



USE OF THE CMAQ MODELING SYSTEM FOR ESTIMATING VISIBILITY PROGRESS IN THE SOUTHEASTERN US FOR COMPLYING WITH THE REQUIREMENTS OF THE REGIONAL HAZE RULE

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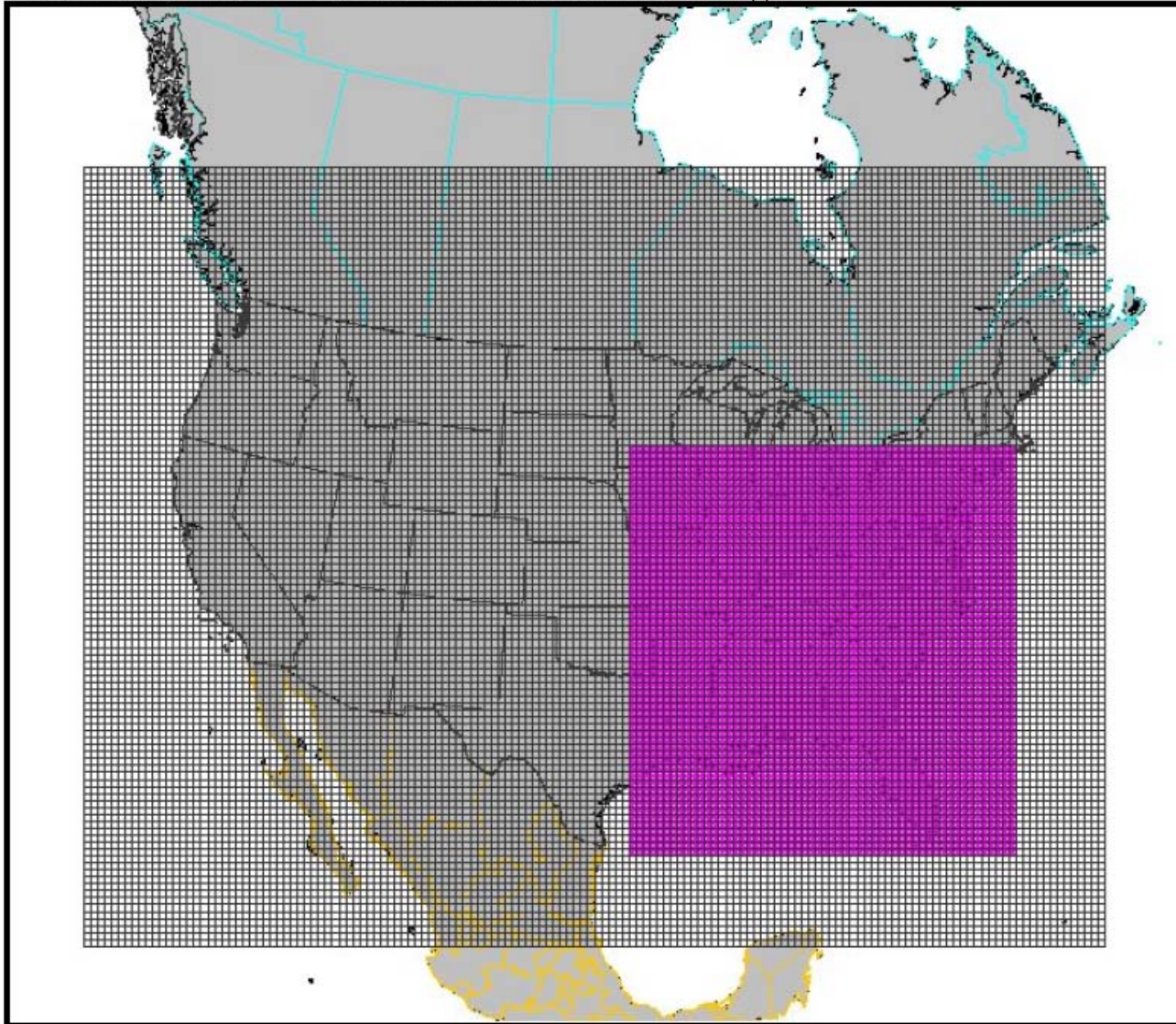
Regional Haze Rule Objectives

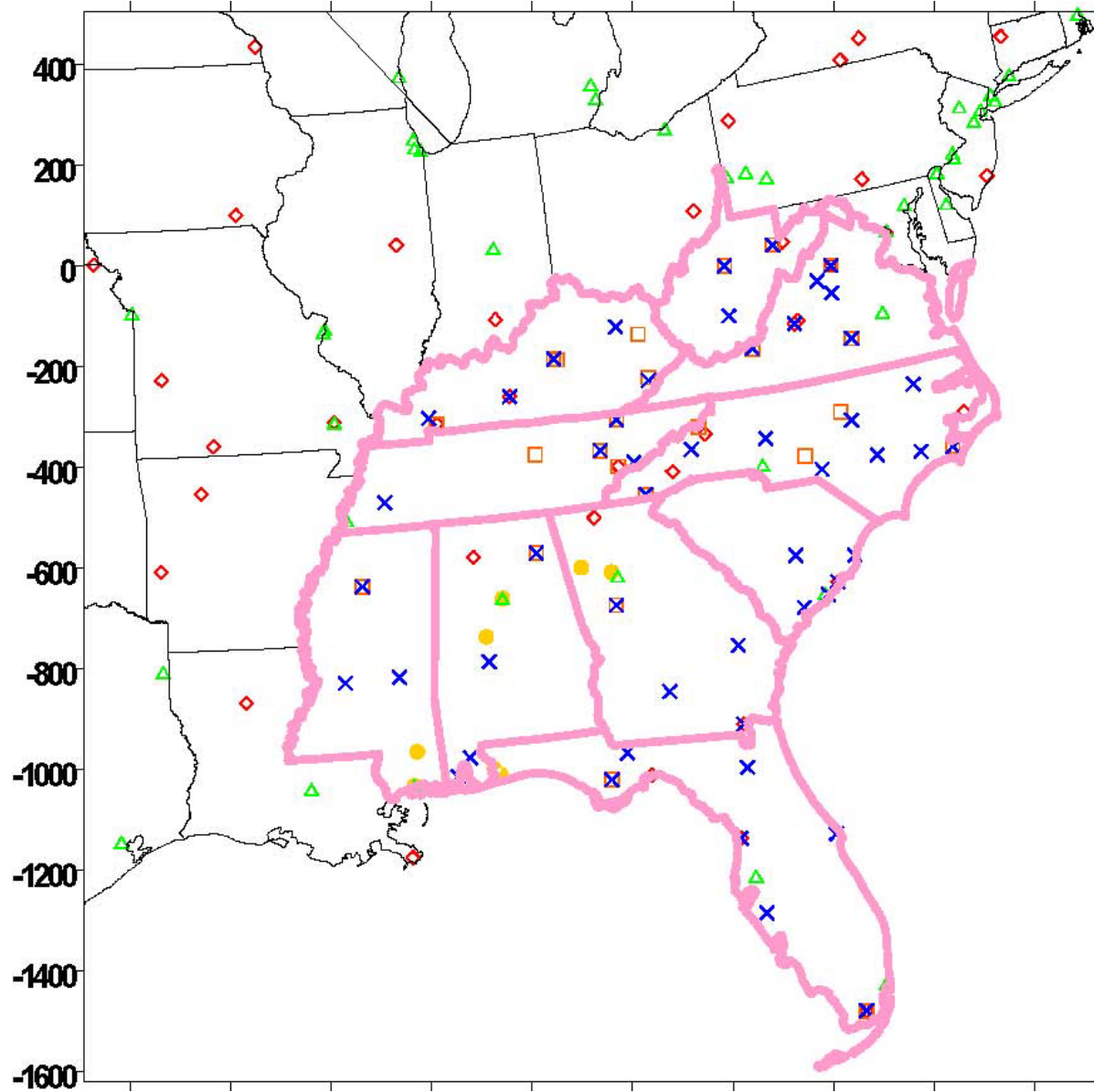
- **Natural Visibility Conditions (no man-made impairment) at 156 Federally mandated Class I areas by 2064**
- **States need to demonstrate progress toward Natural Conditions in State Implement Plans (SIPs) with first SIP due December 2007 that demonstrates progress in 2018:**
 - **Progress toward Natural Conditions for the Worst 20% visibility days at each Class I area**
 - **No degradation in visibility for Best 20% days**
- **Progress is demonstrated using regional modeling of 2002 and 2018 emission scenarios**

VISTAS 2002 Modeling Approach






- **36 km USA and 12 km Eastern USA Grid**
- **MM5 Meteorological & SMOKE Emissions**
- **CMAQ PM/Ozone Air Quality Model**
- **2002 Base Case Simulation (Actual & Typical)**
 - Model Performance Evaluation
 - Speciated PM (SO₄, NO₃, EC, OC, Soil and CM), Wet Deposition and Gaseous Species (O₃, SO₂, NO_x, HNO₃, NH₃)
- **2018 Future-Year Simulations**
 - Visibility Projections at Class I Areas using Relative Reduction Factors (RRFs)
 - Compare with Regional Haze Rule (RHR) Reasonable Progress Goal (RPG)

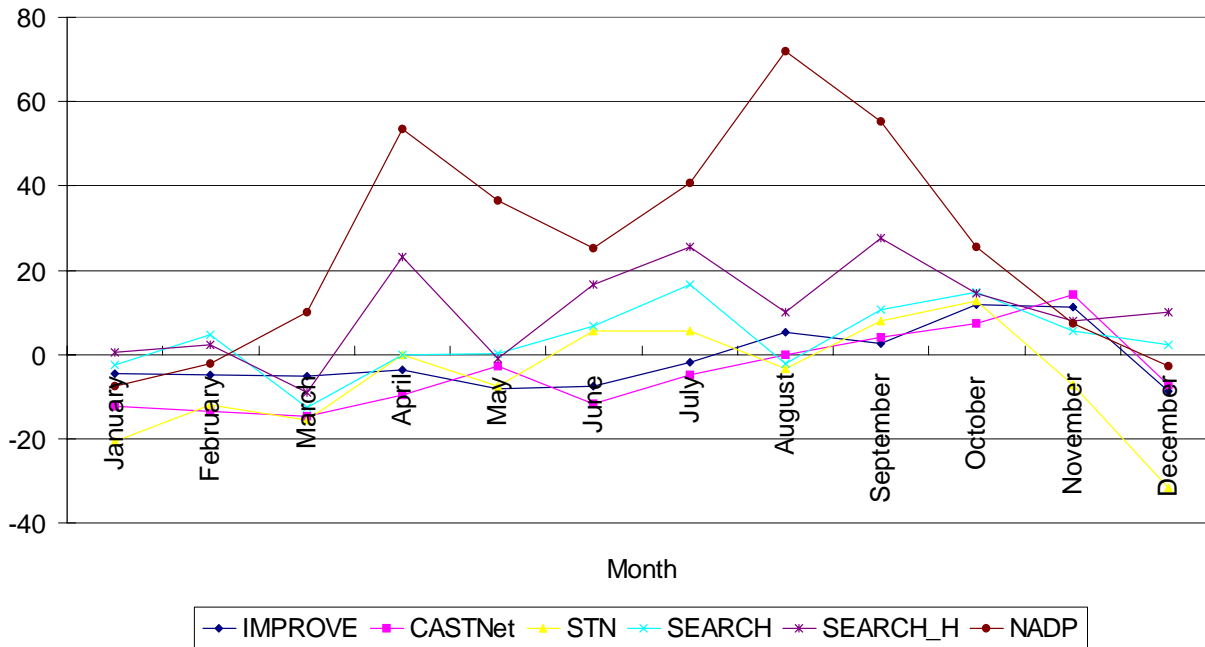
VISTAS 2002 36/12 km Grids





PM Monitors located in the VISTAS States used in the Model Performance Evaluation

