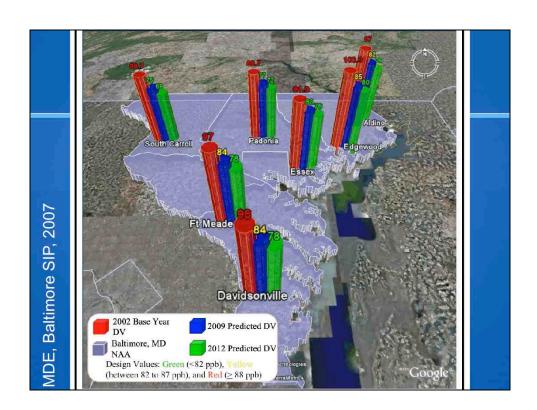
#### Implementing the Clean Air Act

- In 1997, EPA set a standard, 85 ppbv for 8 hour average ozone (now: 75→60-70?)
- Monitoring, states & EPA determine (non)compliance & classify severity
- Severity sets a timeline for compliance with the standard: worse problems get more time
- Figure of merit: 3 year average of each year's 4<sup>th</sup> highest daily maximum 8-hour average ozone at each monitor = Design Value

# Modeling Clean Air Act compliance

- GUIDANCE is set out by EPA
- Do a model run for base (2002) and future (2009) years
- Calculate ratios between future and base year modeled ozone: a relative response factor
- Observations form the baseline → "design value" calculated as a weighted average of 5 years around a base year (2002). This sets your starting point
- Multiply design value by RRF to get future year prediction

#### **Model Predictions** Modeling Attainment Test Using EPA Preferred Methodology DVB RRF DVF Site Name County State Davidsonville MD 98.0 Anne Arundel 0.858 84 0.869 Ft. Meade Anne Arundel MD 97.0 84 Padonia Baltimore 88.7 0.872 MD 77 Essex Baltimore 91.3 0.879 80 MD South Carroll Carroll 88.7 0.847 75 MD Harford 0.852 85 Edgewood MD 100.3 Aldino Harford MD 97.0 0.846 82



#### **Model Evaluation**

- Run the model according to EPA guidance
- Compare the model to ground-level monitoring according to EPA guidance
- Calculate mean error and bias as suggested by EPA guidance
- If they fall within certain limits (set by EPA guidance), then
- THE MODEL IS VALID FOR ANY USE!!

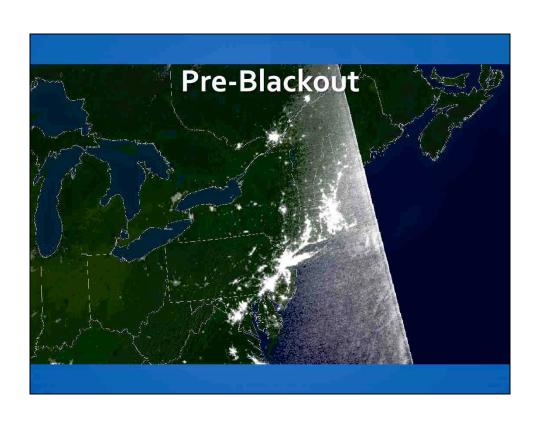
(no!)

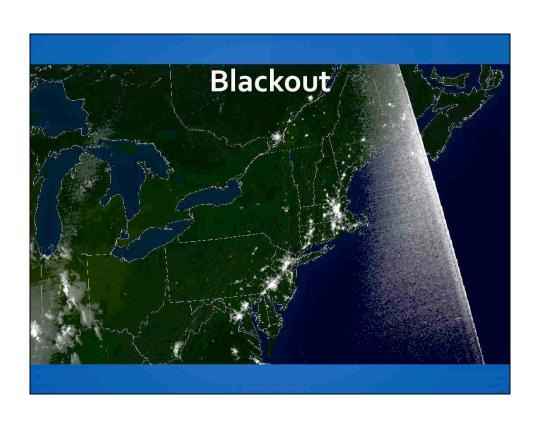
#### The Disconnect

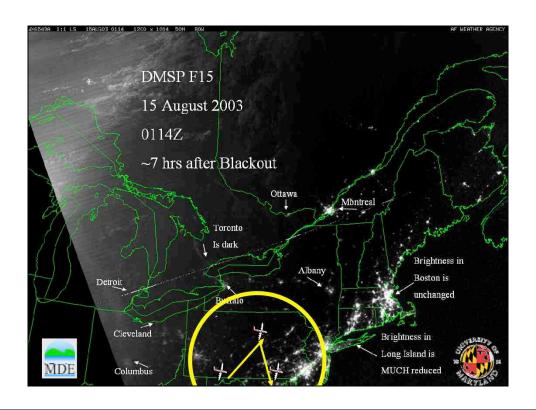
- Base year compared to concentrations at the surface and for that year only to vet performance—a stαtic evaluation
- We evaluate the model based on its static performance, not its ability to predict change
- Then use it dynamically to predict changes

