

Model Performance Evaluation

CENRAP BaseA/St. Louis PM2.5



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ENVIRON International Corporation

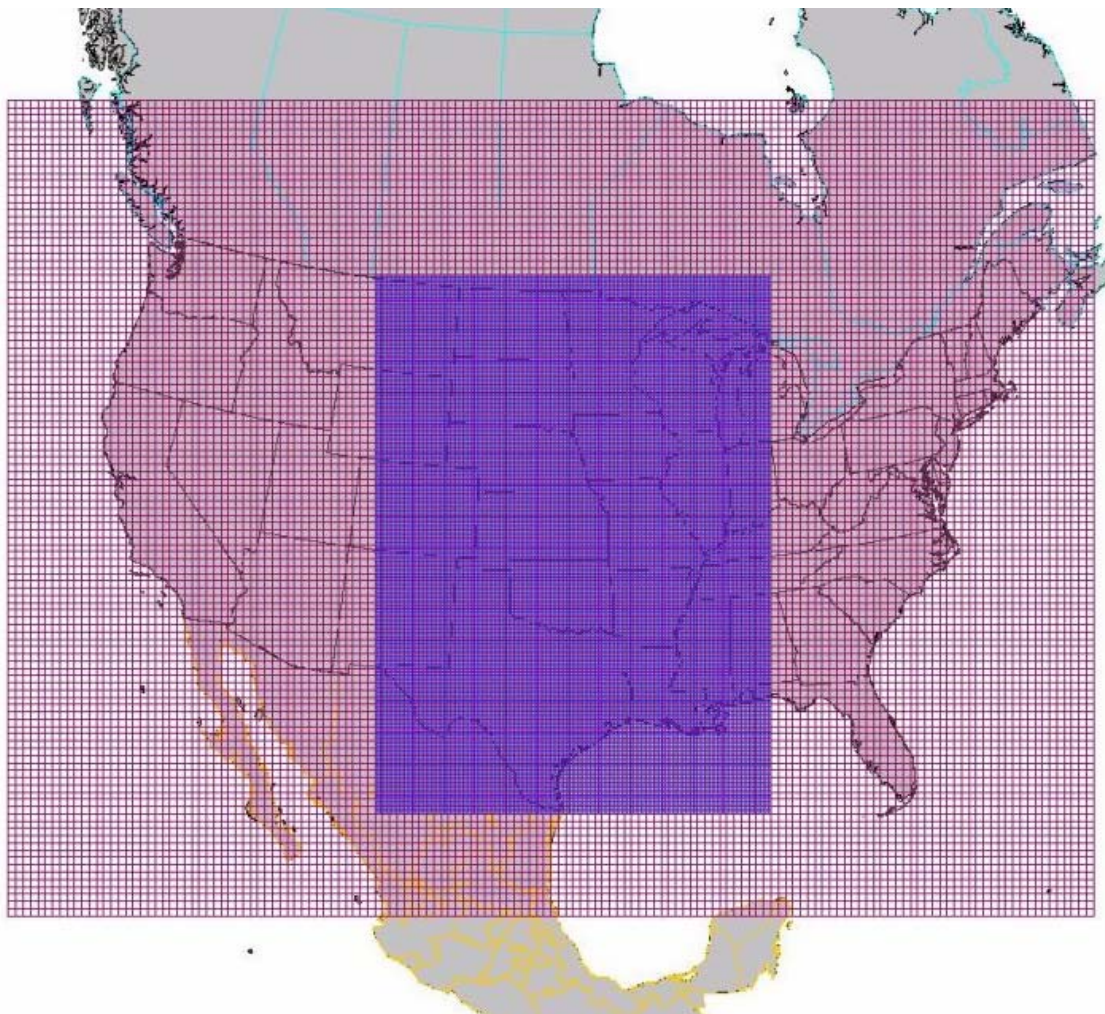
National RPO Meeting
Denver, CO
June 9, 2005

CENRAP Base Case Modeling

- **2002 Annual 36 km modeling - CMAQ and CAMx**
 - BaseA Modeling Report available
 - Results on CENRAP modeling website:
<http://pah.cert.ucr.edu/aqm/cenrap/cmaq.shtml>
 - BaseB is underway which includes emissions & other improvements
- **2002 Episodic 12 km modeling - CMAQ and CAMx**
 - Ongoing
 - Meteorology by OK, TX, R7 - MM5 v3.7

CENRAP Modeling Domains

- Domain 1 (36km)
 - MM5 165x129x34
 - AQ/EM 147x111x19
- Domain 2 (12km)
 - MM5 265x241x34
 - AQ/EM 162x222x19



Proposed PM2.5 Model Performance

Boylan's Rule

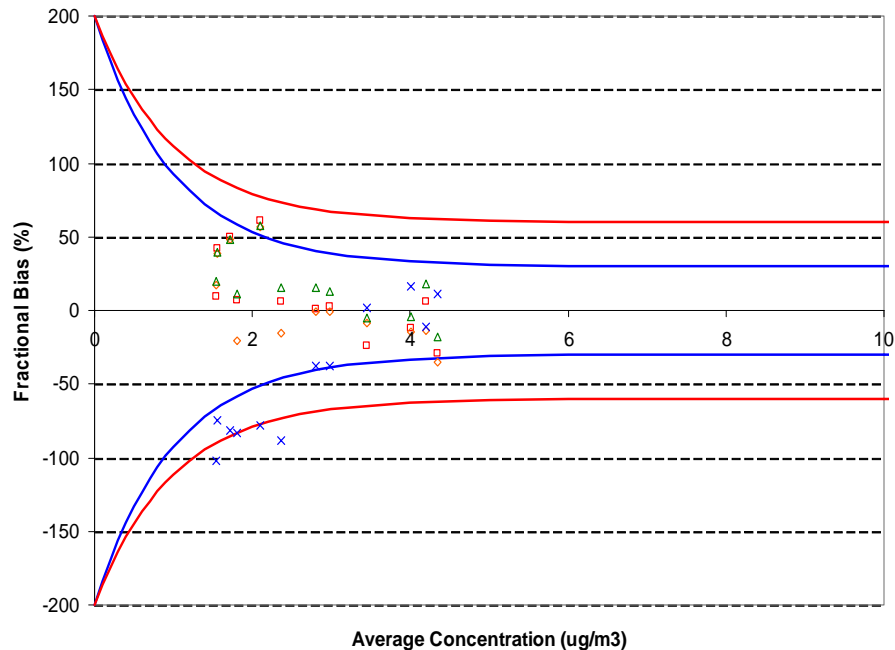
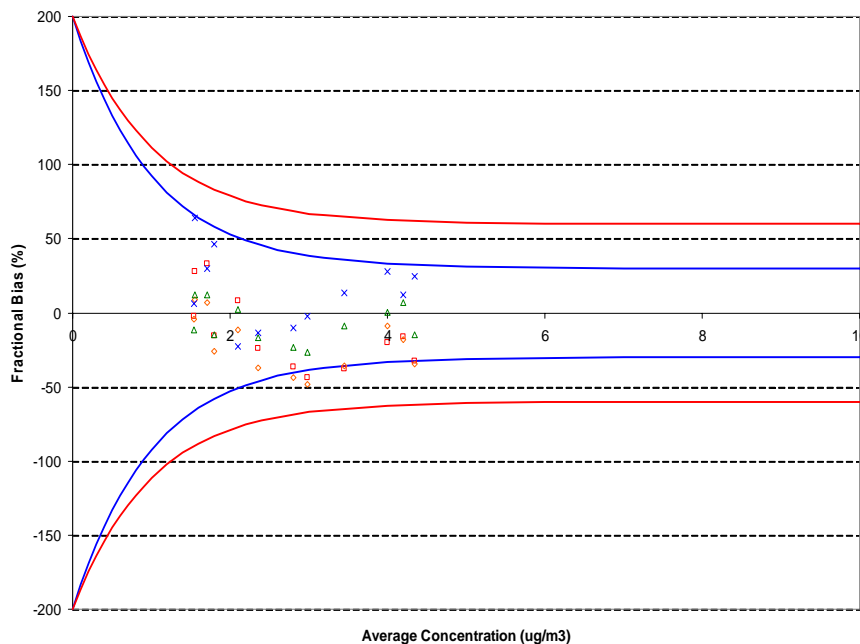


- **Based on MFE and MFB calculations**
- **Vary as a function of species**
 - **Goals:** $\text{MFE} \leq 50\%$ and $\text{MFB} \leq \pm 30\%$
 - **Criteria:** $\text{MFE} \leq 75\%$ and $\text{MFB} \leq \pm 60\%$
- **Less abundant species should have less stringent performance goals and criteria**