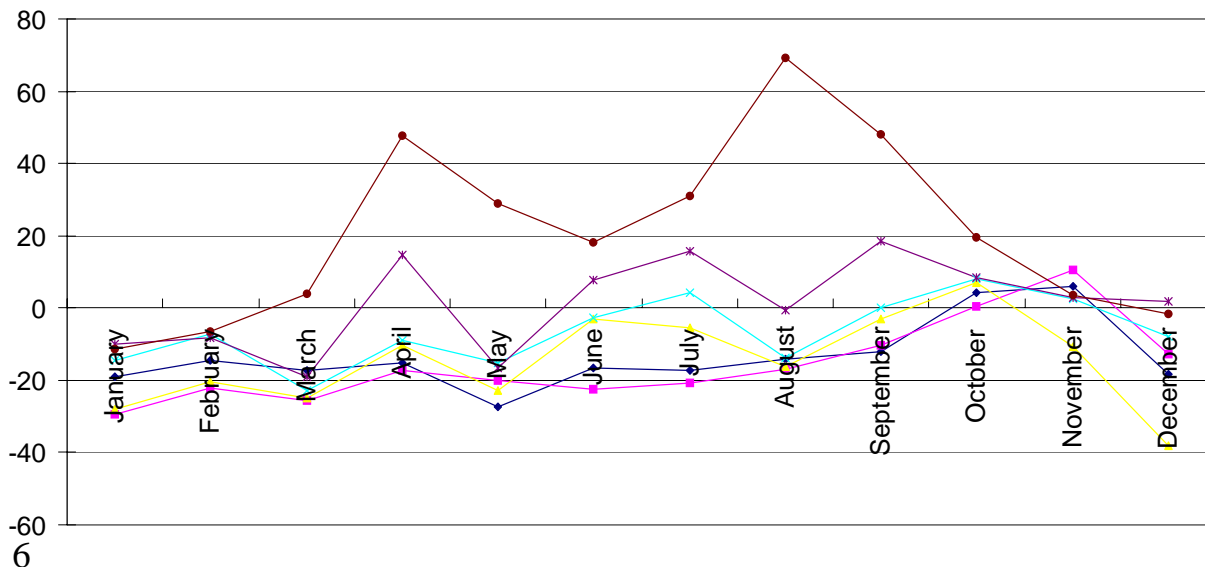
-  **IMPROVE**
-  **CASTNET**
-  **SEARCH**
-  **STN**
-  **NADP**



Sulfate (SO4) CMAQ 36 km Fractional Bias

← Base A CMAQ V4.3

FBias mostly within $\pm 20\%$ for most months except wet dep (NADP)



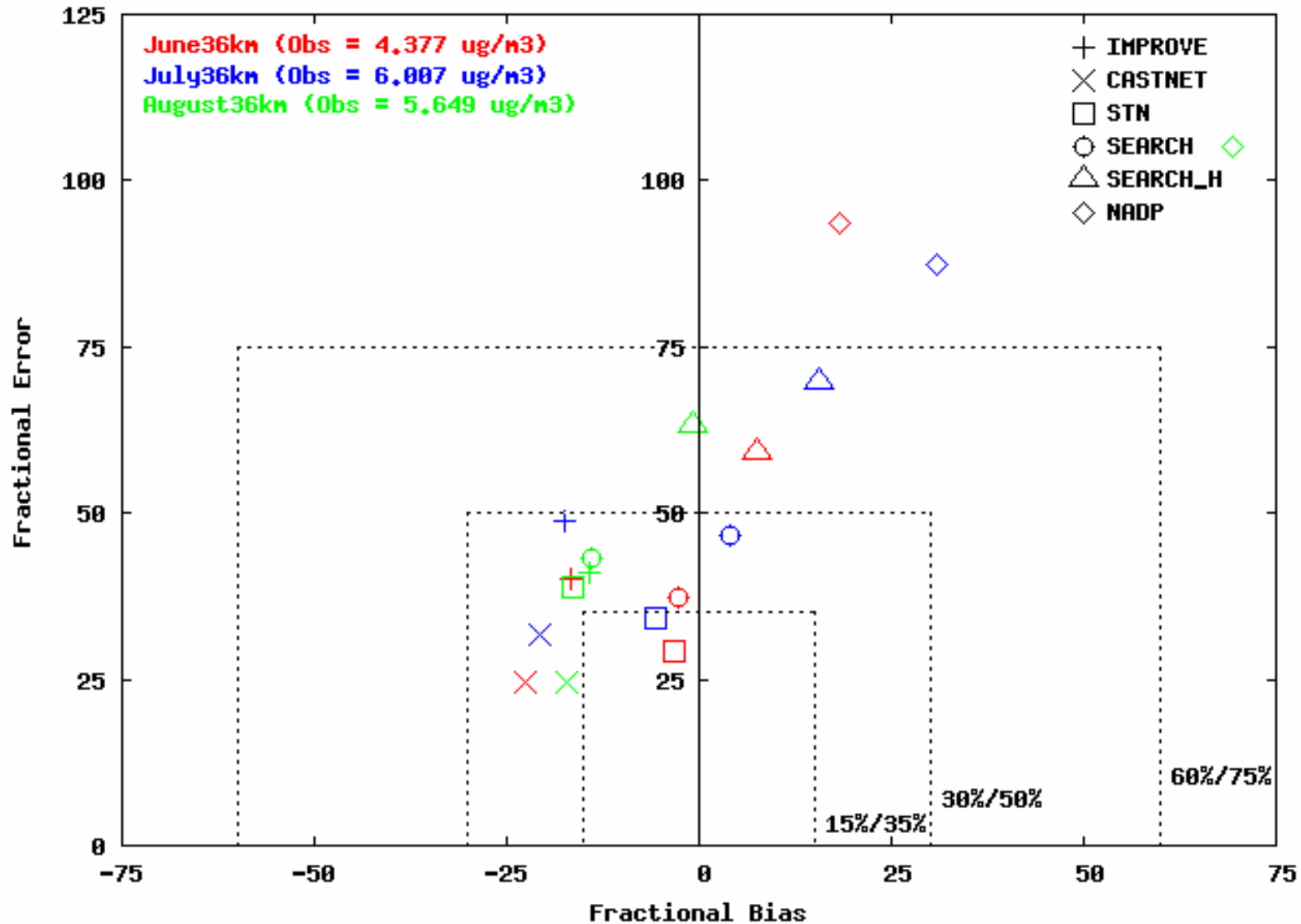
← Base C CMAQ V4.4

Lower SO4, worse performance w/ V4.4

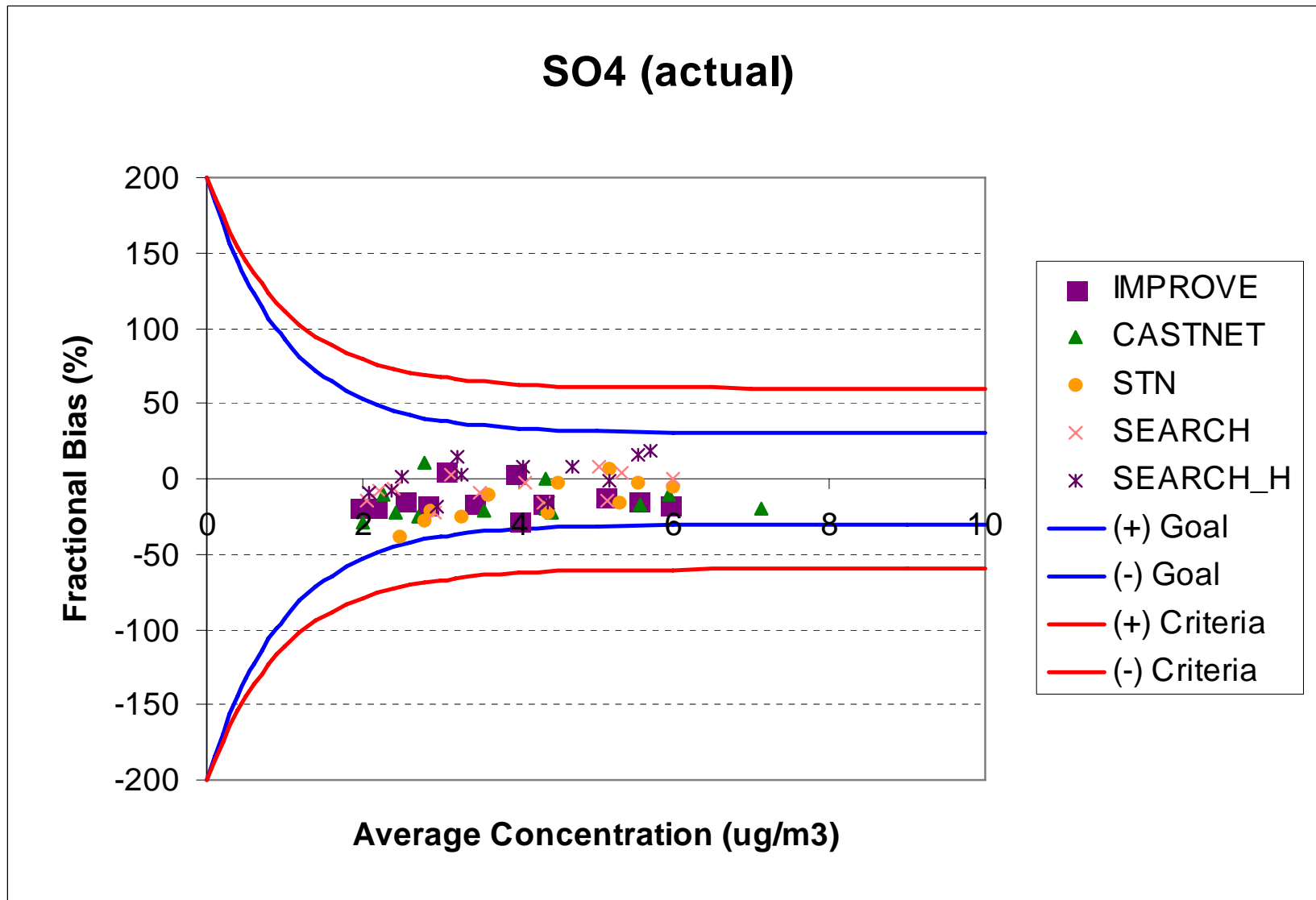
V4,5 further degradation?

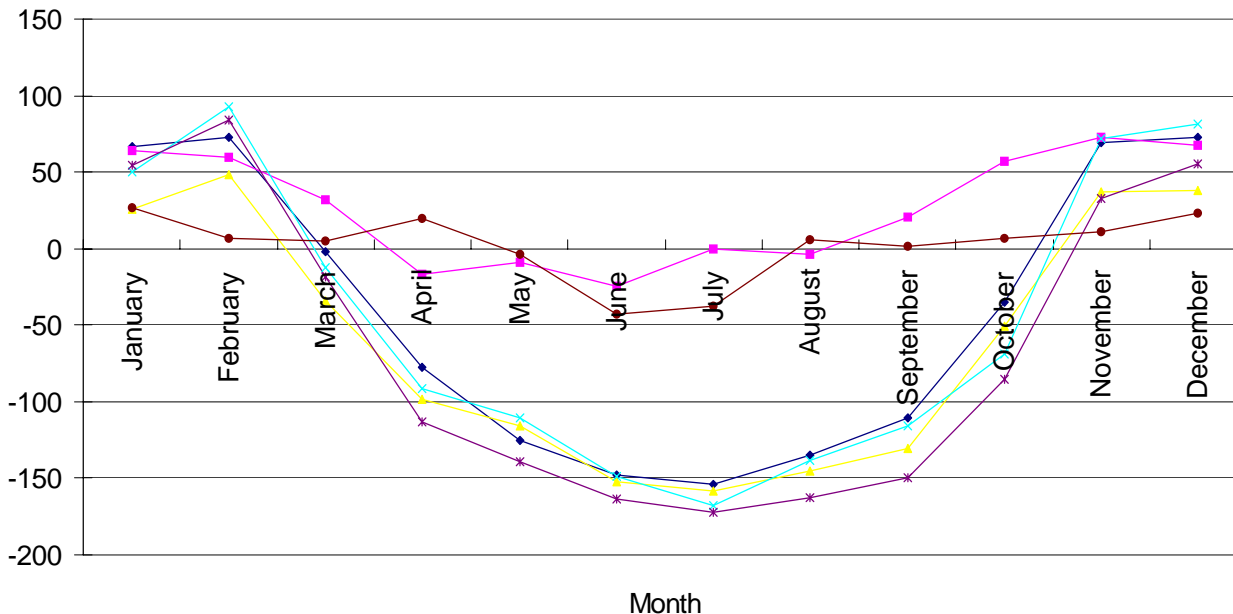
Soccer Plots of Fractional Bias versus Gross Error SO4 Revised 2002 CMAQ 36 km Base C -- Summer