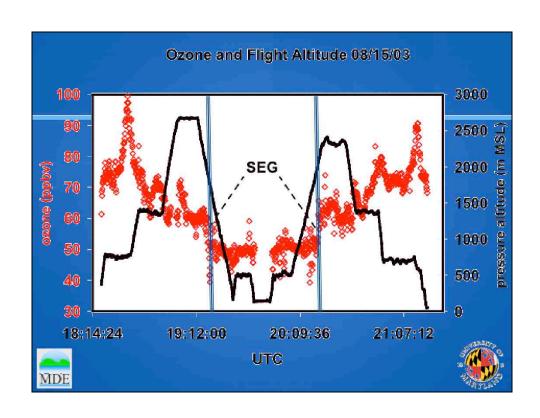
## How about a *dynamic* model evaluation?

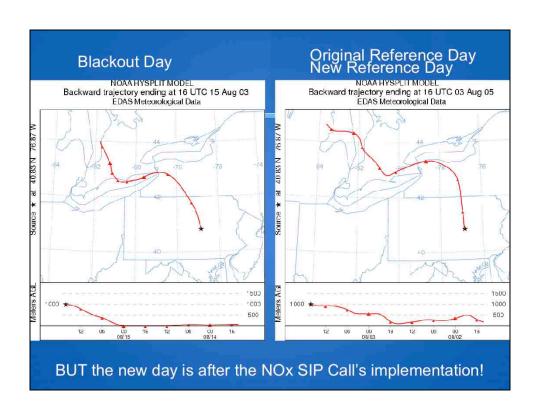
- Sudden changes in emissions are rare, but can be found:
  - 9 2003 Northeast Electrical Blackout
  - NOx controls installed around 2002 (the NOx SIP Call)
- Using the observations differently helps
  - Emphasize diagnostics and changes, not absolute concentrations
  - Diel cycles in ozone
  - Compare model to aircraft vertical profiles of pollutants
    - Transport and mixing of pollution