SO₄ Mean Fractional Bias

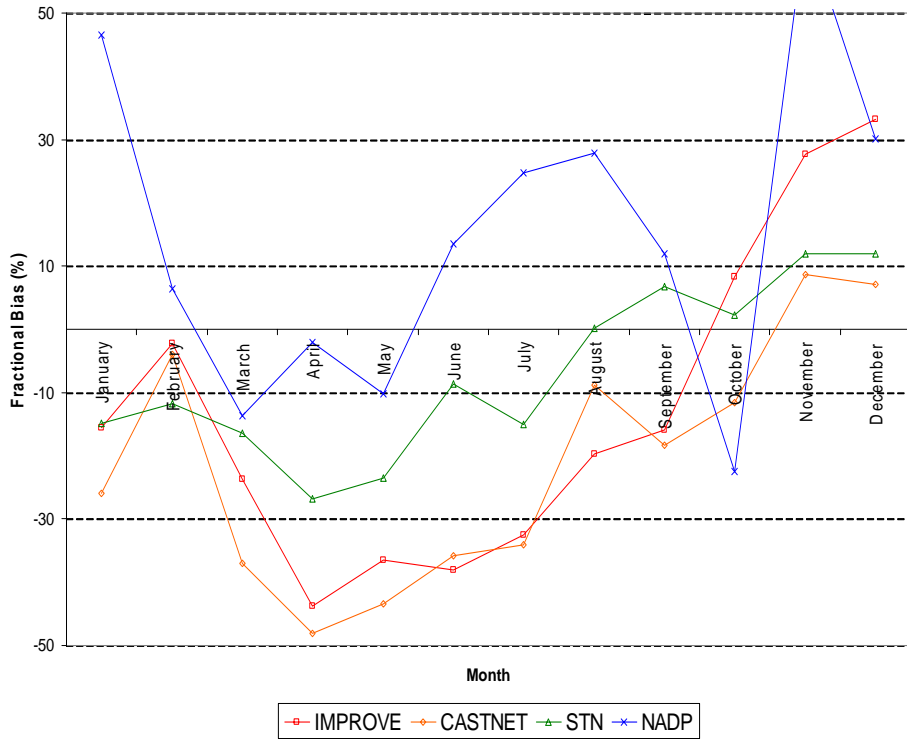
SO4 CMAQ BaseA FB Bugle

SO4 CAMx BaseA FB Bugle

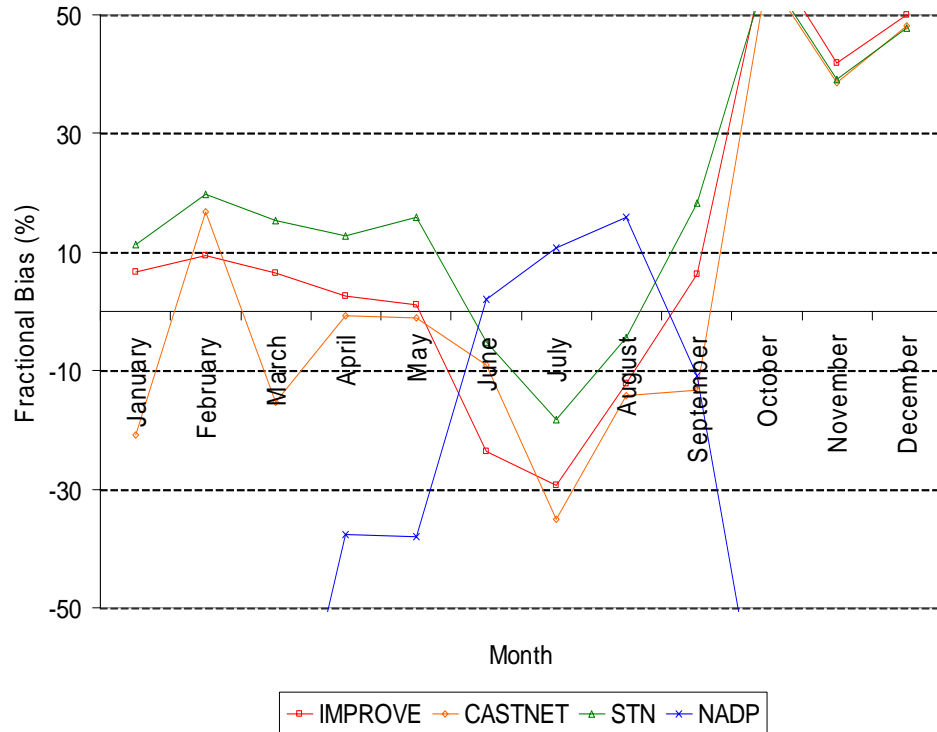


Sulfate Mean Fractional Error

SO4 CMAQ Base A FB Timeseries



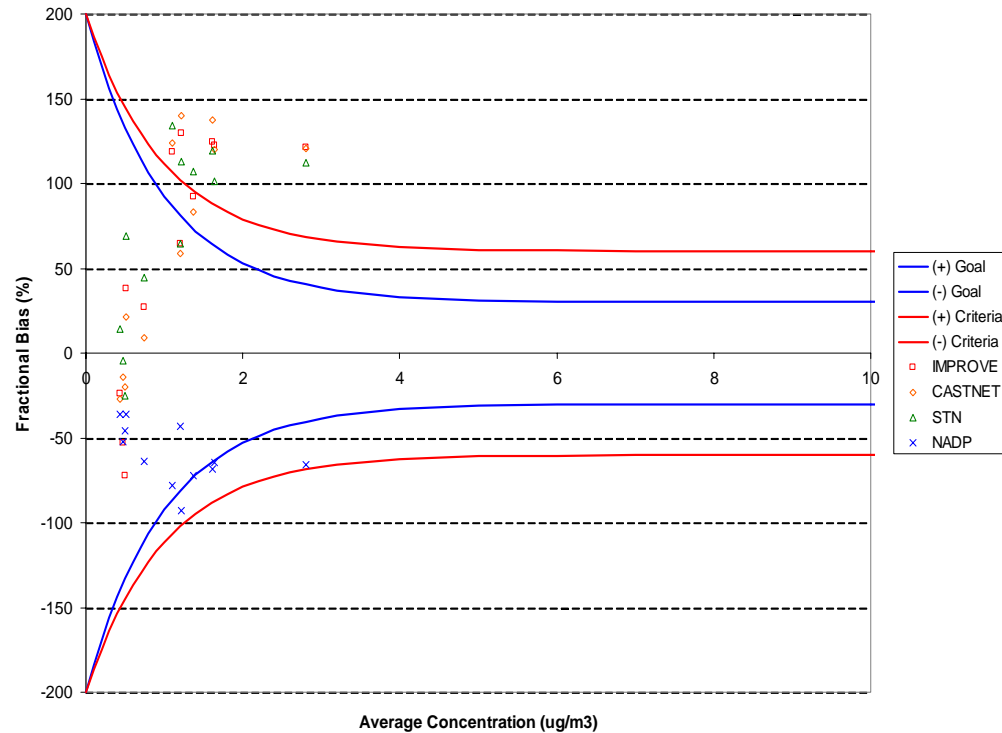
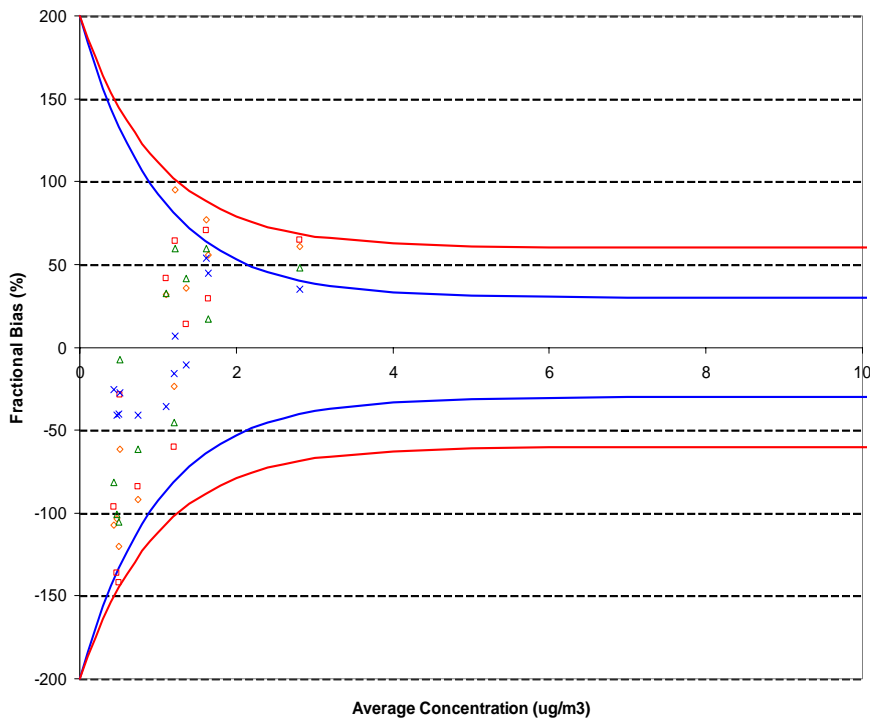
SO4 CAMx Base A FB Timeseries