SO4 : CMAQ 36 km Base C - Summer



Bugle Plots of 2002 Monthly SO₄ Fractional Bias for Sites within the VISTAS States CMAQ V4.4





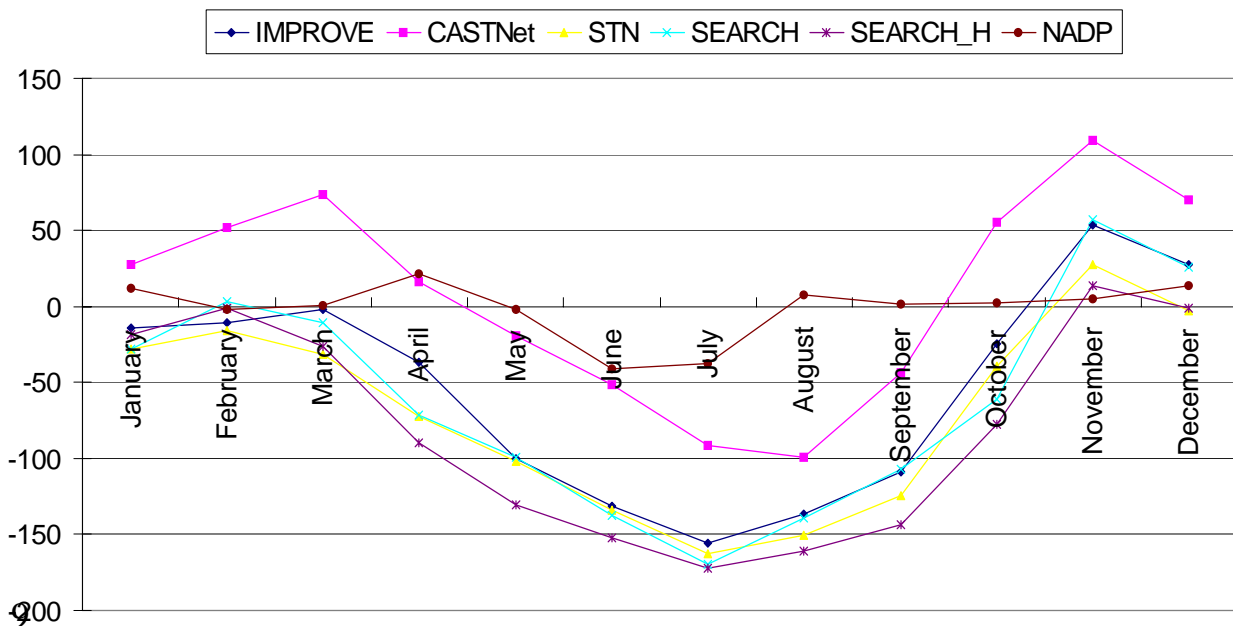
Nitrate (NO3) CMAQ 36 km Fractional Bias

← Base A V4.3

Improved ammonia
emissions between
Base A and C

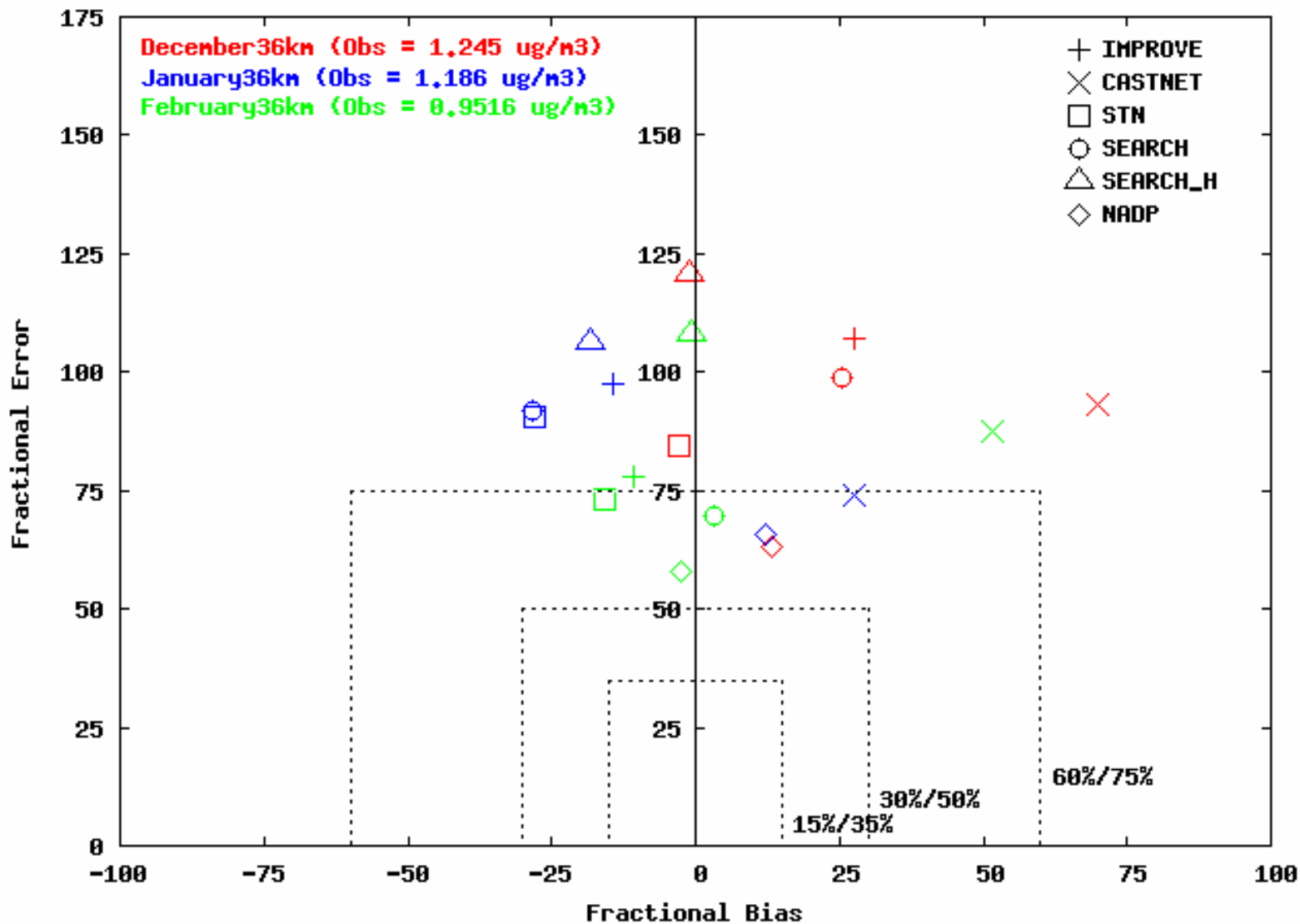
← Base C V4.4

Winter NO3
overestimation bias
summer
underestimation
bias

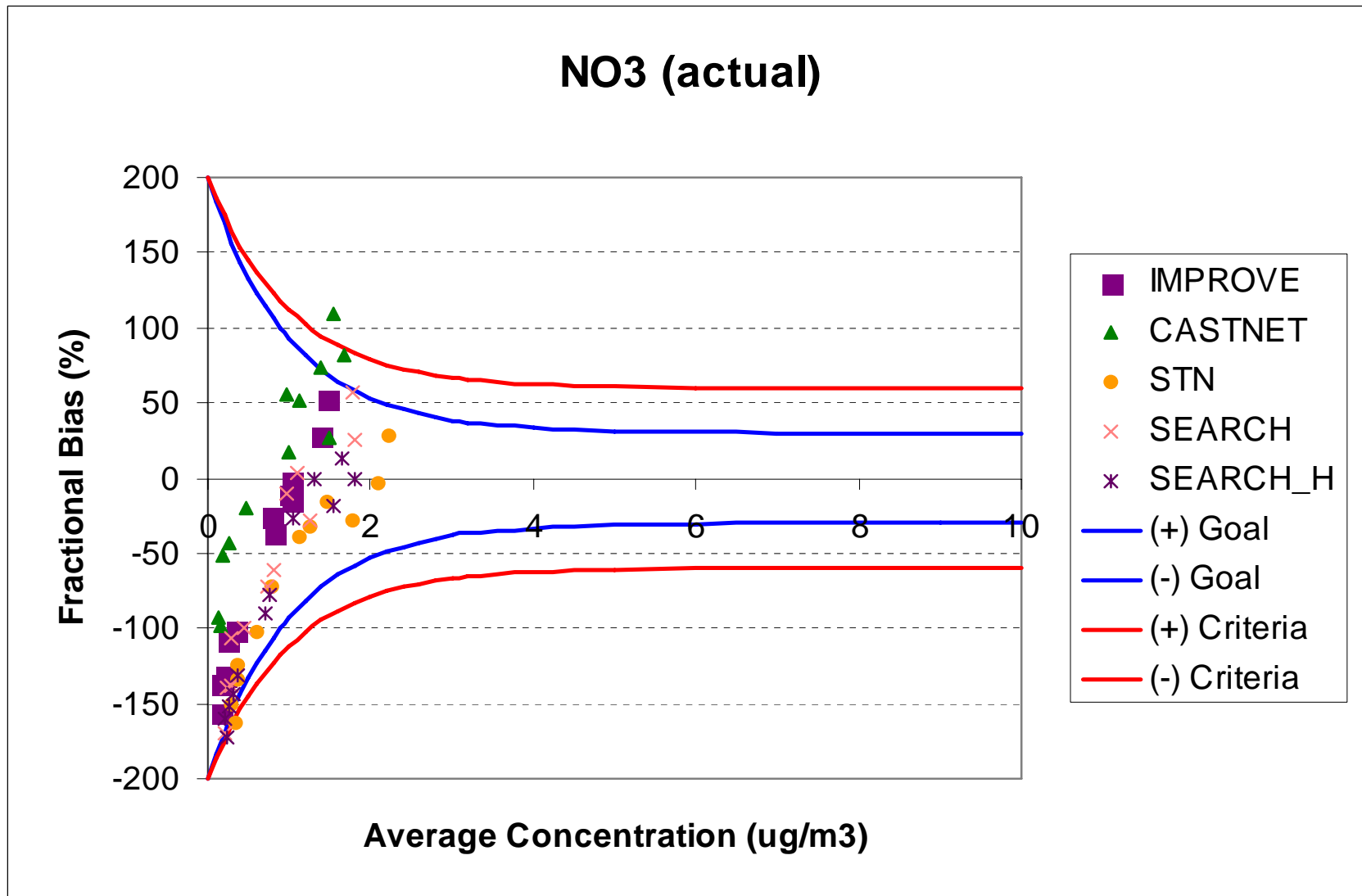


Soccer Plots of Fractional Bias versus Gross Error NO3 Initial 2002 CMAQ 36 km Base C -- Winter