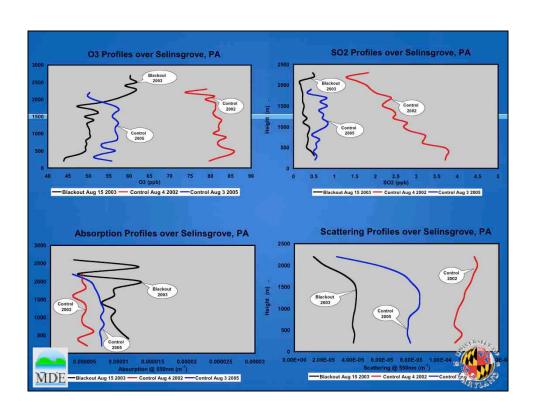


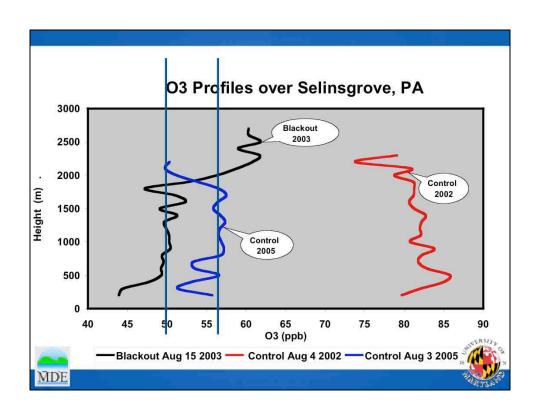






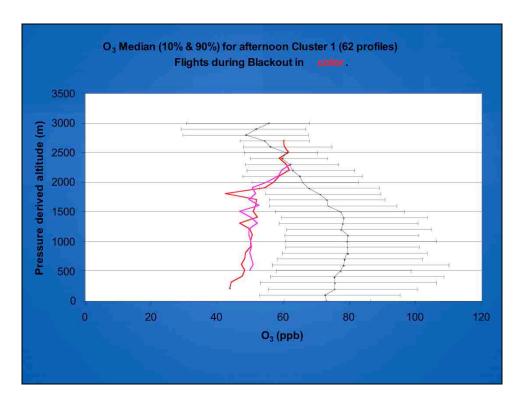






#### Climatology

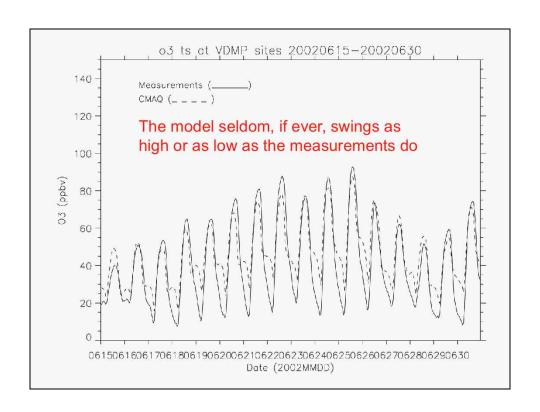
- Compare with historical ozone flights under similar meteorological conditions
- Cluster back-trajectories to determine transport patterns on the days we flew
- Compare blackout ozone profile to statistical summary of all flights within the cluster that contains the blackout flight



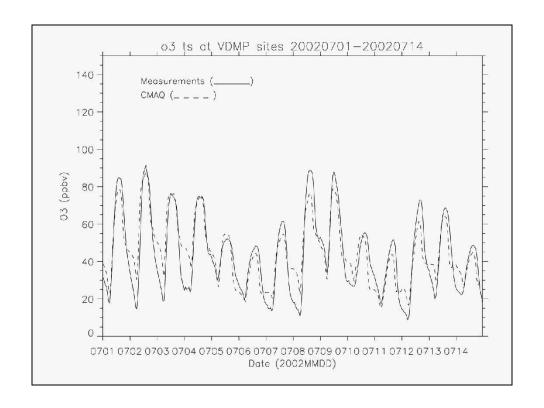


### Dynamic evaluation of the model

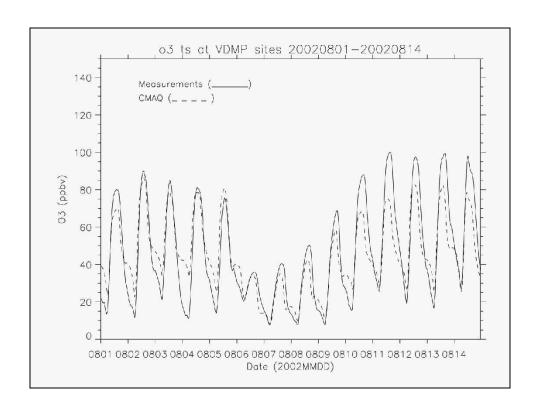
- CMAQ does not reproduce diurnal cycles well
  - Nighttime ozone performance poor, but perhaps expected?
  - Daytime peaks poor as well
- Statistics like mean error and bias necessarily make you look at average performance
  - Model development geared towards these measures!
  - Time to look at some new measures



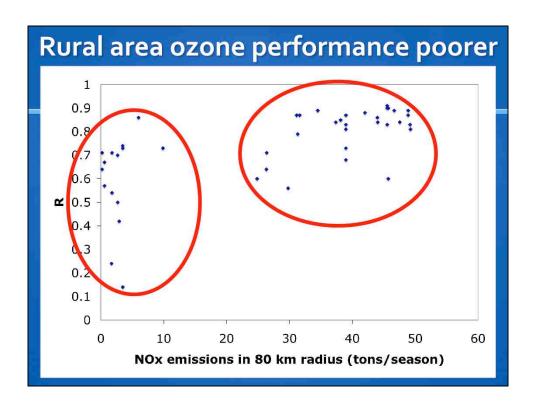
Averages taken at all monitoring stations in Virginia, Maryland, Delaware and Pennsylvania (VDMP); model sampled at those grid cells and averaged. June 15-30, 2002