NO₃ Mean Fractional Bias

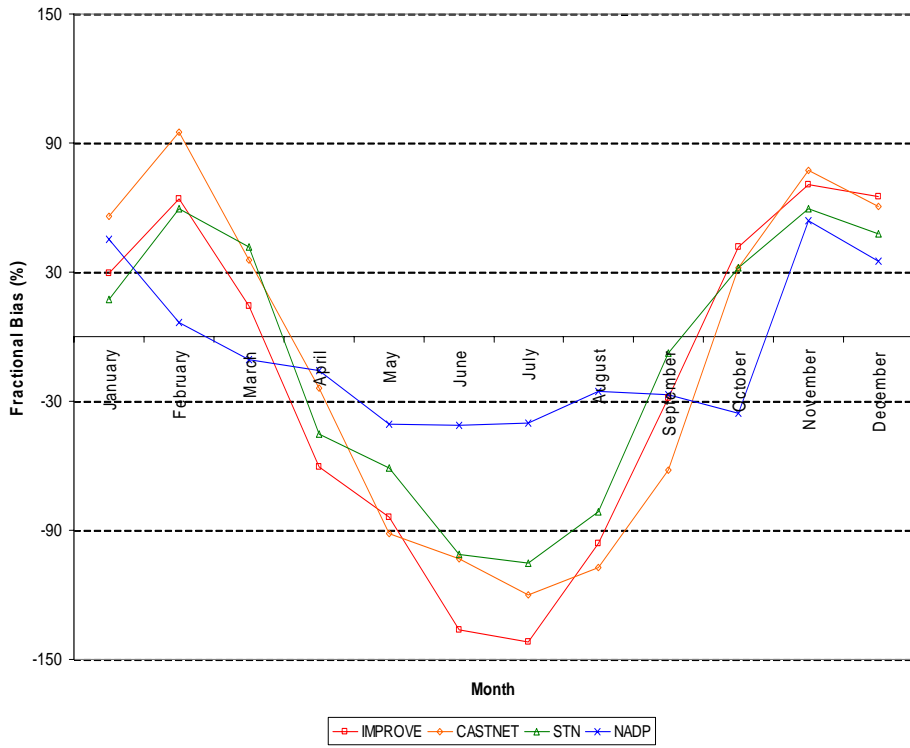
NO₃ CMAQ BaseA FB Bugle

NO₃ CAMx BaseA FB Bugle

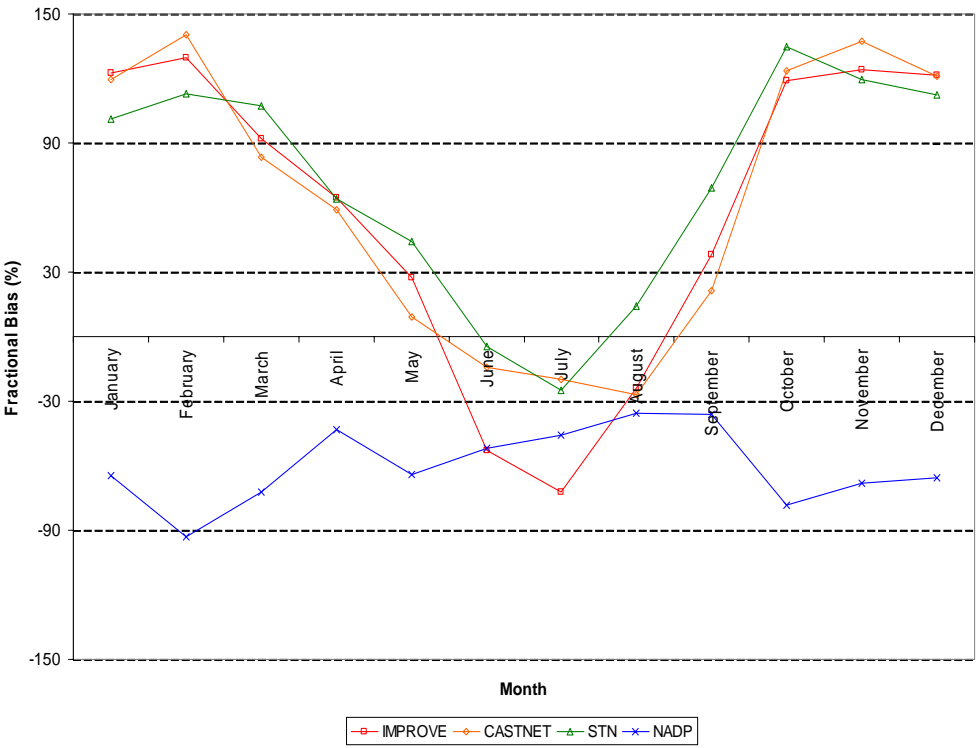


NO₃ Mean Fractional Error

NO3 CMAQ Base A FB Timeseries



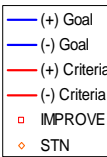
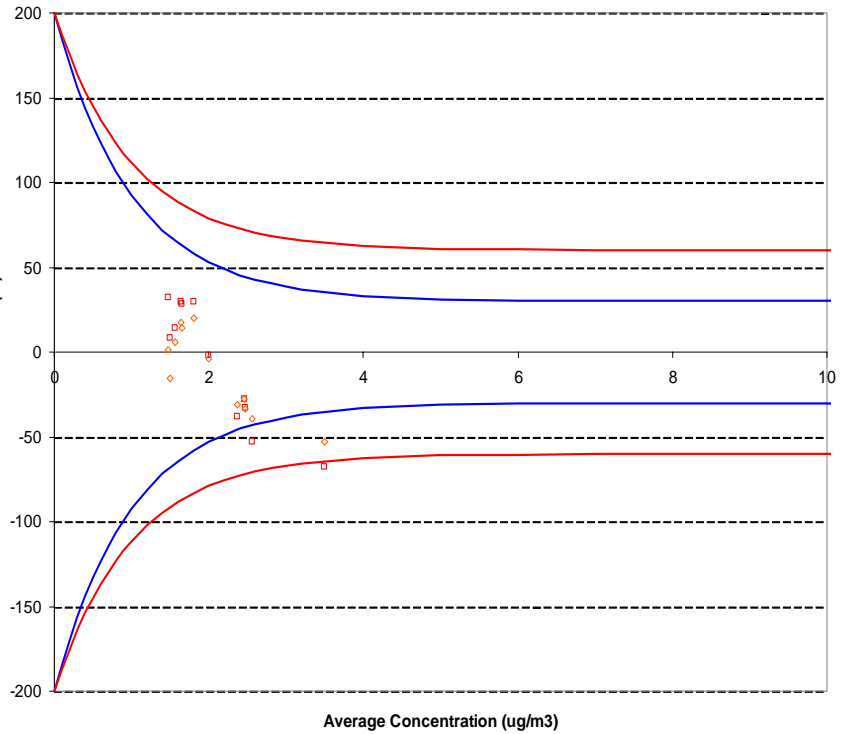
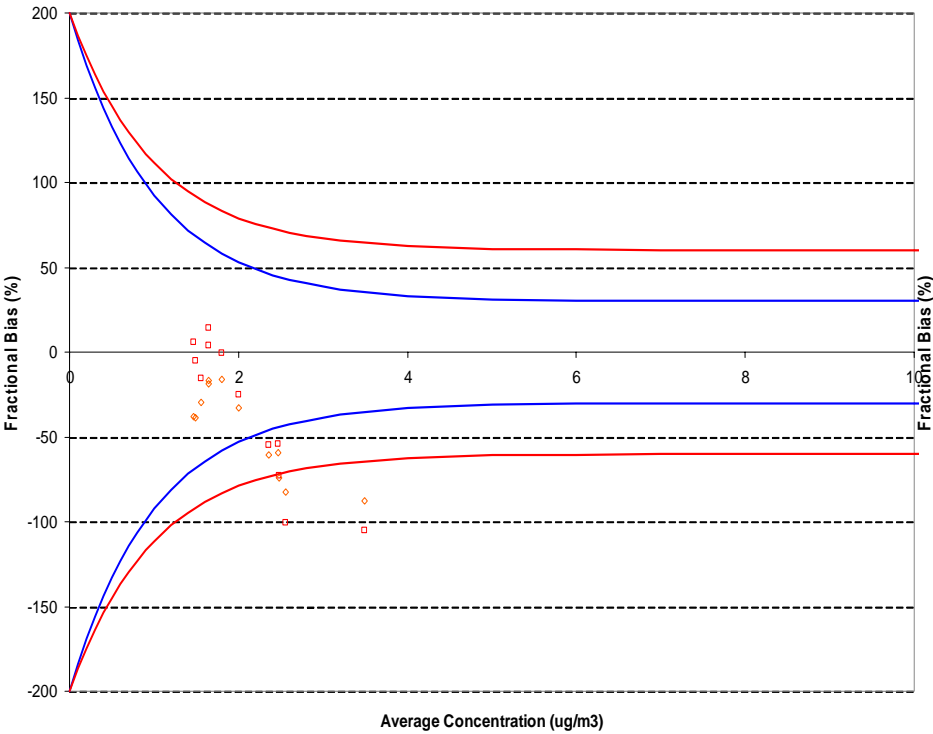
NO3 CAMx Base A FB Timeseries