NO3 : CMAQ 36 km Base C - Winter

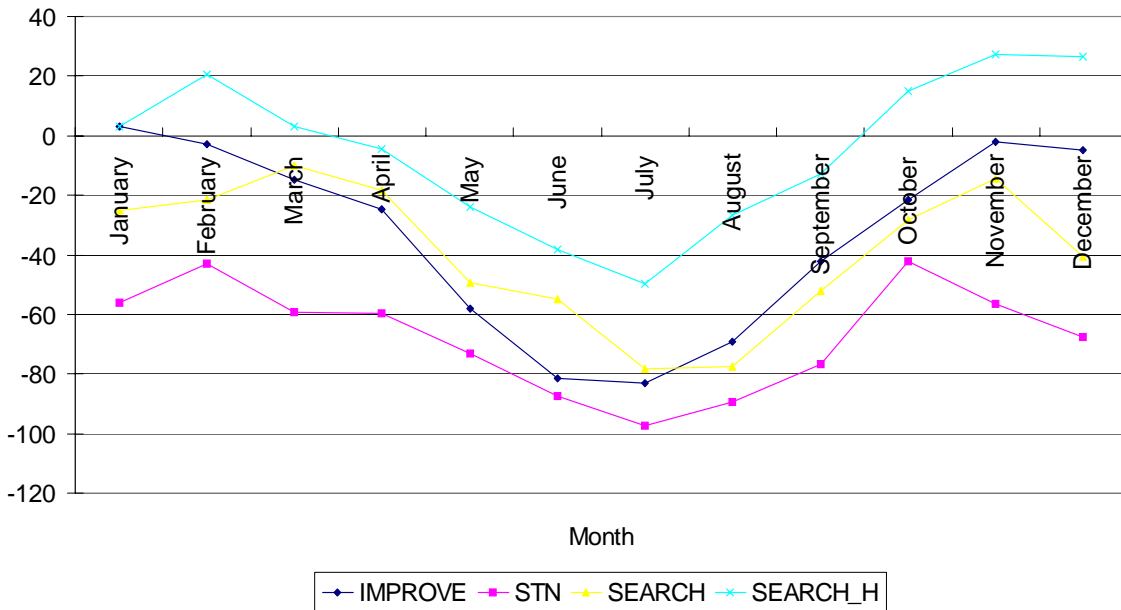


Bugle Plots of 2002 Monthly NO₃ Fractional Bias for Sites within the VISTAS States CMAQ V4.4



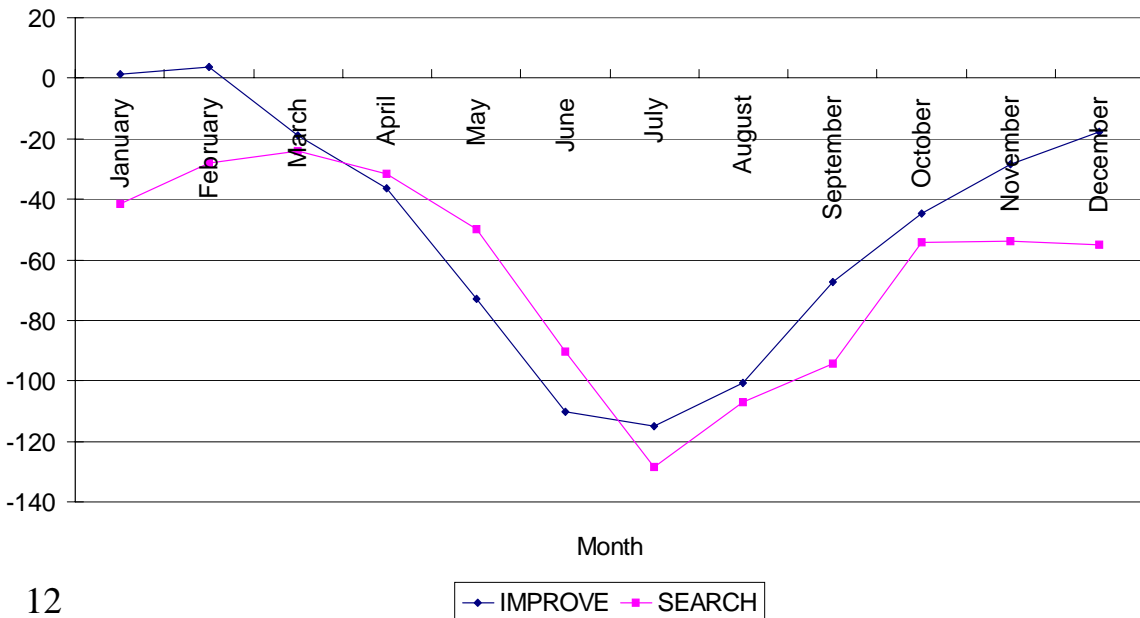
Organic Carbon (OC) CMAQ 36 km Fractional Bias

← Base A V4.3



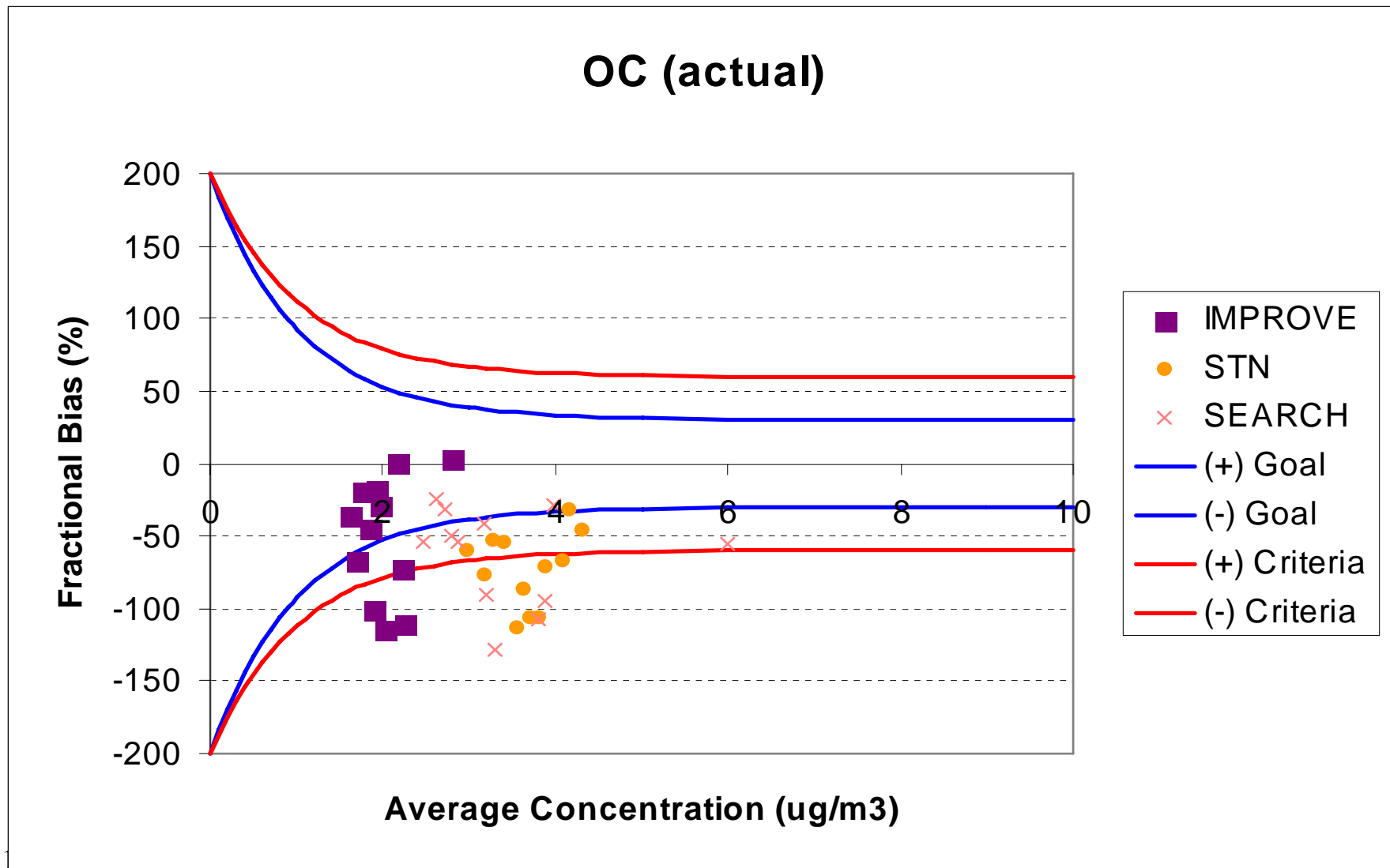
OC summer
underestimation bias
from -80% V4.3 to
-102% V4.4

← Base C V4.4



OC second most
important visibility
degrading pollutant

Bugle Plots of 2002 Monthly OC Fractional Bias for Sites within the VISTAS States CMAQ V4.4



Organic Carbon Sensitivity Analysis

- **CMAQ V4.4 Organic Carbon (OC) summer under-prediction bias (~ -100%) cause for concern; second most important PM_{2.5} and visibility species**
- **Reviewed CMAQ V4.4 treatment of OC species:**
 - **Likely missing or understated primary OC emissions in inventory**
 - **Several process that may be important to the Secondary Organic Aerosol (SOA) formation missing**
- **Decision to enhance CMAQ SOA module and perform emissions investigations**

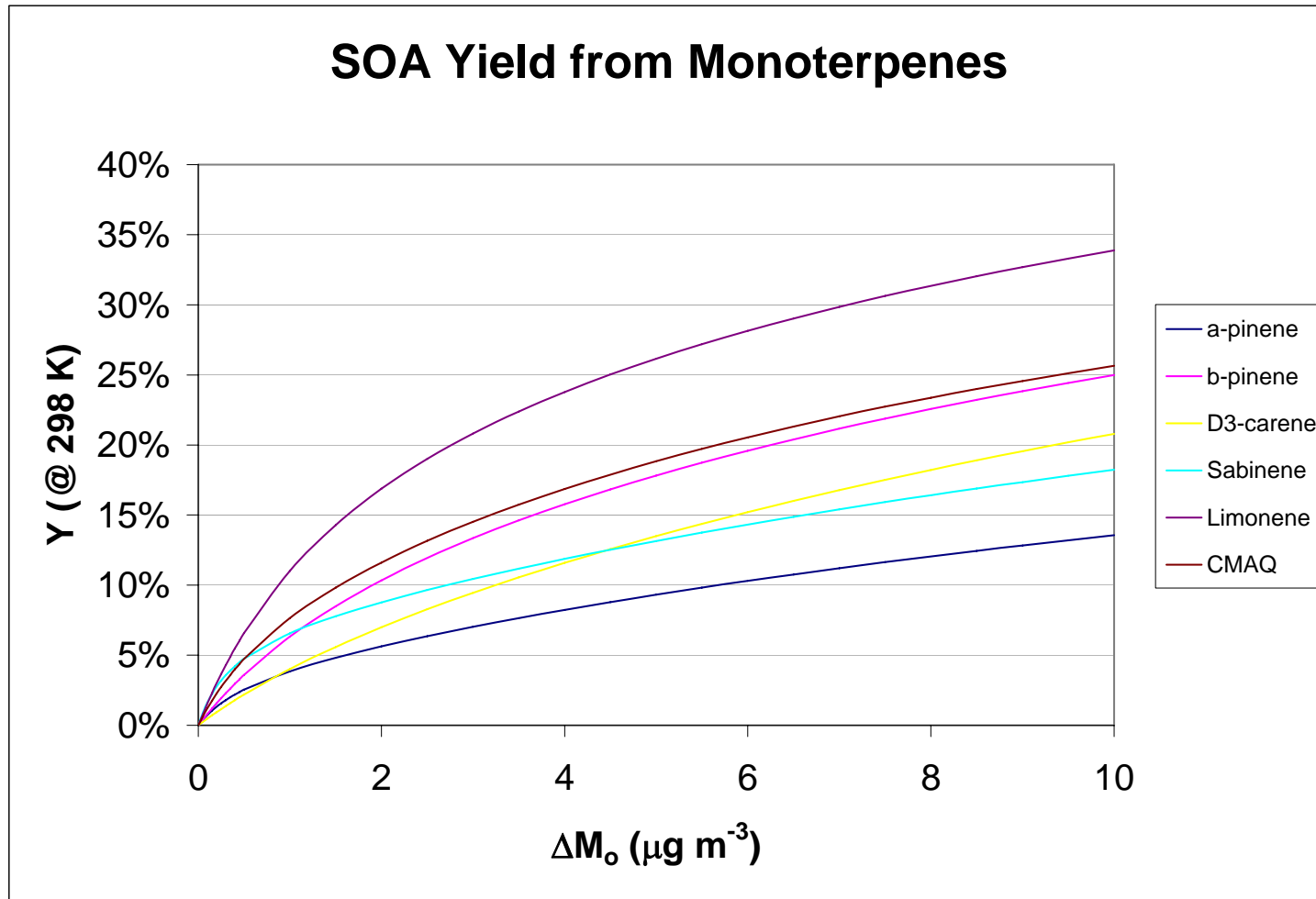
CMAQ V4.4 SOA Module

- **VOC SOA Precursors: Aromatics & Terpenes**
 - Terpenes represented by BEIS3 biogenic TERPM lumped monoterpene species
 - Anthropogenic aromatic represented by CB4 XYL (xylene) and TOL (toluene) species
- **Oxidation: VOC + OH → CG (Condensable Gas)**
- **Equilibrium: CG ⇌ SOA (species and met)**
- **CMAQ transports SGTOT = CG + SOA**
 - Split into CG and SOA in aerosol module and save for output