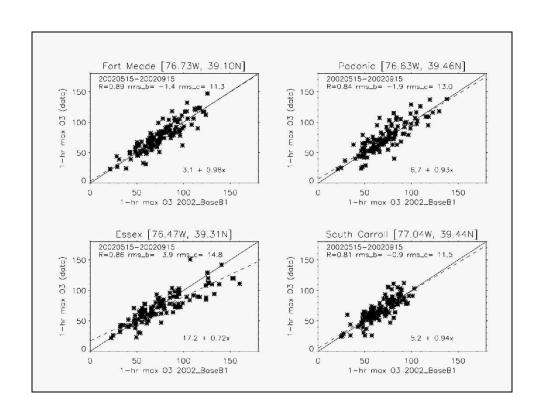
July 1-14, 2002

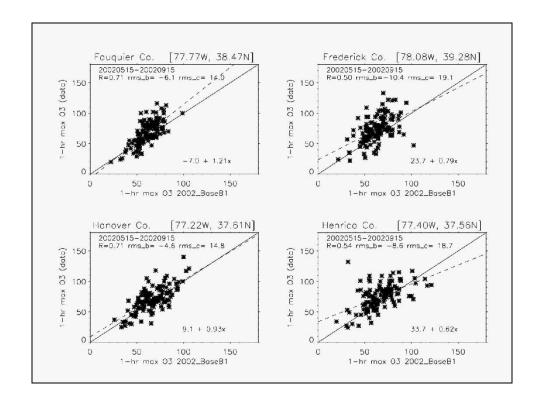


August 1-14, 2002.



Urban areas tend to have lots of cars, rural areas tend to have power plants. If we mess up the rural areas, we mess up the ozone that's coming into the city from outside and emphasize the wrong controls.

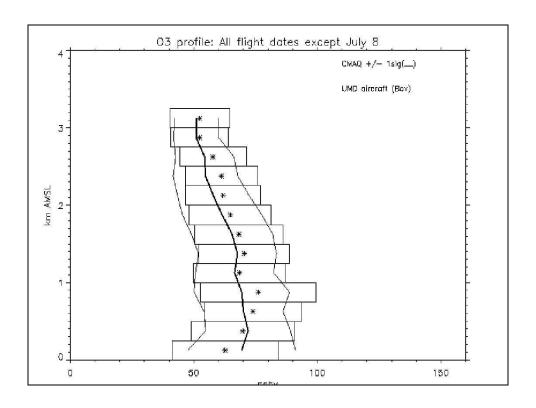




Correlations much poorer at more rural sites.

### **Aloft performance**

- CMAQ generally overpredicts ozone at the surface and underpredicts aloft
- Transport likely underrepresented
- Better than in the past, still not right.



CMAQ underpredicts ozone aloft and overpredicts it at the surface. Graph based on all flights in 2002 except July 8, which was heavily influenced by smoke from forest fires in central Quebec.

### **Dynamic Response Missing**

- Generally falls short of peaks
  - Peaking units? Dyanmics? Chemistry?
- Generally overpredicts nighttime minima
  - NOx titration, sure, but:
    - Everywhere?
    - What about the odd shape?
- Model lacks dynamic range.
- Lack of response due to...?

# Long-term response to emissions changes

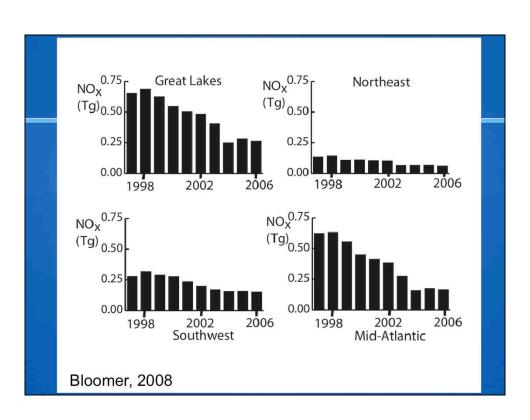
- In New Jersey, 2009 design values arrived in 2006!
- There were still more emissions reductions to come

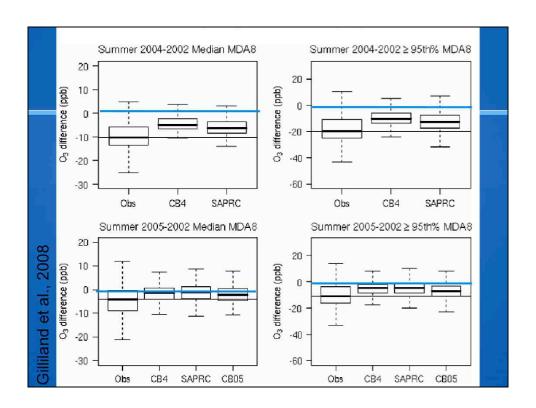
		2006	Mode 2009
COUNTY	OZONE MONITOR LOCATION	2004-2006 DESIGN VALUE	Modeled Predicted O Concentrati (BOTW-v.3)
Atlantic	Nacote Creek	78	75
Passaic	Ramapo	79	79
Monmouth	West Long Beach (Monmouth Univ)	81	83
Morris	Chester	82	85
Camden	Camden Lab	83	89
Bergen	Teaneck	85	87
Cumberland	Millville	85	82
Gloucester	Clarksboro	85	88
Hudson	Bayonne	85	80
Mercer	Rider U	87	87
Middlesex	Rutgers U	88	85
Hunterdon	Flemington	88	84
Camden	Ancora	88	90

The +/-/o signs along the right side indicate where 2006 numbers were with respect to 2009

#### Response to the NOx SIP Call

- Around 2002-2004, HUGE emissions controls went in on power plants, many upwind of Maryland—the NOx SIP Call
- EPA and collaborators modeled 2002, 2004 and 2005 meteorology, emissions, and chemistry
- Look at CMAQ's response to the NOx SIP Call





The model never shows the same level of change that the measurements indicate between 2002 and 2004/2005. Generally, the response is about half that measured in reality.