TCM Mean Fractional Bias

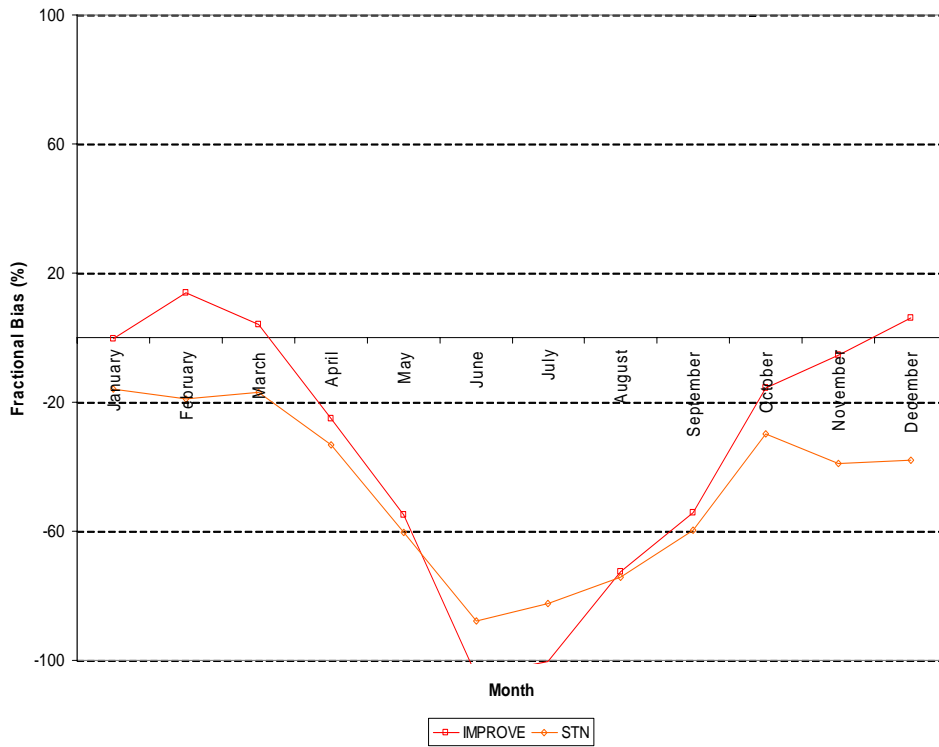
TCM CMAQ BaseA FB Bugle

TCM CAMx BaseA FB Bugle

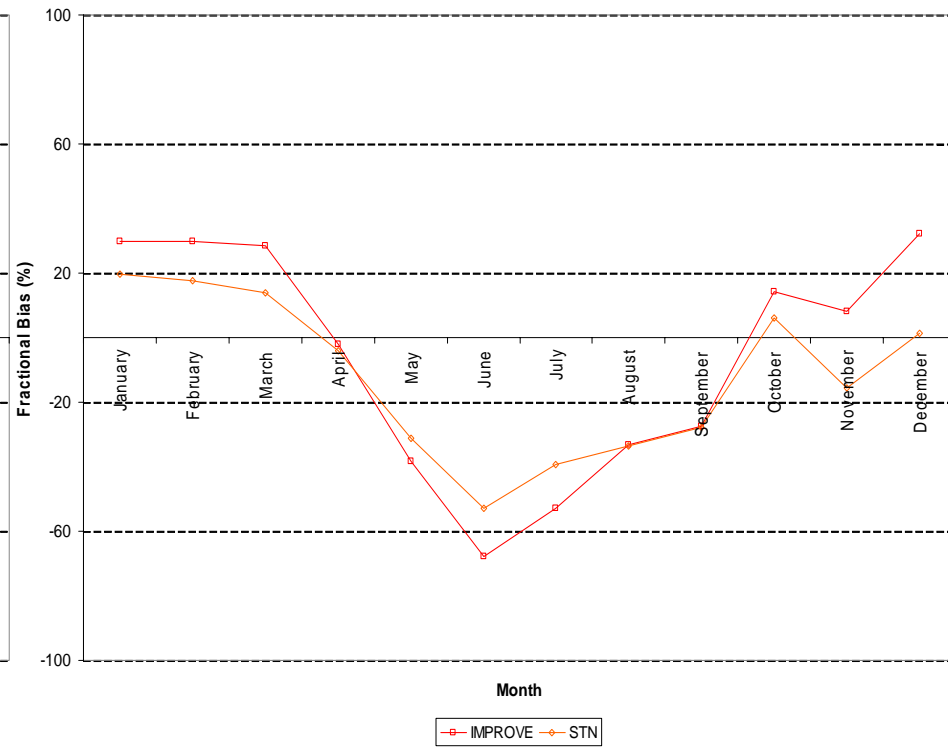


TCM Mean Fractional Error

TCM CMAQ Base A FB Timeseries



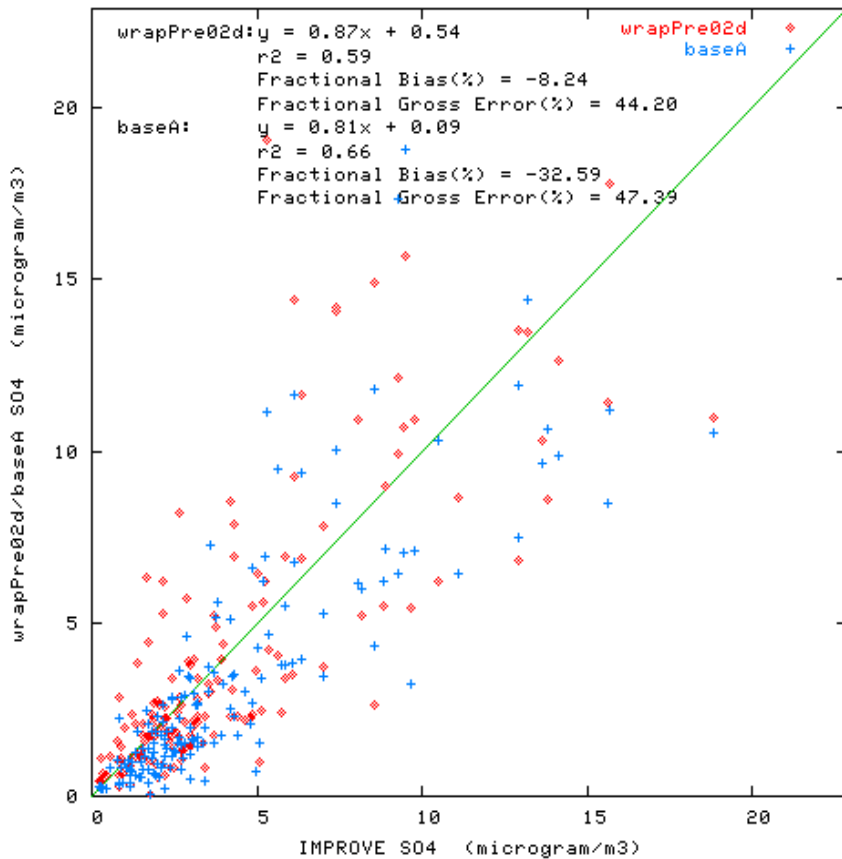
TCM CAMx Base A FB Timeseries



Sulfate July 2002 @ IMPROVE Sites

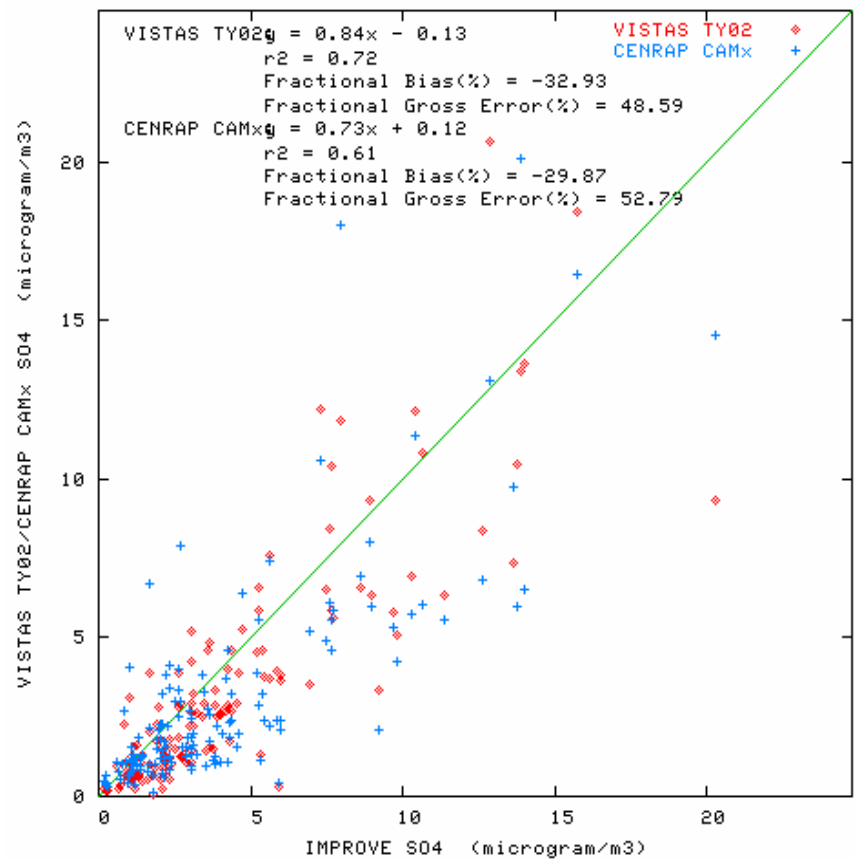
CMAQ WRAP vs. CMAQ CENRAP

IMPROVE vs. wrapPre02d/baseA S04 at 21 stations on 2002182-200221



CMAQ VISTAS vs. CAMx CENRAP

IMPROVE vs. VISTAS TY02/CENRAP CAMx S04 at 17 stations on 2002182-200221

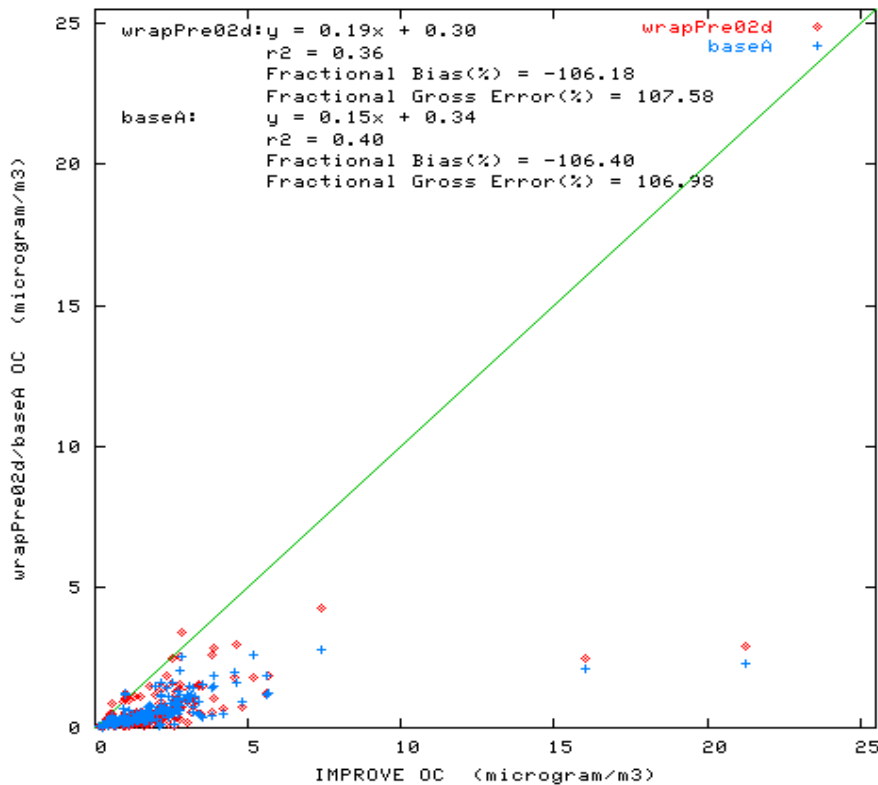


Organic Carbon July 2002 CENRAP IMPROVE Sites

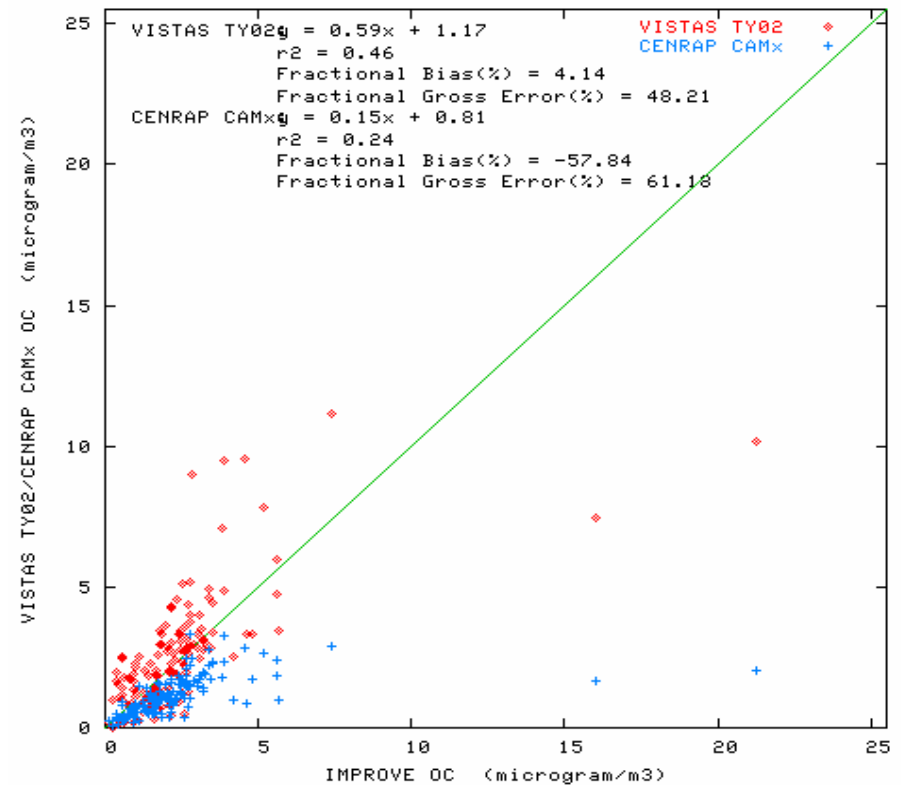
CMAQ WRAP vs. CMAQ CENRAP

CMAQ VISTAS vs. CAMx CENRAP

IMPROVE vs. wrapPre02d/baseA OC at 21 stations on 2002182-20022



IMPROVE vs. VISTAS TY02/CENRAP CAMx OC at 17 stations on 2002182-20022



CMAQ VISTAS w/ SOAmods update best performing (+4%) followed by CENRAP CAMx (-58%) with CENRAP/WRAP CMAQ worse (-106%)

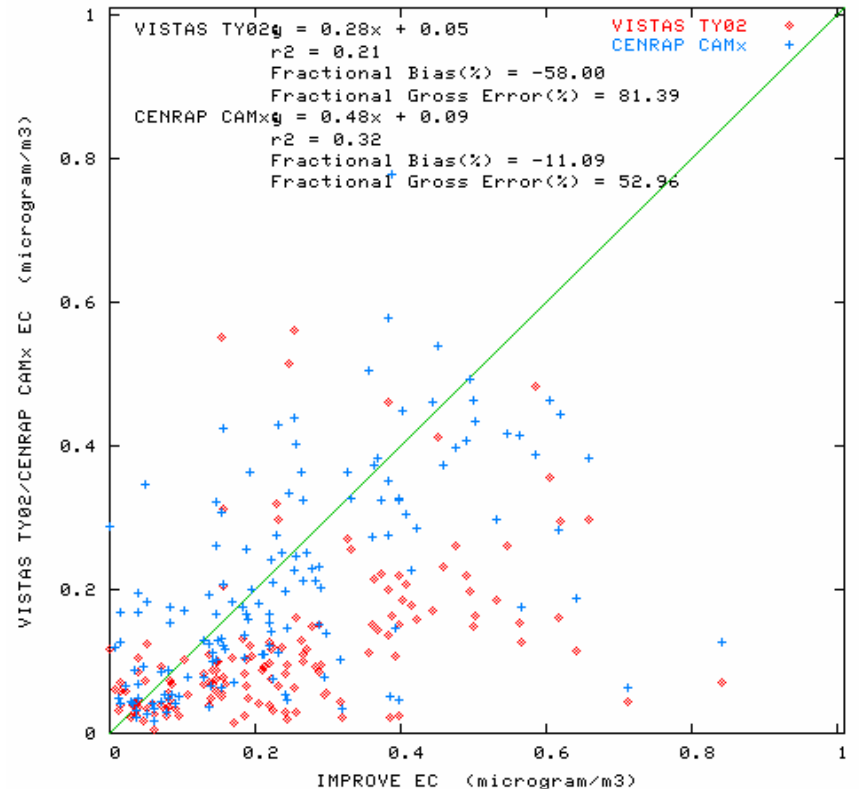
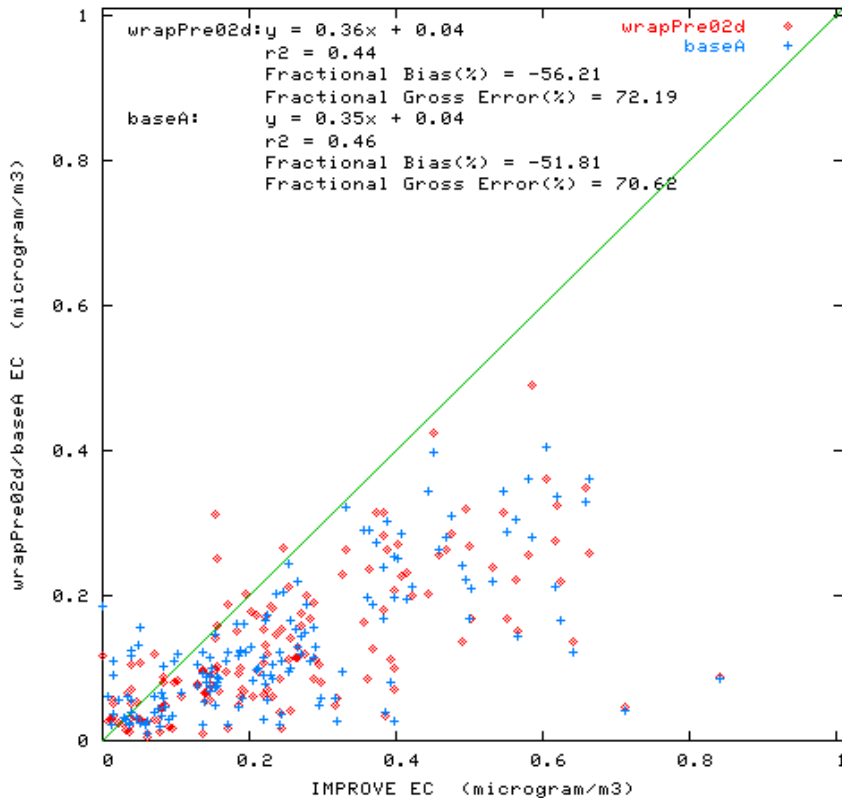
EC July 2002 CENRAP IMPROVE Sites

CMAQ WRAP vs. CMAQ CENRAP

CMAQ VISTAS vs. CAMx CENRAP

IMPROVE vs. wrapPre02d/baseA EC at 21 stations on 2002182-200221

IMPROVE vs. VISTAS TY02/CENRAP CAMx EC at 17 stations on 2002182-200221



CMAQ underestimates summer EC by -52% to -58% with errors of 71% to 81% (WREAP, VISTAS and CENRAP), whereas CENRAP CAMx underestimates EC by -11% with 53% error