CMAQ V4.4 SOA Module

- **BEIS3 TERPB Biogenic Terpenes**
 - Based on measured monoterpene (MT) species that are overstated
 - Does not include higher yield sesquiterpenes (SQT)
- **CMAQ TERPB SOA parameters based on fit to monoterpene data from CalTech smog chambers**
 - Monoterpene species only
 - Two product representation
 - Chamber artifacts introduces uncertainties, but best data available

CMAQ SOA Module fit to Chamber



CMAQ SOA Module Parameters fit to monoterpenes:

-  **α-pinene**
-  **β-pinene**
- D3-carene**
- Sabinene**
- Limonene**

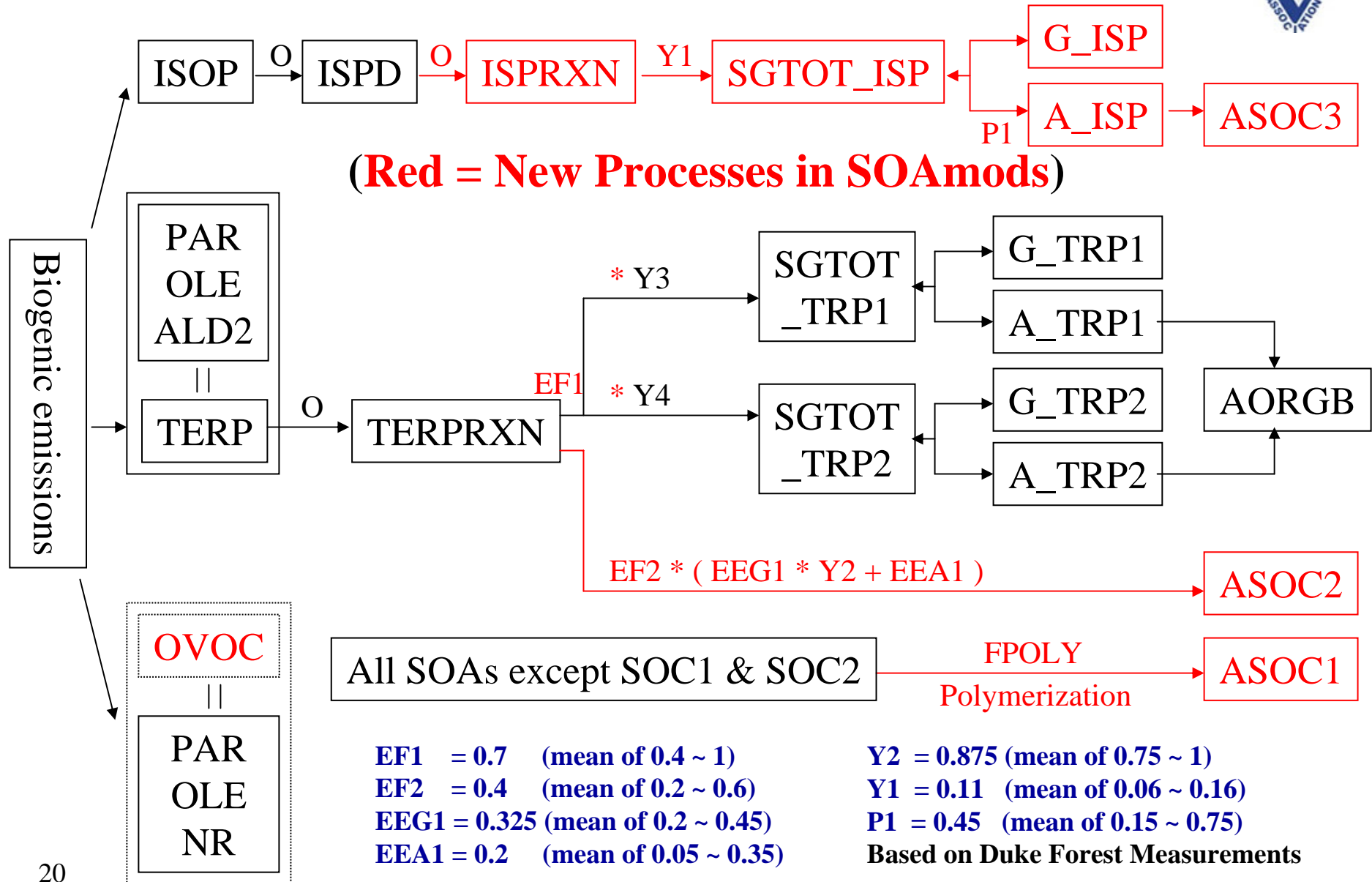
Missing SOA Processes in CMAQ

- **Polymerization**: SOA becomes nonvolatile
 - Kalberer et al (2004) saw 50% SOA polymerized in 20 hours
- **Sesquiterpenes**: Not included, known important SOA precursor
 - Important for VISTAS Class I areas
- **Isoprene**: Not included, high in southeastern US
 - New evidence that isoprene may be SOA precursor that appears to be sensitive to SO₂/SO₄
- **Biogenic OVOC**: Also SOA precursor (Nonanal)
- **Acid Catalyzed Formation**: Some biogenic SOA formation higher under acidic conditions

Development of Enhanced SOA Module

- **Added to existing CMAQ SOA module for monoterpenes**
- **Analyze Duke Forest ambient field study data to develop range of parameters for sesquiterpenes and isoprene**
 - **Select midpoint of data range**
 - **Alex Guenther (NCAR) analyzed data**
 - **Bonyoung Koo (ENVIRON) implement algorithms**
- **Other parameters from literature**

Enhanced CMAQ V4.4 SOA Module



CMAQ SOAmods Testing

- **Applied to January 2002 and July 2002**
 - Standard CMAQv4.4
 - CMAQv4.4 with SOAmods
- **Examined Organic Matter Carbon (OMC=1.4 x OC)**
- **Examined various U.S. sub-domains**
 - VISTAS, MRPO, MANE-VU, CENRAP, WRAP
- **Annual 2002 Base Case run**

OMC at VISTAS (July 2002) IMPROVE & SEARCH

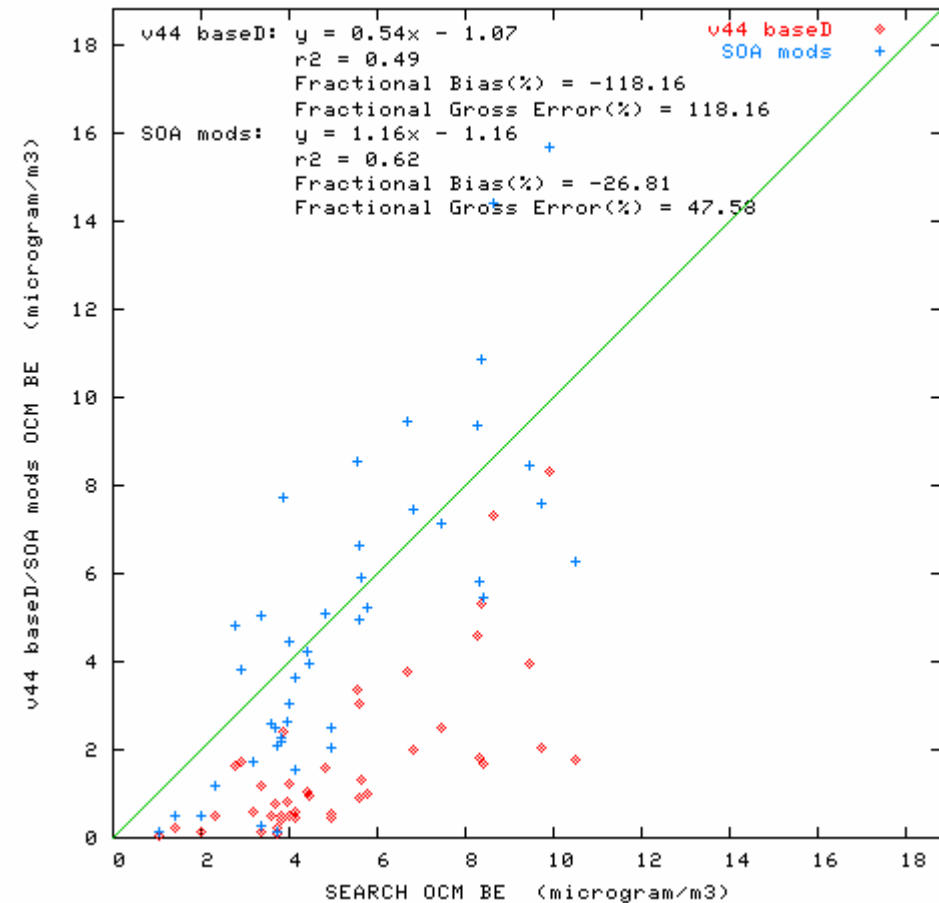
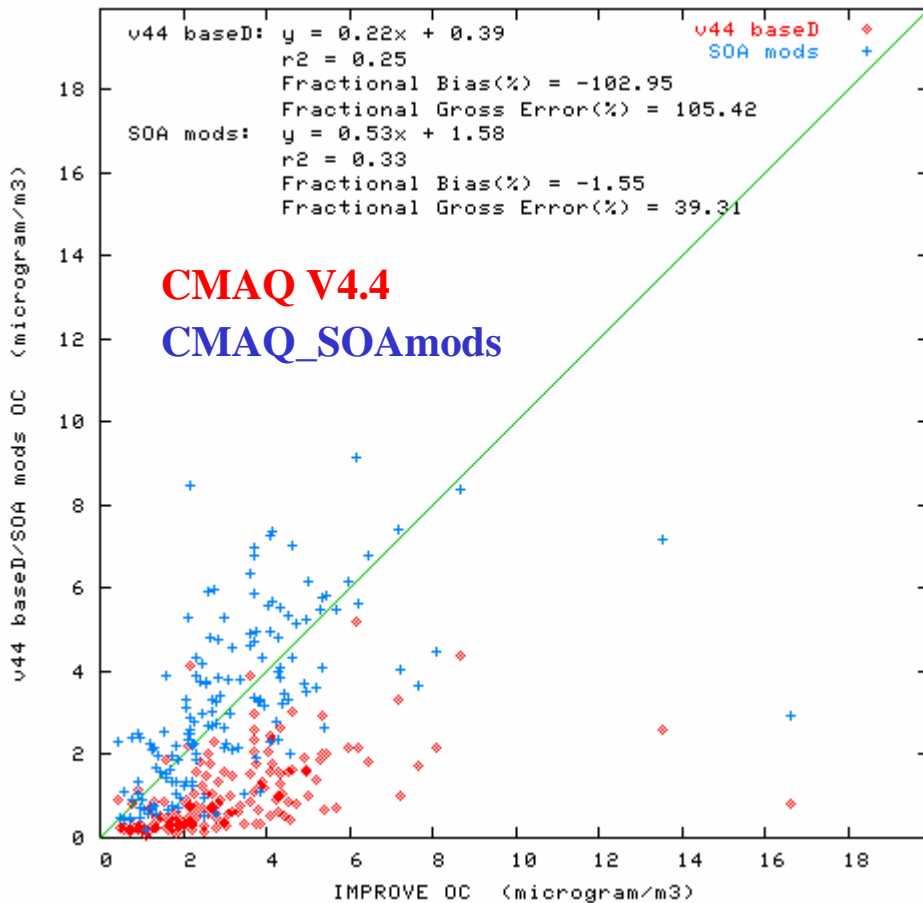