## Dynamic evaluation results

#### Blackout:

- Using the 2005 reference day: A minimum of 7 ppbv ozone throughout a deep column, likely higher
- Using comparisons to areas outside the blackout on the same day:
   10 ppb, possibly 20-25 ppb.
- Using comparisons to climatology: ozone levels were very unusual for those conditions
- Hu et al.: 4%: some from power plants, more from assumed weekend traffic patterns on the blackout day (~2 ppb)
- Measurement-based estimates of the change in ozone due to the blackout are at least twice the model-based estimate

Hu et al. is a paper from Georgia Tech that simulated the effects of the blackout by examining the measured emissions from the blacked out plants and assuming weekend travel patterns on that day (toll booth records and measurements of species other than ozone suggest otherwise) throughout the affected area. They got a 4% reduction in ozone from the blackout.

## **Dynamic Evaluation Results**

- Dynamic model evaluation
  - CMAQ underpredicts the peaks, overpredicts nighttime lows: poor response to emissions changes
  - Performance poorer in upwind rural areas
- New Jersey effect
  - 2009 modeled design values at the highest monitors (New Jersey) were already there by 2006

### **Make Predictions**

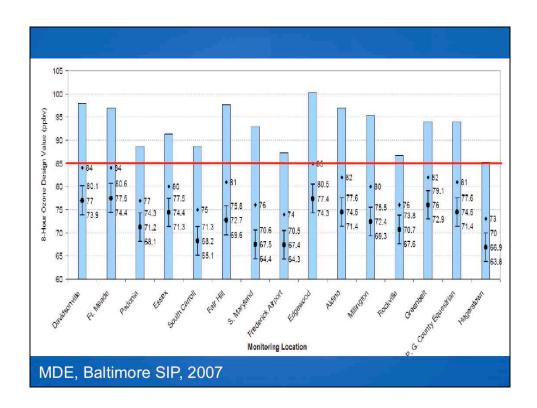
- Use EPA-approved guidance to calculate 2009 future design values
- For Maryland, things looked close
- Blackout suggests double the response
- Gilliland et al suggests a larger response as well
- Take a conservative estimate: 50% more response to emissions changes than CMAQ predicts.
- This is what EPA calls a Weight of Evidence argument

Weight of evidence is essentially arguing. If your prediction is that you will be close to the standard (below or above) in the future, you have to argue why your area should be able to attain the standard using more than just model results. In my view, this amounts to "prove the model is right".

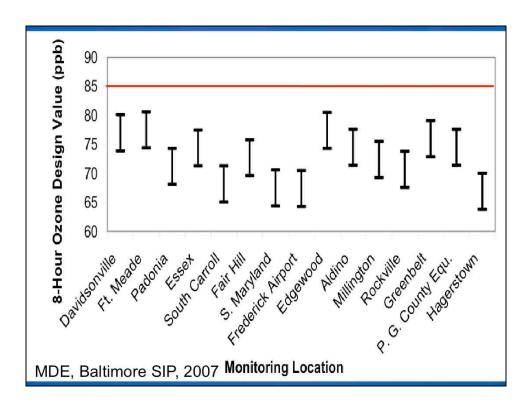
## **Maryland Model Predictions**

- Also include a RANGE of possible future outcomes
- Spread in model runs using estimates of future year emissions
- Spread in 4<sup>th</sup> highest ozone from years around the base year\*