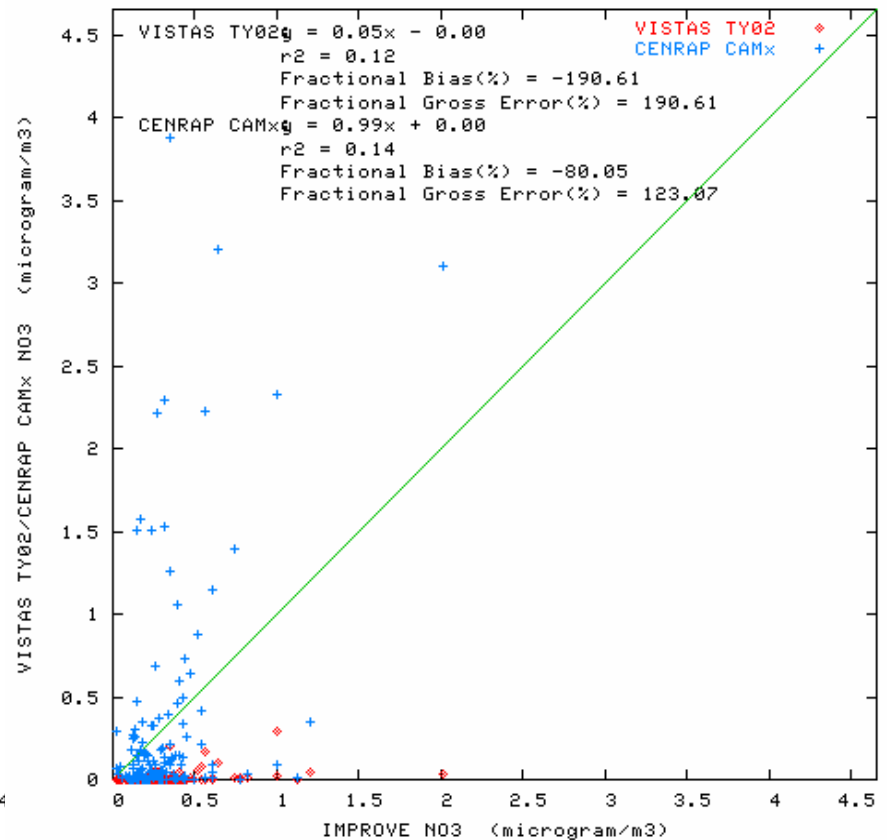
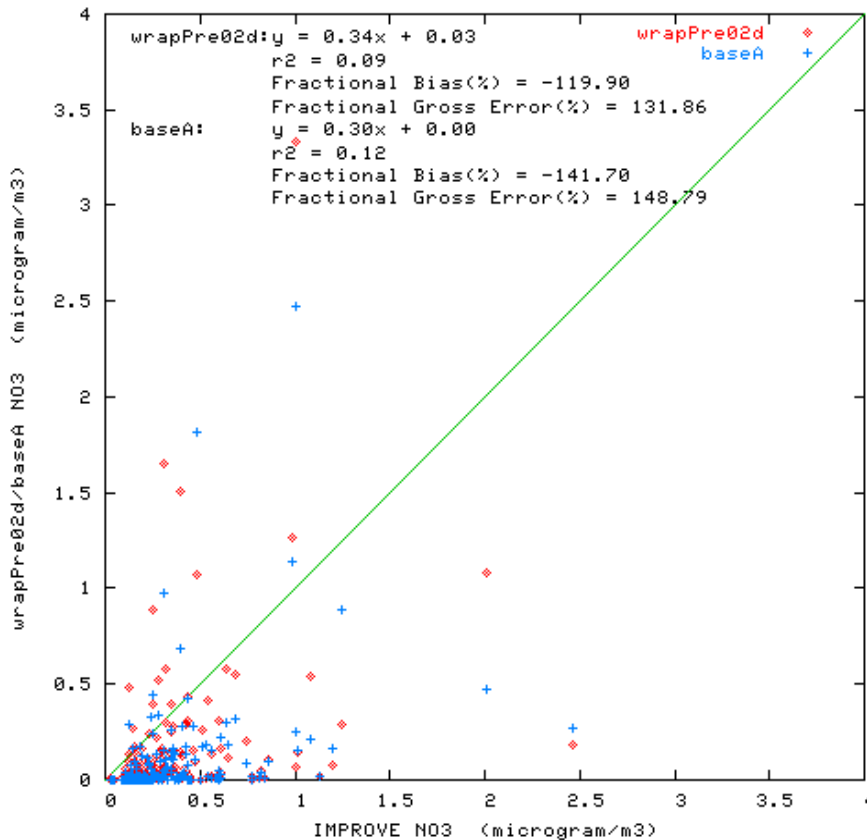
Nitrate July 2002 CENRAP IMPROVE Sites

CMAQ WRAP vs. CMAQ CENRAP

CMAQ VISTAS vs. CAMx CENRAP

IMPROVE vs. wrapPre02d/baseA NO3 at 21 stations on 2002182-2002

IMPROVE vs. VISTAS TY02/CENRAP CAMx NO3 at 17 stations on 2002182-2002



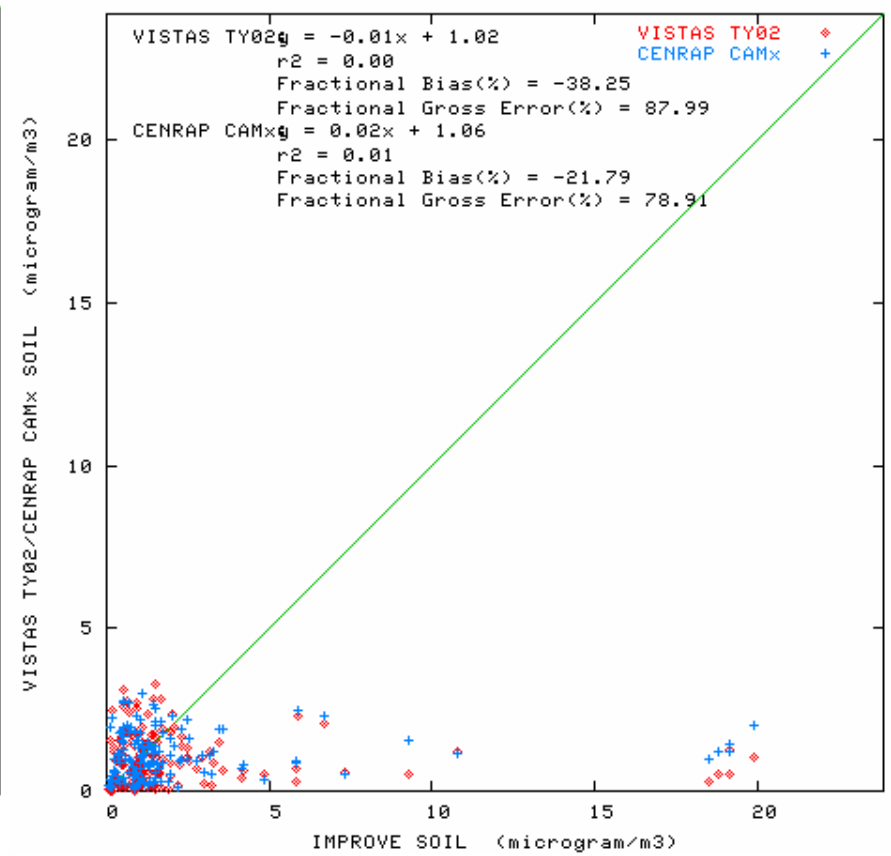
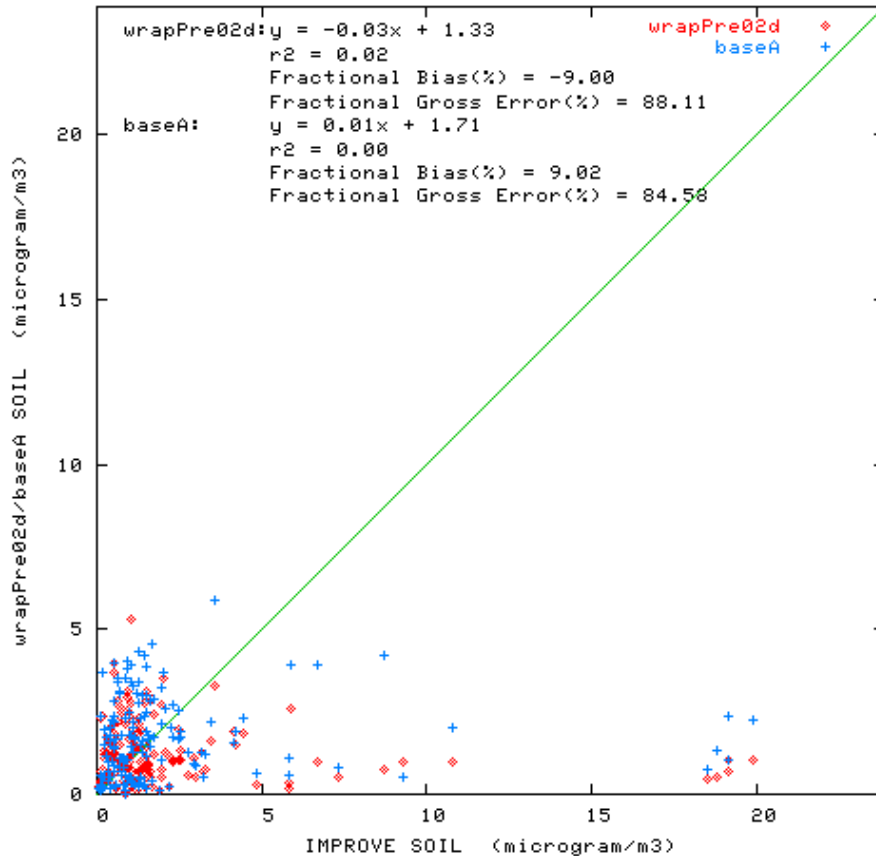
All models underestimate summer NO3 with CMAQ bias of -120%, -142% and -191% for WRAP, CENRAP and VISTAS and CENRAP CAMx bias of -80%

SOIL July 2002 CENRAP IMPROVE Sites

CMAQ WRAP vs. CMAQ CENRAP

CMAQ VISTAS vs. CAMx CENRAP

IMPROVE vs. wrapPre02d/baseA SOIL at 21 stations on 2002182-2002 IMPROVE vs. VISTAS TY02/CENRAP CAMx SOIL at 17 stations on 2002182-2002

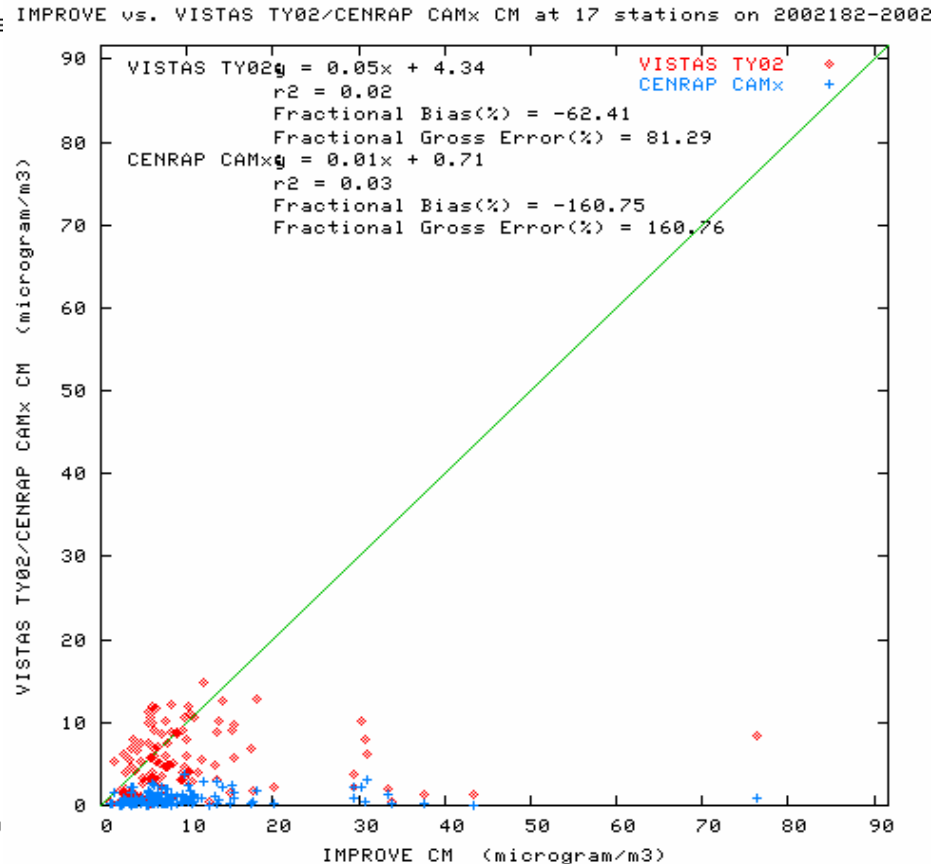
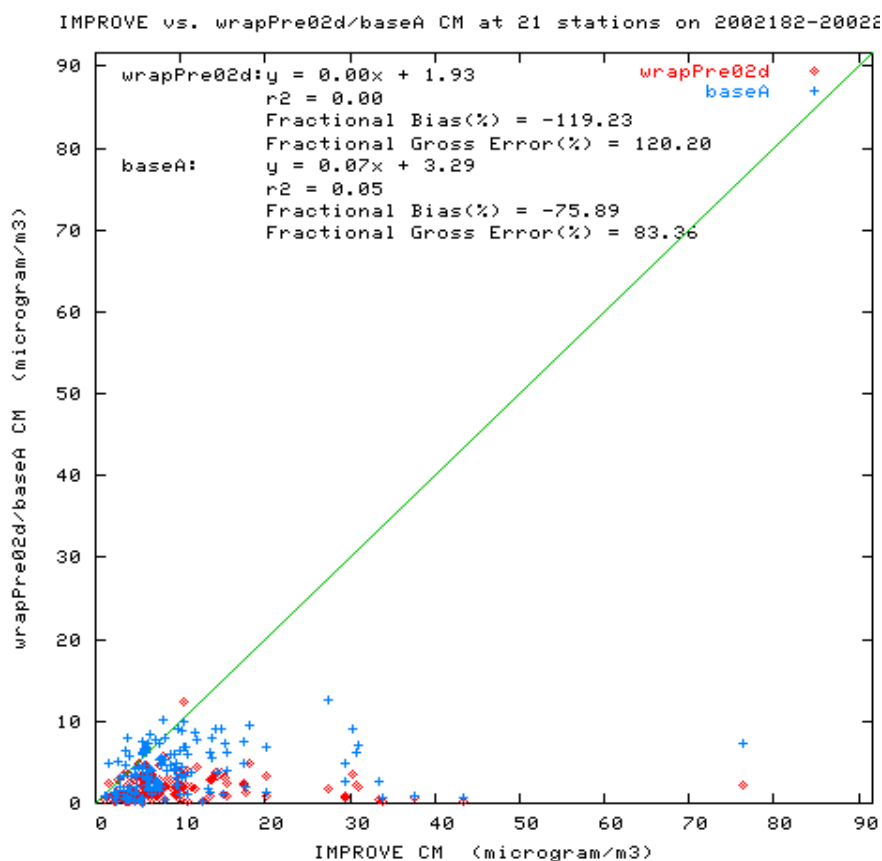