FB: **-103%** → **-2%**

FB: **-118%** → **-27%**

IMPROVE vs. v44 baseD/SOA mods OC at 16 stations on 2002182-20022

SEARCH vs. v44 baseD/SOA mods OCM BE at 8 stations on 2002182-2002



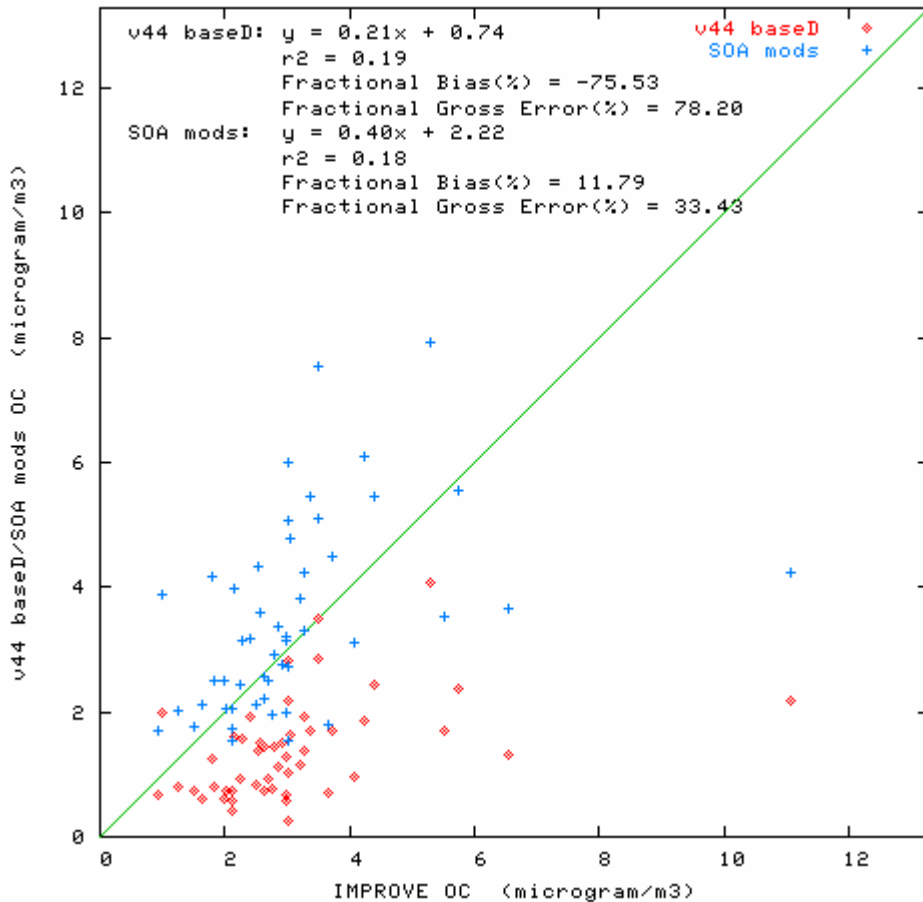
OMC/TCM at MRPO (July 2002)

IMPROVE & STN

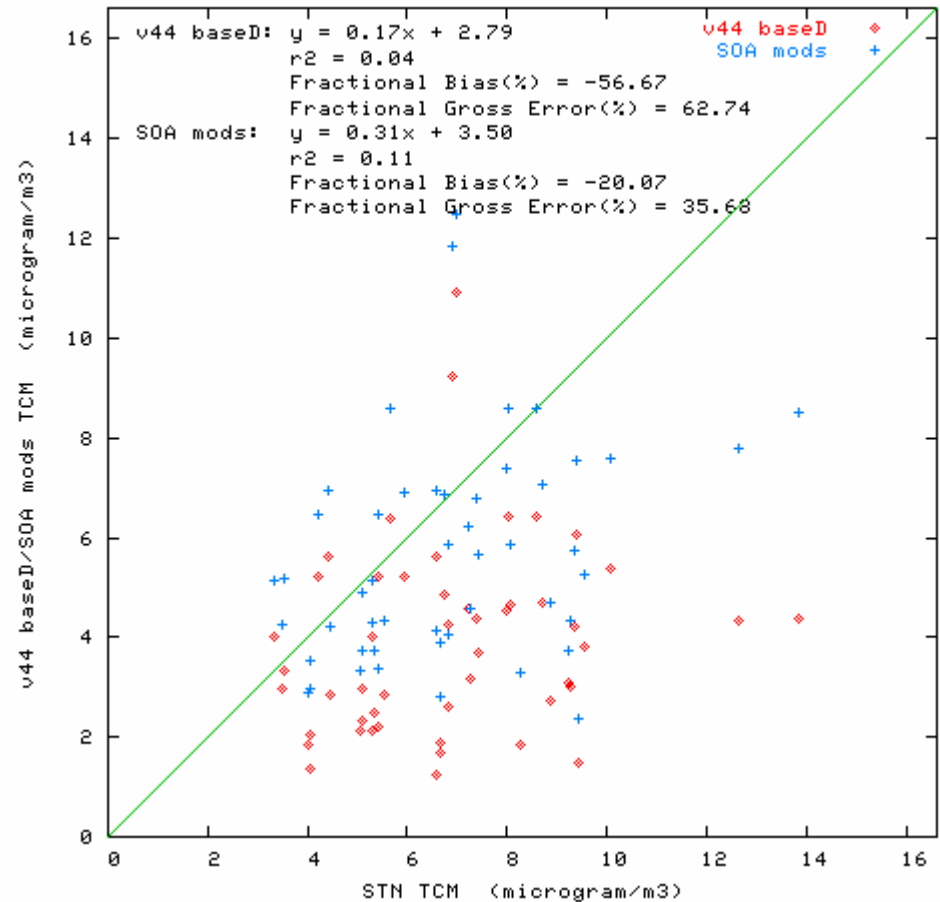
OMC FB: -76% → +12%

TCM FB: -57% → -20%

IMPROVE vs. v44 baseD/SOA mods OC at 5 stations on 2002182-2002212



STN vs. v44 baseD/SOA mods TCM at 6 stations on 2002182-2002212



CMAQ V4.4 vs. SOAmods

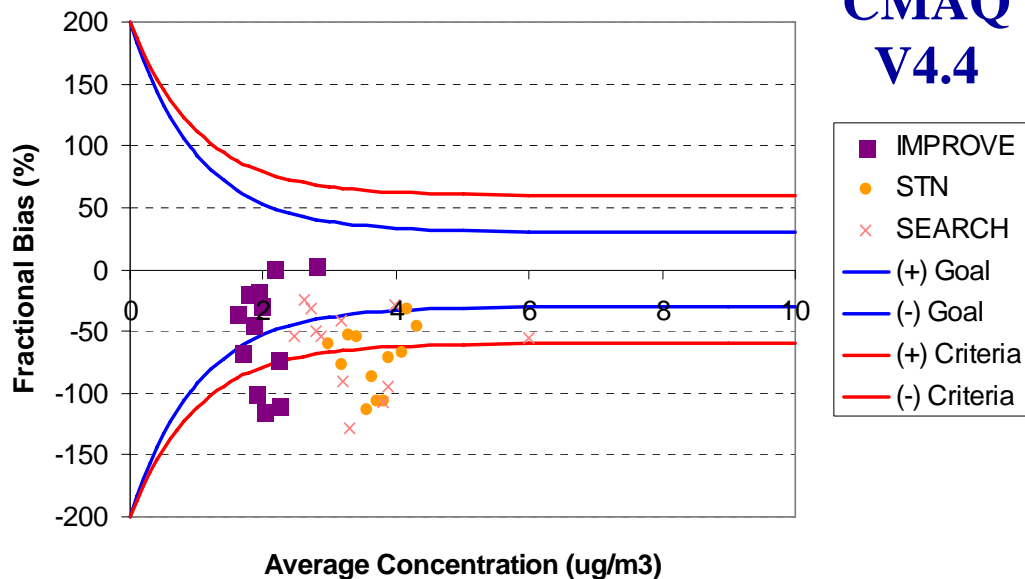
IMPROVE (OMC)

STN (TCM)

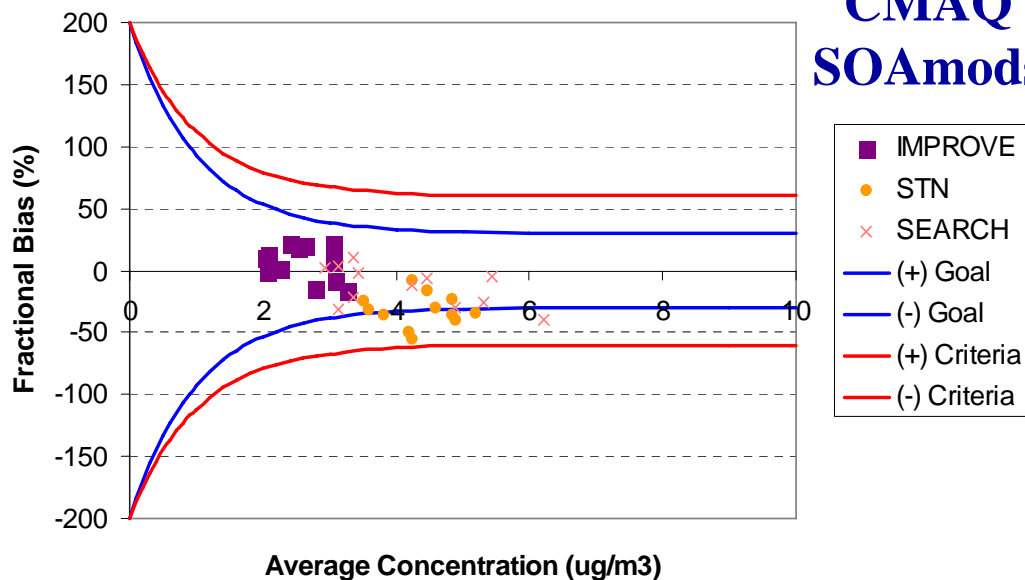
F. BIAS	CMAQv4.4	SOAmods	CMAQv4.4	SOAmods
VISTAS	-103%	-2%	-93%	-30%
MRPO	-76%	+12%	-57%	-20%
M-VU	-82%	-14%	-82%	-40%
CENRAP	-98%	+8%	-69%	-23%
WRAP	+40%	+84%	-6%	+22%

F. ERROR	CMAQv4.4	SOAmods	CMAQv4.4	SOAmods
VISTAS	105%	39%	96%	46%
MRPO	78%	33%	63%	36%
M-VU	88%	52%	89%	52%
CENRAP	100%	49%	82%	48%
WRAP	83%	94%	52%	49%