\*The only idea EPA liked



The red line was the ozone standard for this SIP = State Implementation Plan



MDE = Maryland Department of the Environment

Table 3. Current and Projected Design Values and Their Uncertainties for Maryland Monitors Observed Modeled Probable Monitor 2002 2009 2012 2009 2009 2009 AIRS-ID Name Design Design Design Design Lower Upper Value Value Value Value **Bound** Bound Davidsonville 240030014 98.0 84 78 77.0 73.9 80.1 Ft. Meade 240030019 97.0 84 78 77.5 74.4 80.6 88.7 Padonia 240051007 77 72 71.2 68.1 74.3 240053001 91.3 Essex 80 76 74.4 71.3 77.5 South Carroll 240130001 88.7 75 69 68.2 65.1 71.3 240150003 97.7 75 72.7 Fair Hill 81 69.6 75.8 240170010 93.0 76 70 67.5 70.6 64.4 S. Maryland Frederick 240210037 87.3 74 68 67.4 64.3 70.5 Airport 100.3 Edgewood 240251001 85 80 77.4 74.3 80.5 240259001 97.0 76 74.5 71.4 77.6 82 Aldino 240290002 95.3 72.4 Millington 80 74 69.3 75.5 240313001 Rockville 86.7 76 71 70.7 67.6 73.8 Greenbelt 240330002 94.0 82 76 76.0 72.9 79.1 P. G. County 240338003 94.0 81 76 74.5 71.4 77.6 Equestrian 240430009 85.3 73 67 66.9 70.0 Hagerstown 63.8

		Jersey t by year and		
Site	2007	2008	2009	2 07-200
Ancora	91	82	71	81
Bayonne	92	81	69	80
Brigantine	78	72	71	73
Chester	88	81	68	79
Clarksboro	89	89	71	83
Colliers Mills	86	85	71	80
Flemington	88	85	70	81
Leonia	<u>(=)</u>	82	72	-
Millville	83	79	72	78
Monmouth	88	83	72	81
Newark	<b>—</b>	æ	64	- 1
Ramapo	85	76	69	76
Rider University	94	79	71	81
utgers University	90	83	67	80
	7			1
·				

All sites in attainment!!

A COLUMN	I				
IN O	ew Jei	rsey i	n 20	09	
COUNTY	OZONE MONIT	TOR		2004-2006 DESIGN	Modeled Predicted O3 Concentration (BOTW-v.3)
COUNTY	LOCATION	Site	Average	VALUE	(50111-1.0)
		Site	2007-2009		i i
Atlantic	Nacote Cree	Nacote Creek	-	78	75
Passaic	Ramapo	Ramapo	76	79	79
Monmouth	West Long B	Monmouth	81	81	83
Morris	Chester	Chester	79	82	85
Camden	Camden Lab	Camden Lab	-	83	89
Bergen	Teaneck	Teaneck	2	85	87
Cumberland	Millville	Millville	78	85	82
Gloucester	Clarksboro	Clarksboro	83	85	88
Hudson	Bayonne	Bayonne	80	85	80
Mercer	Rider U	Rider U	81	87	87
Middlesex	Rutgers U	Rutgers U	80	88	85
Hunterdon	Flemington	Flemington	81	88	84
Camden	Ancora	Ancora	81	88	90
Ocean	Colliers Mills	Colliers Mills	80	92	93
			*****		

Note how many sites were projected to be far out of attainment

	Design Value (ppb)		4th Maximum Concentration (ppb)			Modeled		Probable			
Site Name	2008	2009	2006 2007 2008 2009		2009 DV	2012 DV	2009 DV	2009 Lower Bound	2009 Upper Bound		
Southern											
Maryland		75	85	83	78	66	76	70	67.5	64.4	70.6
Frederick Airport			85	86	75	69	74	68	67.4	64.3	70.5
Rockville	84		88	88	76	70	76	71	70.7	67.6	73.8
PG Equestrian											
Center	87		95	88	79	67	81	76	74.5	71.4	77.6
Mount Vernon	87		88	88	85	69					
Franconia	85		87	85	85	70					
McMillian											
Reservoir	87		90	87	84	71					
Davidsonville	87	80	92	89	81	70	84	78	77	73.9	80.1
Padonia	80	75	81	72	87	68	77	72	71.2	68.1	74.3
Essex	85		91	83	81	71	80	76	74.4	71.3	77.5
South Carroll	83	78	82	89	78	68	75	69	68.2	65.1	71.3
Edgewood	91	87	95	90	88	83	85	80	77.4	74.3	80.5
Aldino	89		90	92	85	69	82	76	74.5	71.4	77.6
Millington		78	82	83	85	66	80	74	72.4	69.3	75.5
Hagerstown		73	79	81	75	65	73	67	66.9	63.8	70
Fairhill	90		92	92	88	72	81	75	72.7	69.6	75.8
Colliers Mills	87		91	86	85	71					
Bucks Co PA	91	87	87	102	85	74					