Variable SOIL bias from +9% (CENRAP CMAQ) to -38% (VISTAS CMAQ).
 CENRAP CAMx used Fugitive Dust Transport Factor of 0.25 for a bias of -22%

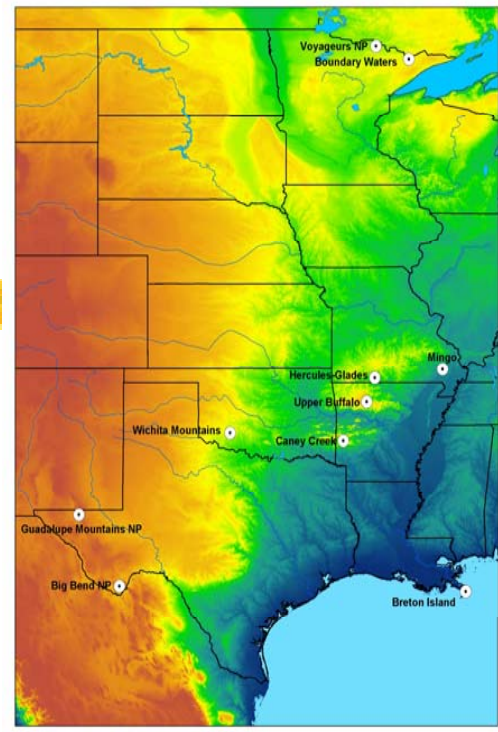
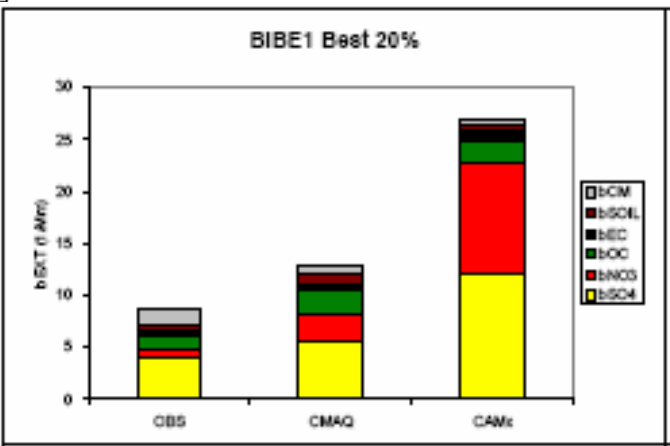
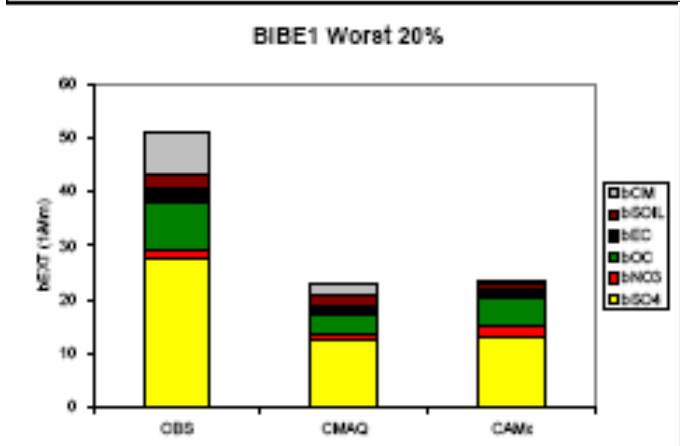
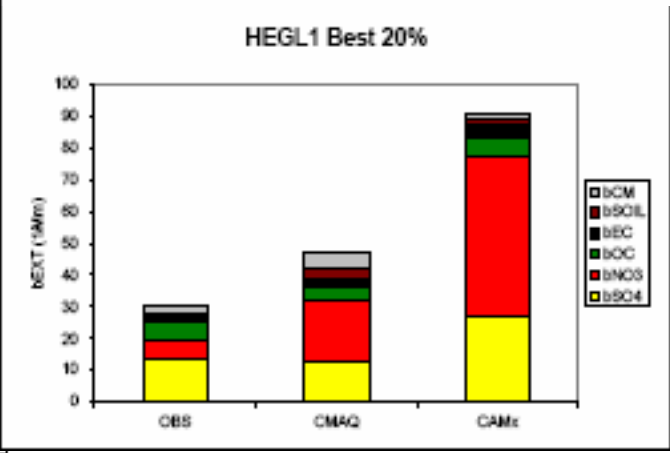
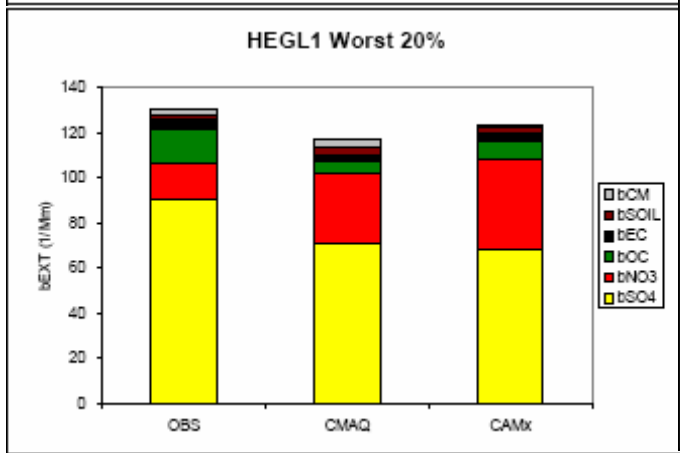
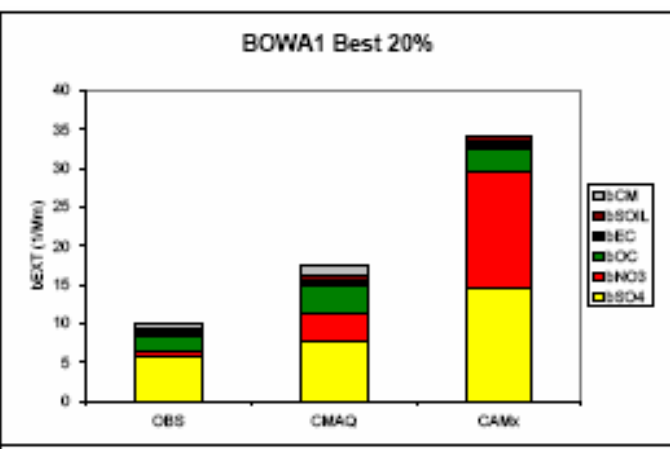
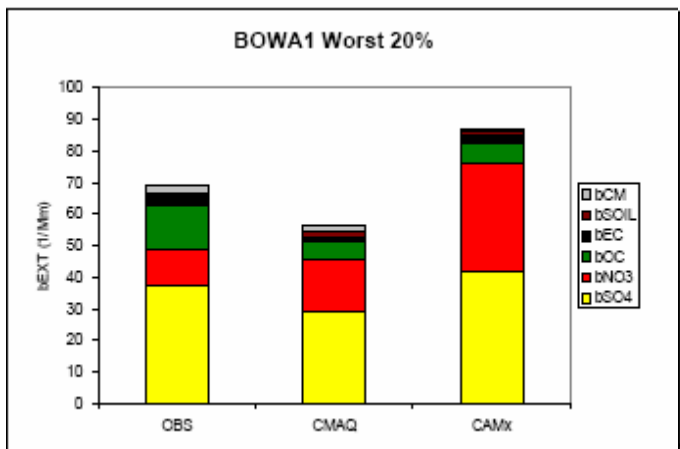
Coarse Matter July 2002 CENRAP IMPROVE Sites

CMAQ WRAP vs. CMAQ CENRAP

CMAQ VISTAS vs. CAMx CENRAP



No Fugitive Dust Transport Factor (FDTF) applied in CMAQ runs with -62% to -119% underestimation bias. 0.25 FDTF applied in CAMx runs for -161% bias.



36 km CMAQ and CAMx Base Case Summary

- **Comparable model performance, difficult to select on model as performing better than the other across all species and times**
 - SO₄ performance fairly good across all models
 - NO₃ performance poor
 - VISTAS CMAQ w/ SOAmods performing best for summer OC followed by CAMx
 - CAMx CM underestimation, does not justify use of 0.25 FDTF?
- **Performance varies by Class I area**
 - Severe underprediction for two Texas Class I areas
 - Overestimation of extinction for 20% best days at ALL Class I areas

Next Steps EM & AQ Modeling



■ Revised 2002 Base Case Modeling (Base B)

- Emissions updates include data from CENRAP, MRPO, WRAP, VISTAS, Mexico, etc.
- Should include SOAmods update from VISTAS

■ Diagnostic Model Evaluation?

- Process Analysis, model tracers and source apportionment, sensitivity studies, etc.

■ 2018 Base Case Simulation

- Use Base B inventory for 2018 emission projection?
- Annual 36 km - both CMAQ & CAMx, or 36/12 km but CMAQ or CAMx only?