CMAQ V4.4



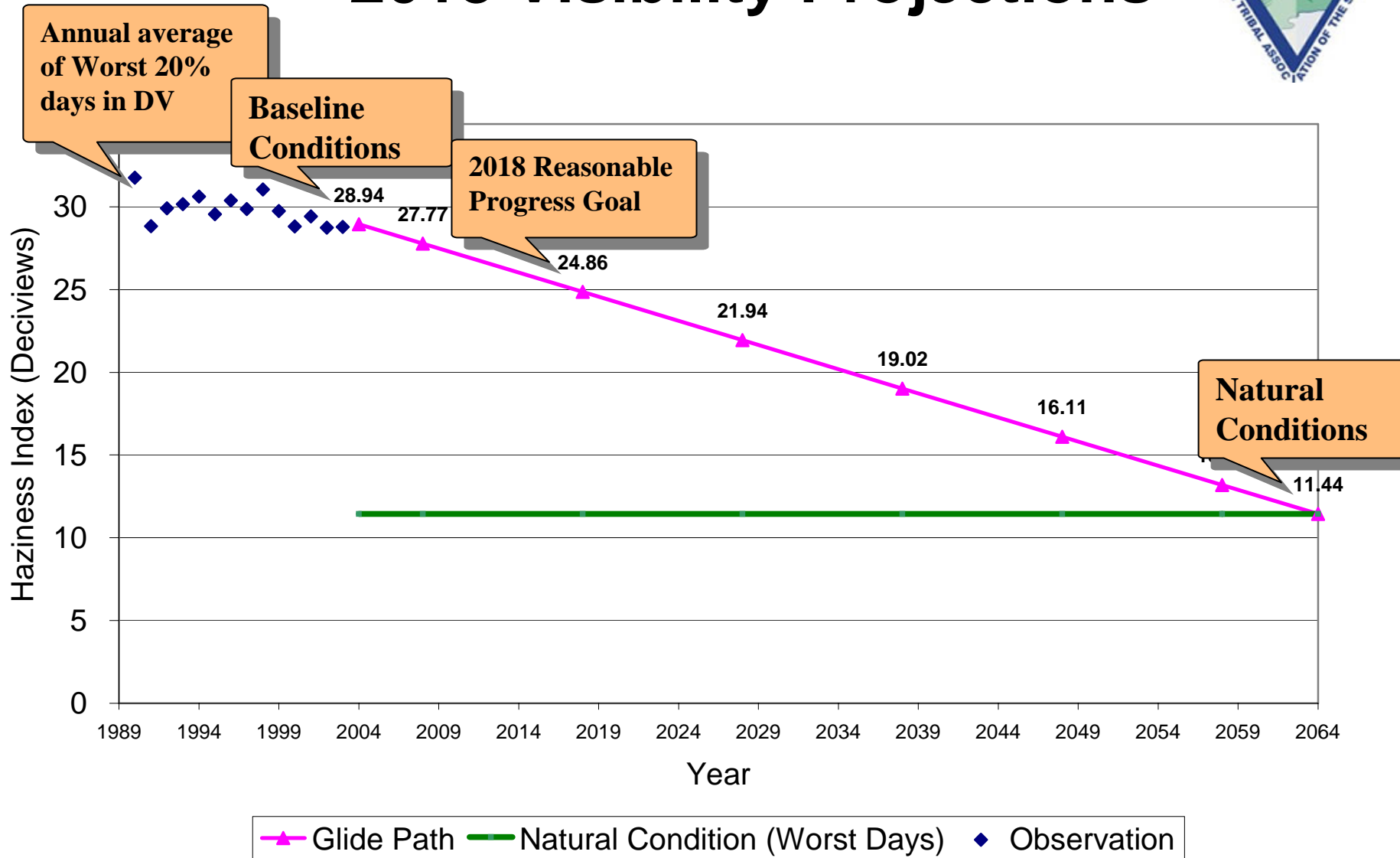
CMAQ SOAmods



**CMAQ with SOAmods
update much improve OC
model performance over
CMAQ V4.4 (V4.5)**

More research needed to develop more definitive SOA mechanism, but SOA from sesquiterpenes, isoprene, and polymerization are real processes that need to be accounted for in order to obtain proper future year visibility and $PM_{2.5}$ projections

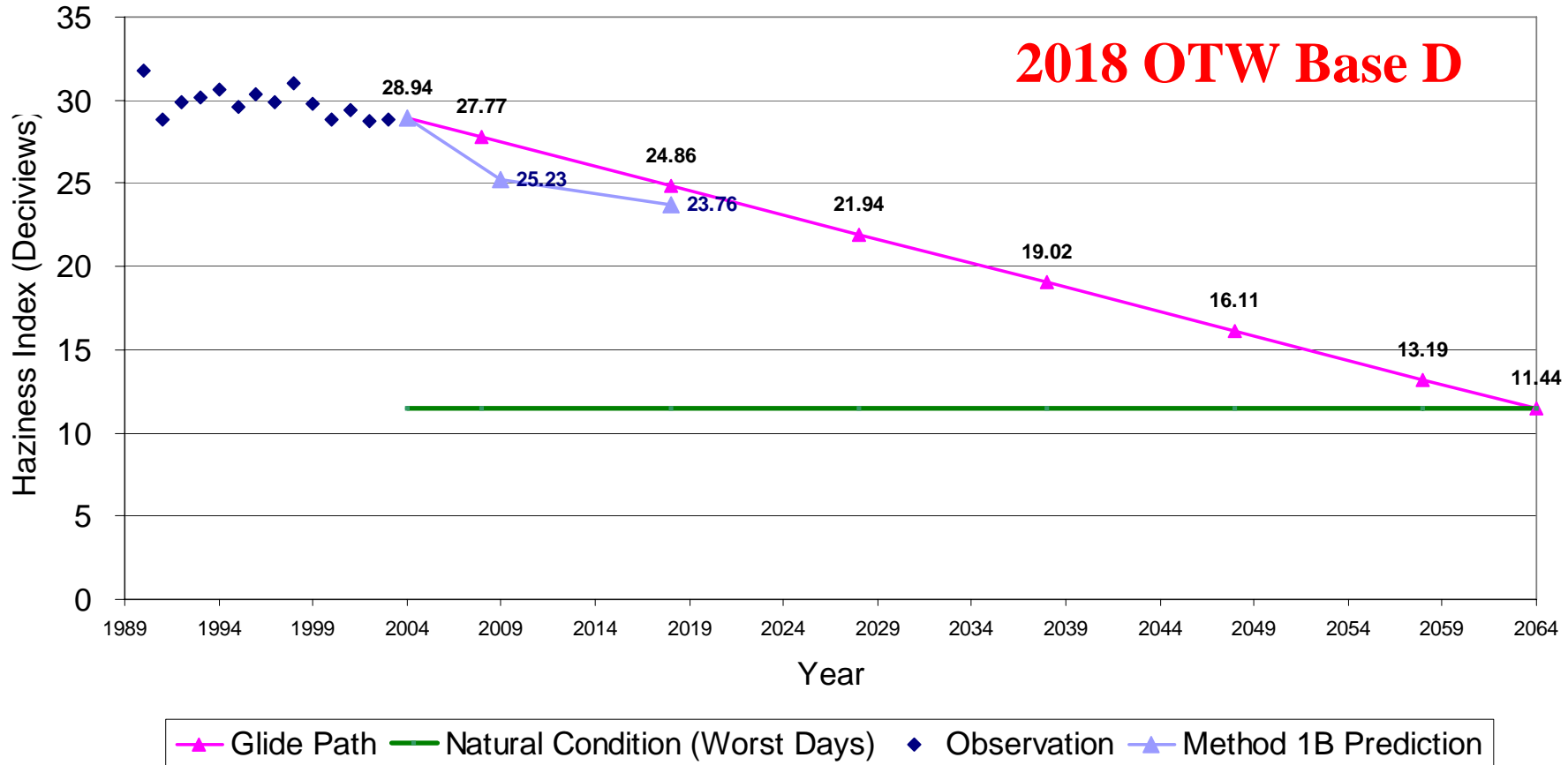
2018 Visibility Projections



Glide Path/Slope to Natural Conditions

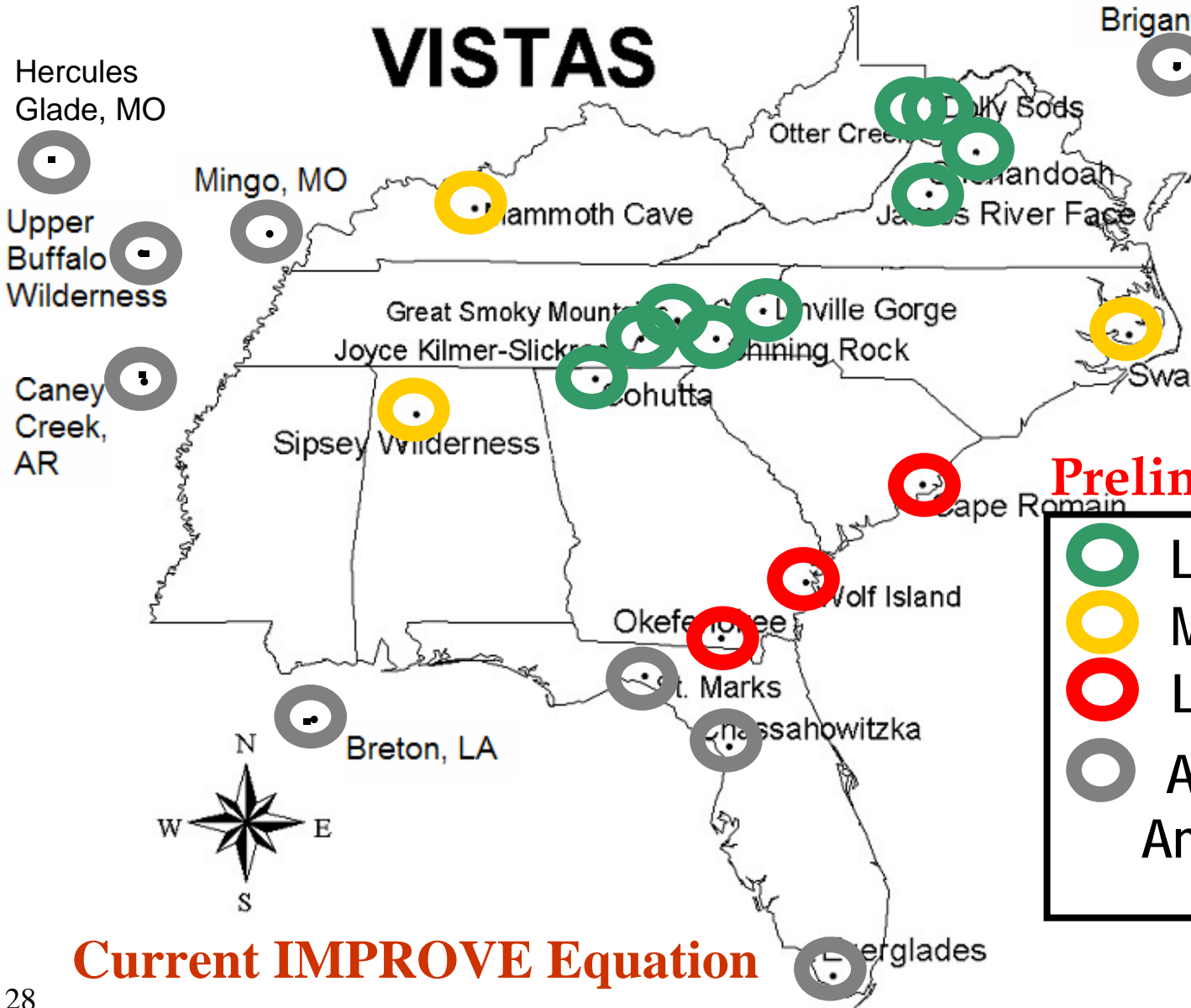
2018 Visibility Projections for GRSM

Uniform Rate of Reasonable Progress Glide Path
Great Smoky Mountains NP (TN) - 20% Worst Days



Baseline Conditions = 28.9 dv **2018 Reduction Goal = 4.1 dv**
Natural Conditions = 11.4 dv **2018 Modeled Reduction = 5.2 dv**
2018 Target = 24.9 dv **GRSM achieves 2018 RPG**