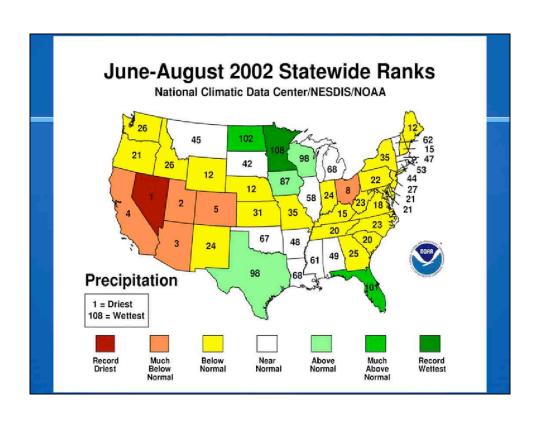
Note the boxes in pink and blue in the 2009 DV column. Four of our predictions were too high for 2009 and only one was too low. Clearly something is unusual about Edgewood.

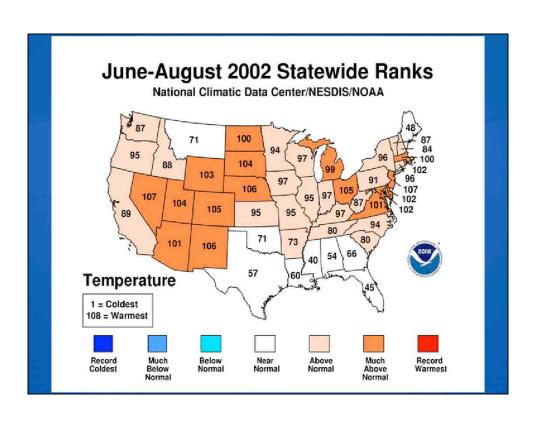
	Design Value (ppb)	4th Maximum Concentration (ppb)	Modeled	Most Probable
Site Name	2009	2009	2009 DV	2009 DV
Southern				
Maryland	75	66	76	67.5
Frederick Airport	76	69	74	67.4
Rockville	78	70	76	70.7
PG Equestrian				
Center	78	67	81	74.5
Mount Vernon	80	69		
Franconia	80	70		
McMillian				
Reservoir	80	71		
Davidsonville	80	70	84	77
Padonia	75	68	77	71.2
Essex	78	71	80	74.4
South Carroll	78	68	75	68.2
Edgewood	87	83	85	77.4
Aldino	82	69	82	74.5
Millington	78	66	80	72.4
Hagerstown	73	65	73	66.9
Fairhill	84	72	81	72.7
Colliers Mills	80	71		
Bucks Co PA	87	74		

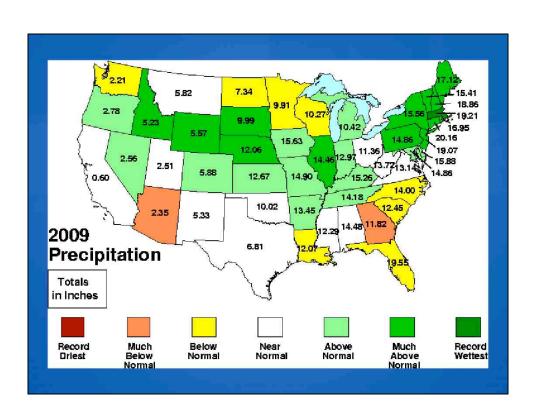
Even the 3 year average "design values" were close. (Colliers Mills (NJ) and Bucks County (PA) are particularly difficult sites in the Philadelphia nonattainment area)

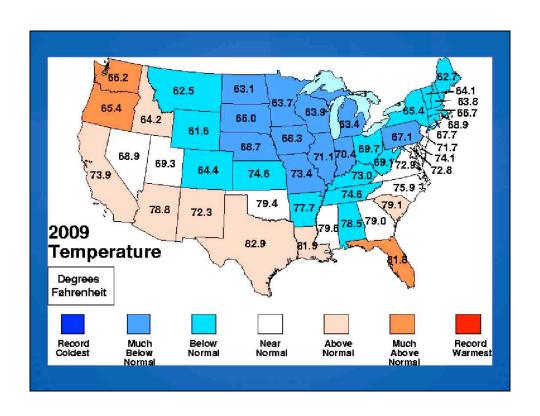
# Lucky or good?