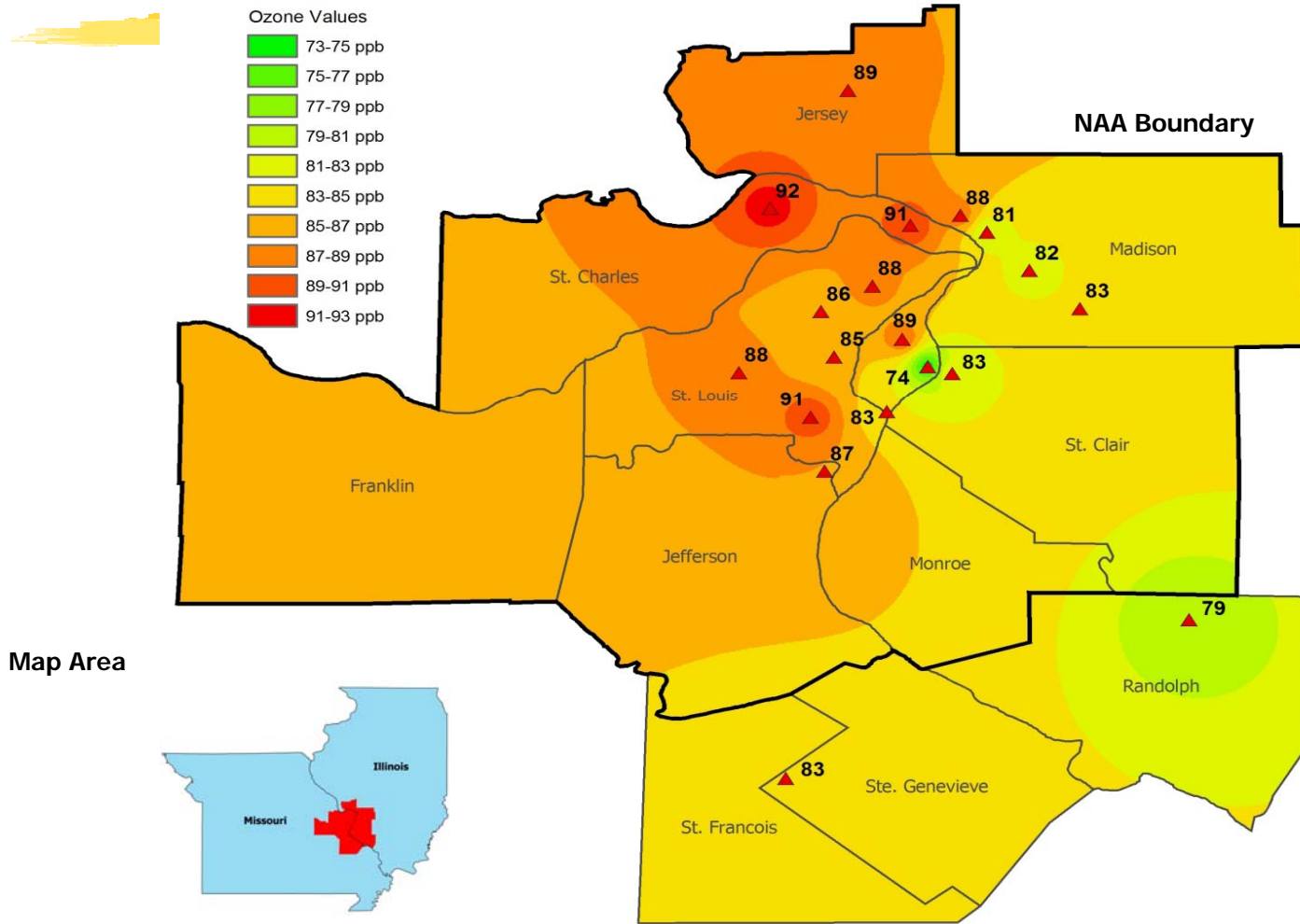
St. Louis Ozone/PM2.5 SIP Modeling



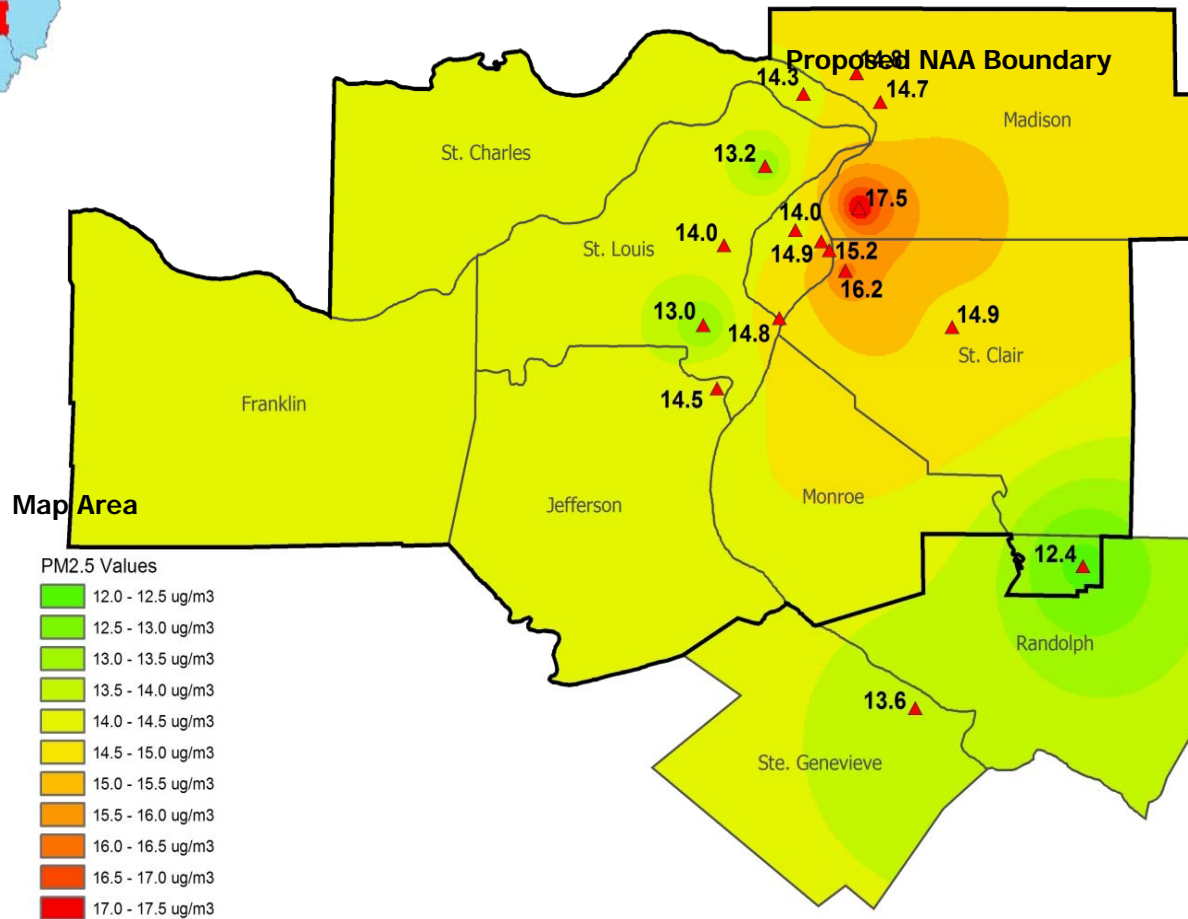
■ St. Louis Modeling Team

- Missouri DNR, Illinois EPA, American, EPA Region 7
- EMVIRON/Alpine Geophysics

St. Louis Region 2001-2003 8-hour Ozone Design Values



St. Louis Region 2001-2003 Annual PM2.5 Design Values

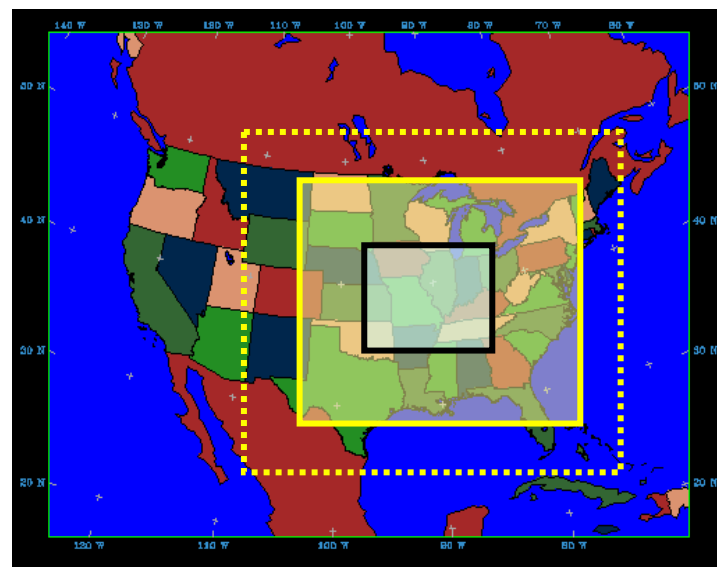
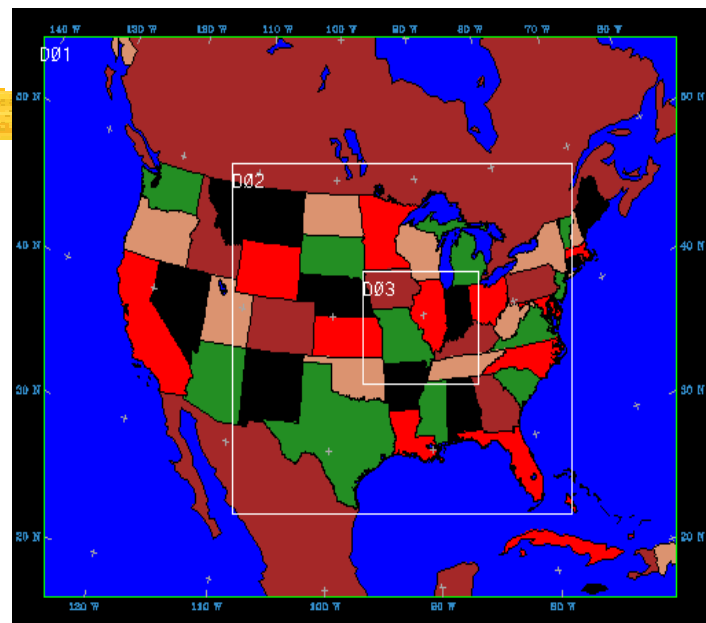


St. Louis Modeling Domains

MM5 Vertical Layers=34
MM5 Horizontal Structure:
36 km = 165 x 129
12 km = 265 x 241
4 km = 271 x 235
Total Grid Cells = 5.0 mil

AQ Vertical Layers=16
Aq Horizontal Structure
36 km = 148 x 112
12 km = 203 x 200
4 km = 254 x 218
Total Grid Cells = 1.8 mil

Episodic 4 km
Annual 12 km
CMAQ v4.4/CAMx v4.11s



Episode Days Modeled for MM5

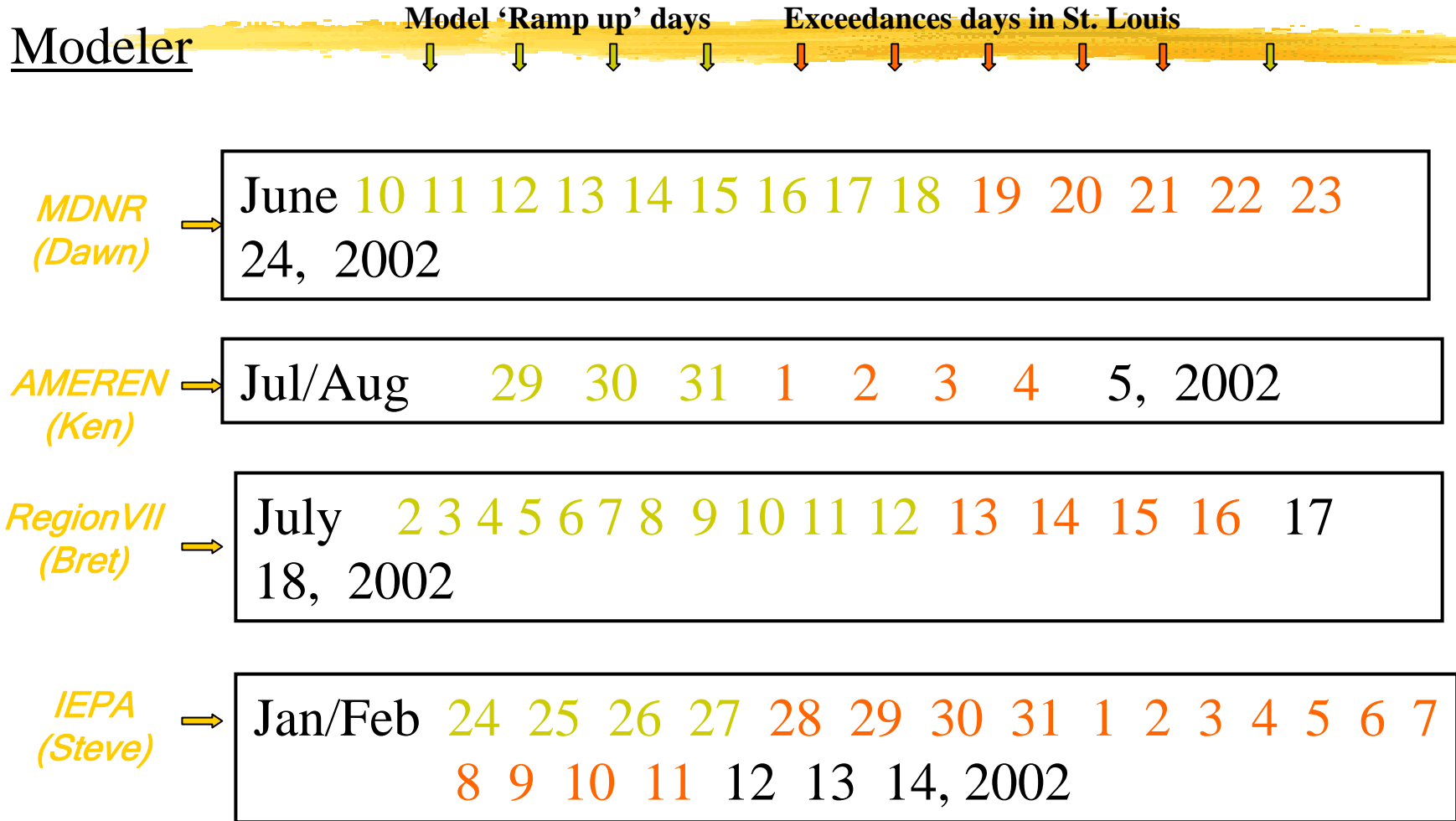


Table 5-2. CMAQ Model Configuration to be Used in the St. Louis Modeling.