VISTAS



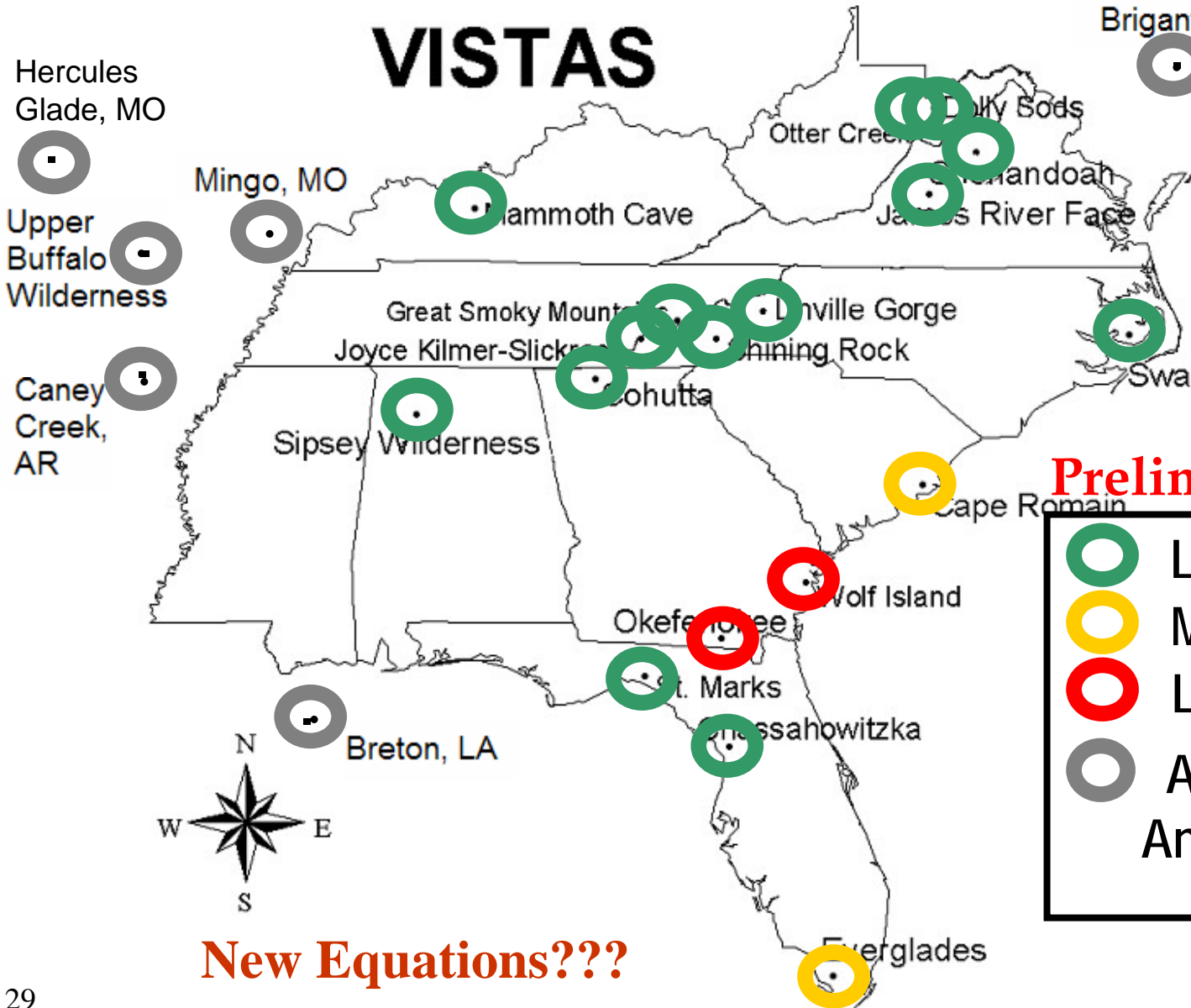
**2018 OTWd
 Visibility
 Projections
 2018 Base D**

Preliminary Results

- Likely to meet
- May meet
- Likely not met
- Additional Analyses Needed

Current IMPROVE Equation

VISTAS



**2018 OTWd
 Visibility
 Projections
 2018 Base D**

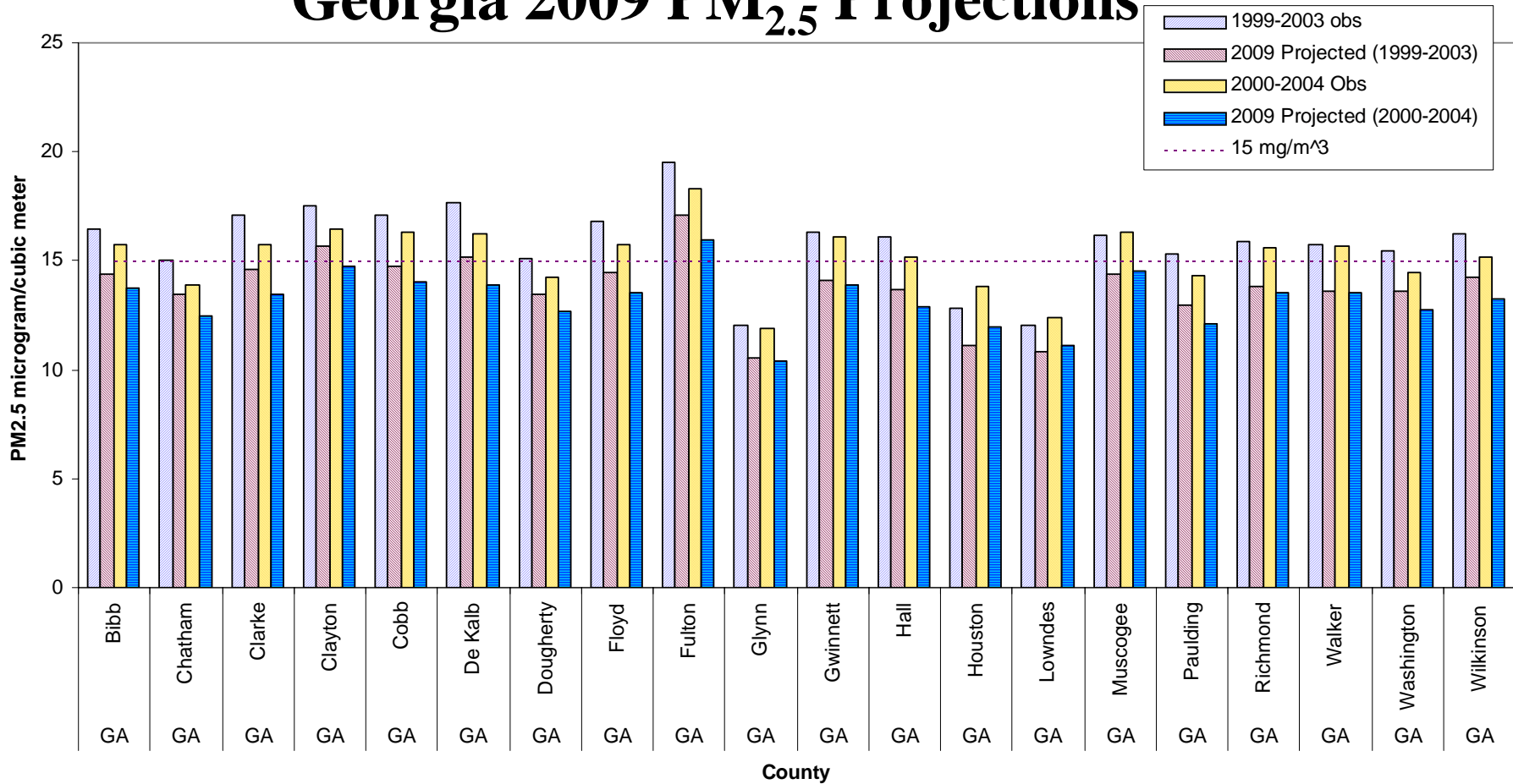
Preliminary Results

- Likely to meet
- May meet
- Likely not met
- Additional Analyses Needed

New Equations???

VISTAS/ASIP Regional Haze Modeling also used to Provide Information for PM_{2.5}

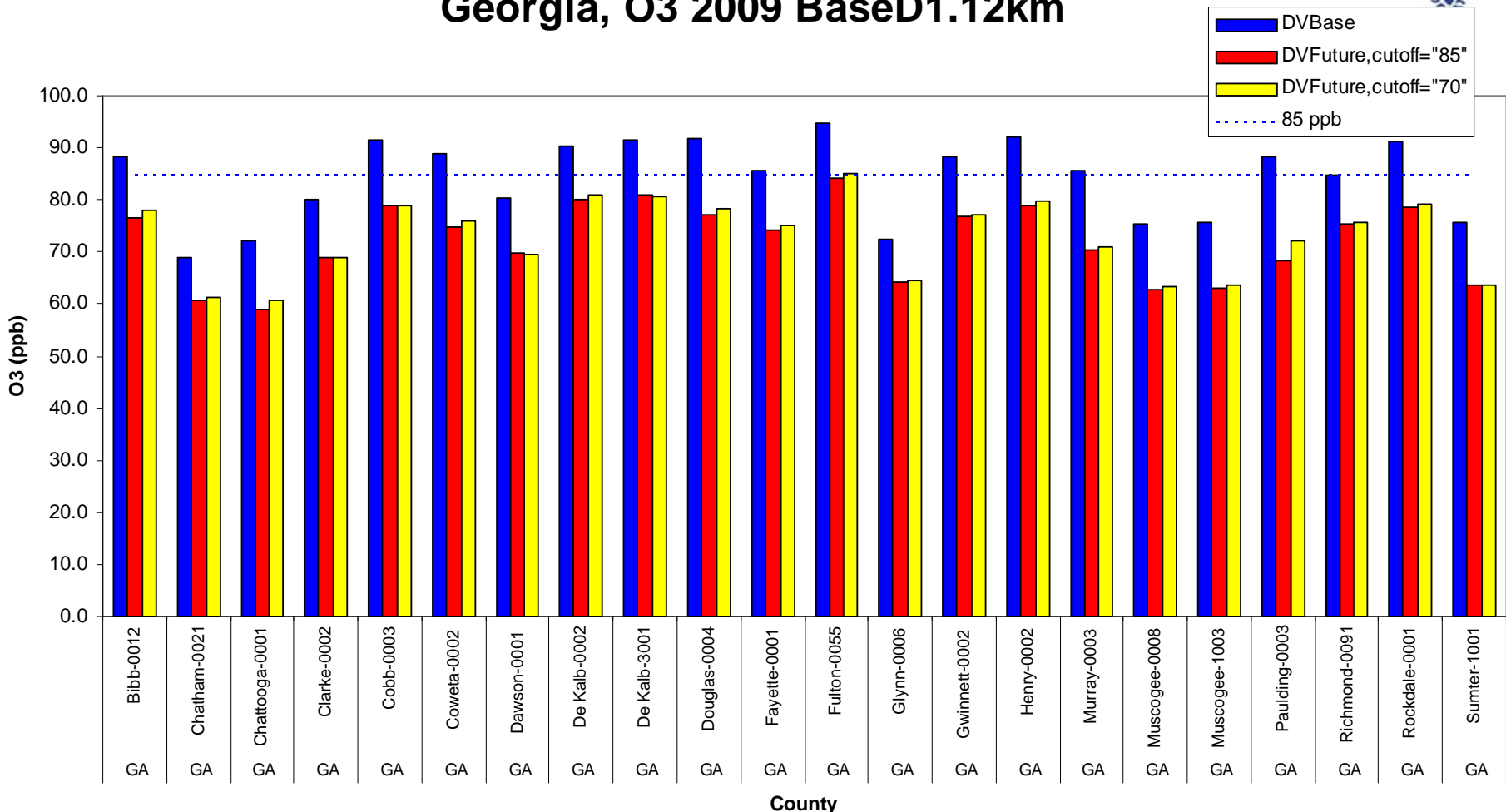
Georgia 2009 PM_{2.5} Projections



Fulton County still a problem area, possibly Clayton and DeKalb Counties (all part of Atlanta MSA)

VISTAS/ASIP 2009 8-hr Ozone Projections

Georgia, O3 2009 BaseD1.12km



GA 12 sites with AvgDV > 85 ppb almost all projected attainment in 2009; Fulton Co. (Confederate Ave. Atlanta on cusp with 2009 AvgDVs: 84.2, 85.0, 82.0, 83.1 ppb

VISTAS/ASIP Next Steps

- **2018 Visibility Projections using Base F Inventories using CMAQ V4.4 w/ SOAmods**
- **Evaluate CMAQ V4.5**
 - Implementation of SOAmods in V4.5?
 - Test & Evaluate CMAQ V4.5 w/ SOAmods?
 - Adopt CMAQ V4.5 w/ SOAmods or keep CMAQ V4.4 SOAmods?
 - **Rerun 2018 OTW Base F?**
- **2002 & 2009 Base F Emissions and CMAQ Modeling**
- **2018 & 2009 Control Strategies**