- 2009 was not 2002
- o 2009 unusually wet, cool...
- o 2002 unusually hot, dry









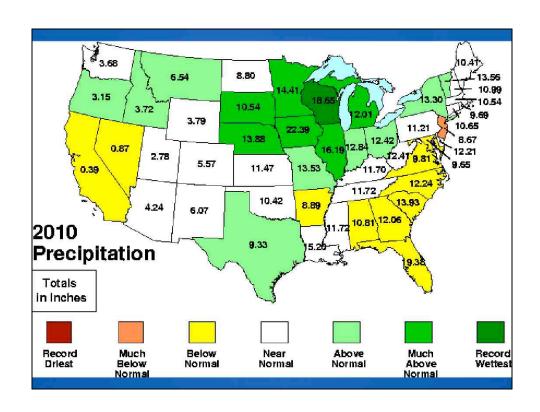
## Lucky or Good? Both!

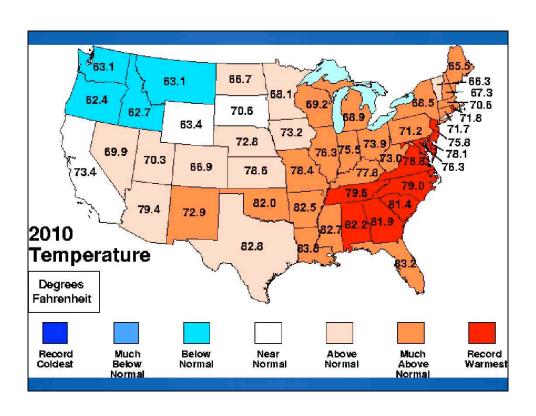
- Substantial power plant emission reductions were installed in Maryland for the summer of 2009
- Summer of 2009 was cool and wet, then just cool, then warm and convectively active
- Summer of 2002 was very hot and dry
- Predictions for 2012 suggest greatly improved air quality due to ongoing automobile fleet turnover & better exhaust systems

	Design Value (ppb)	4th Maximum Concentration (ppb)	Modeled	Mos	st Probable
Site Name	2009	2009	2012 DV	2009 DV	2009 Upper Bound
Southern					
Maryland	75	66	70	67.5	70.6
Frederick Airport	76	69	68	67.4	70.5
Rockville	78	70	71	70.7	73.8
PG Equestrian					
Center	78	67	76	74.5	77.6
Mount Vernon	8.0	69			
Franconia	80	70			
McMillian					
Reservoir	80	71			
Davidsonville	80	70	78	77	80.1
Padonia	75	68	72	71.2	74.3
Essex	78	71	76	74.4	77.5
South Carroll	78	68	69	68.2	71.3
Edgewood	87	83	80	77.4	80.5
Aldino	82	69	76	74.5	77.6
Millington	78	66	74	72.4	75.5
Hagerstown	73	65	67	66.9	70
Fairhill	84	72	75	72.7	75.8
Colliers Mills	80	71			
Bucks Co PA	87	74	April 1		

Da	re I a	sk ab	out 2	010?
	0000 PV	0040 DV	2010 4th	
Aldian	2009 DV	2010 DV	highest	
Aldino	82	78	80	
Davidsonville	80	79	87	
Edgewood -	87	89	96	
Essex	78	79	84	
Furley ES, Baltimore	67		<75	
Padonia	75	78	78	All 2010 design
South Carroll	78	76	83	A 200 PAGE 10 A
Calvert County	74		87	values are below
PG Equestrian Center	78	77	85	81 ppb except
Frederick County	76	76	83	Edgewood: 89
Howard U Beltsville	78		85	Lagewood. 65
Rockville	78	74	77	
Southern Maryland	75	75	82	
Fair Hill	84	81	82	
Millington	78	*	<75	
Hagerstown	73	73	78	
Piney Run	71	*	<75	

We're going to start thinking of Edgewood as its own private nonattainment area.





## Lucky or Good? Both!

- Taking model predictions at face value, we needed a little help in 2009 and we got it.
- We didn't get that much help!
- We got no help in 2010, and with the exception of one site, we were fine
- Two very interesting/irritating sites: Edgewood, MD and Bucks Co, PA.
- The standard will probably fall to 60-70 ppbv in the near future, which will be difficult to achieve

## **Conclusions**

- Dynamic model evaluation produced more reasonable results for most sites
- Edgewood is clearly quite different
  - Think of it as its own area with its own problems?
- Fine particles did NOT work this way (attainment was easy)
- Models only develop the way we push them to
- If we're going to use a model to predict change, we must evaluate its ability to do so and develop the model accordingly.

## **Acknowlegements**

- Lackson Marufu, Jennifer Hains, Russ Dickerson, Charles Piety,
   Dale Allen, Brett Taubman, Bruce Doddridge, Bob Hudson, Shunli
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- Christian Hogrefe, everyone else at NYDEC
- Ray Papalski, Andy Mikula NJDEP