Model Option	CMAQ
Model Version	Version 4.4 (October 2004)
Horizontal Resolution	36/12/4 km
No. Vertical Layers	NZ = 19 (36 km) TBD (12/4 km)
Horizontal Advection	PPM
Vertical Advection	PPM
Horizontal Diffusion	Spatially Varying
Vertical Diffusion	K_V (Eddy Diffusion)
MM5 Configuration	Pleim-Xiu/ACM
MM5 Processing	MCIP2.2 Pass Through
Gas-Phase Chemistry	CB4
Gas-Phase Chemistry Solver	EBI
Secondary Organic Aerosol	SORGAM
Aqueous-Phase Chemistry	RADM
Aerosol Chemistry	AE3/ISORROPIA
Dry Deposition	Pleim-Xiu
Plume-in-Grid	Off
Initial Concentrations	CMAQ Default
Boundary Conditions	3-Hourly 2002 GEOS-CHEM
Emissions	CENRAP States 2002 Other States 2002 from RPOs

Table 5-3. CAMx Model Configuration to be Used in the St. Louis Modeling.

Model Option	CAMx
Model Version	Version 4.10s (August 2004) or Version 4.2 if available
Horizontal Resolution	36/12/4 km
No. Vertical Layers	NZ = 19 (36 km) TBD (12/4 km)
Horizontal Advection	PPM
Vertical Advection	PPM
Horizontal Diffusion	Spatially Varying
Vertical Diffusion	K _v (OB70 and CMAQ)
MM5 Configuration	Pleim-Xiu/ACM
MM5 Processing	MM5CAMx
Gas-Phase Chemistry	CB4
Gas-Phase Chemistry Solver	CMC
Secondary Organic Aerosol	SOAP
Aqueous-Phase Chemistry	RADM
Aerosol Chemistry	ISORROPIA
Dry Deposition	Wesley
Plume-in-Grid	Off
Initial Concentrations	CMAQ Default
Boundary Conditions	3-Hourly 2002 GEOS-CHEM
Emissions	CENRAP States 2002 Other States 2002 from RPOs

Existing Modeling Analyses



- Can we use the existing modeling analysis for attainment demonstrations, or for supplemental demonstrations as a WOE?
 - RPOs, EPA, other States modeling?
 - Ozone and PM2.5?

Existing Regional Modeling Study

	VISTAS	CENRAP	St. Louis
Episodes	January & June 2002	January & June 2002	Episodic 4 km & Annual 12 km
Met Model (MM5)	ver. 3.6.3	ver. 3.6.3	ver. 3.7
Emissions Inventory	2002 BaseC	2002 BaseA	CENRAP/MWRPO/ VISTAS
Emissions Model	SMOKE2.1	SMOKE2.1	SMOKE2.1 & EMS2004
AQ Model	CMAQ4.4 w/ SOAmd	CMAQ4.4 & CAMx4.10	CMAQ4.4 & CAMx4.11s
Domain Horizontal Grid	Nat. RPO (36 km) VISTAS (12 km)	Nat. RPO (36 km)	(36 km/12 km/4 km)
Vertical Layers (mm5/AQ)	34/19	34/19	34/16
Boundary Conditions	GEOS-CHEM	GEOS-CHEM	GEOS-CHEM
Model Performance			

PM2.5 - VISTAS 36/12 km

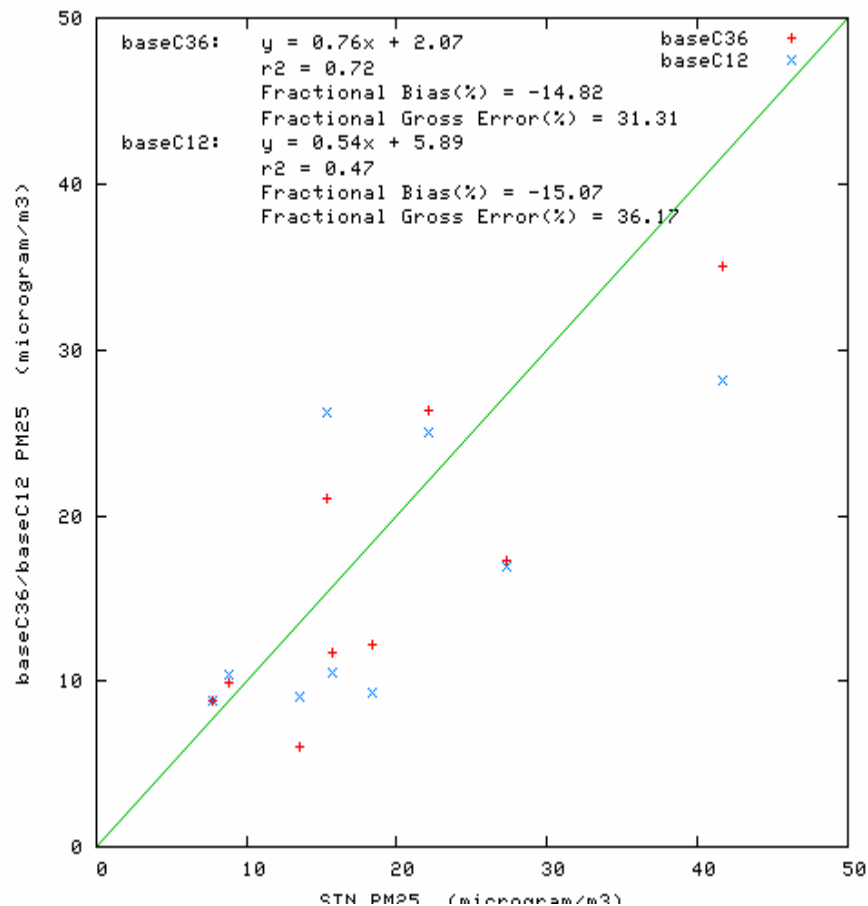
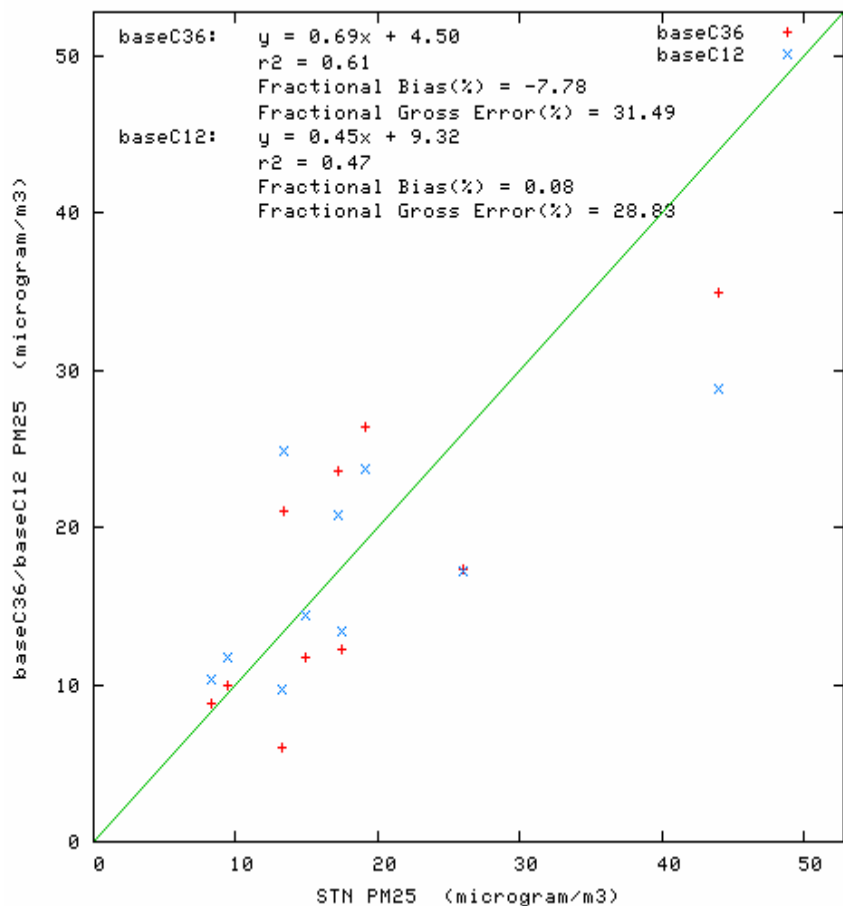
June 02 Episode

Blair St.

Grant

STN vs. baseC36/baseC12 PM25 at station 29 510 0085 on 2002152-2002181

STN vs. baseC36/baseC12 PM25 at station 29 510 0089 on 2002152-2002181

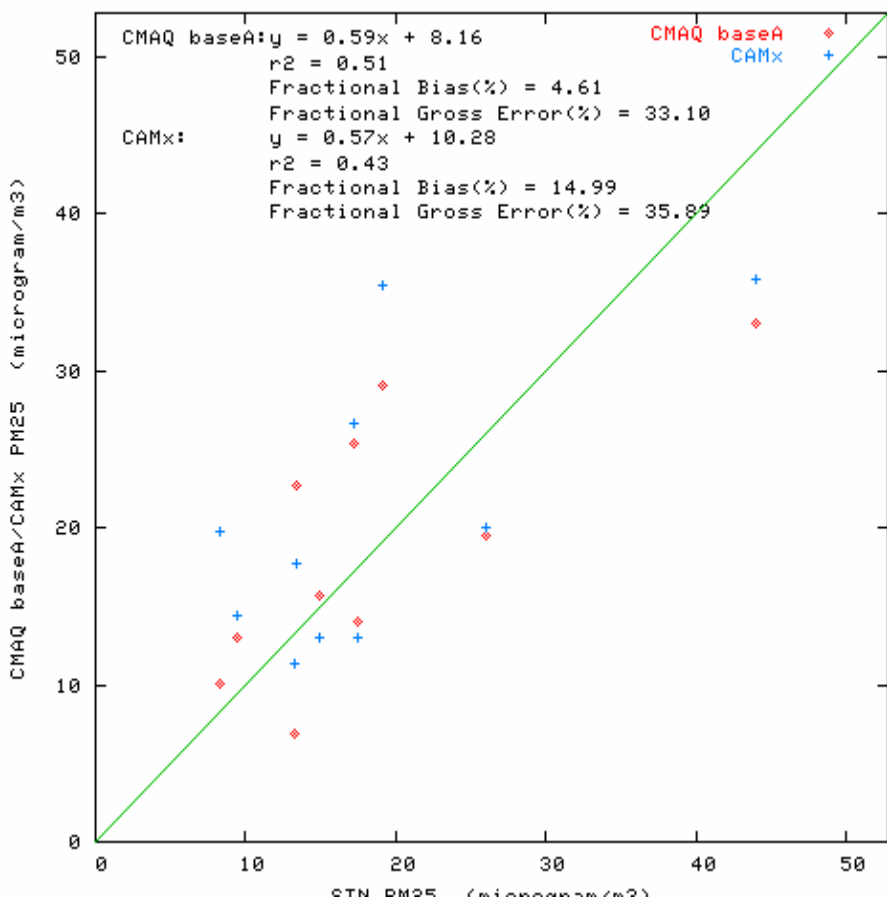


PM2.5 - CENRAP 36 km

June 02 Episode

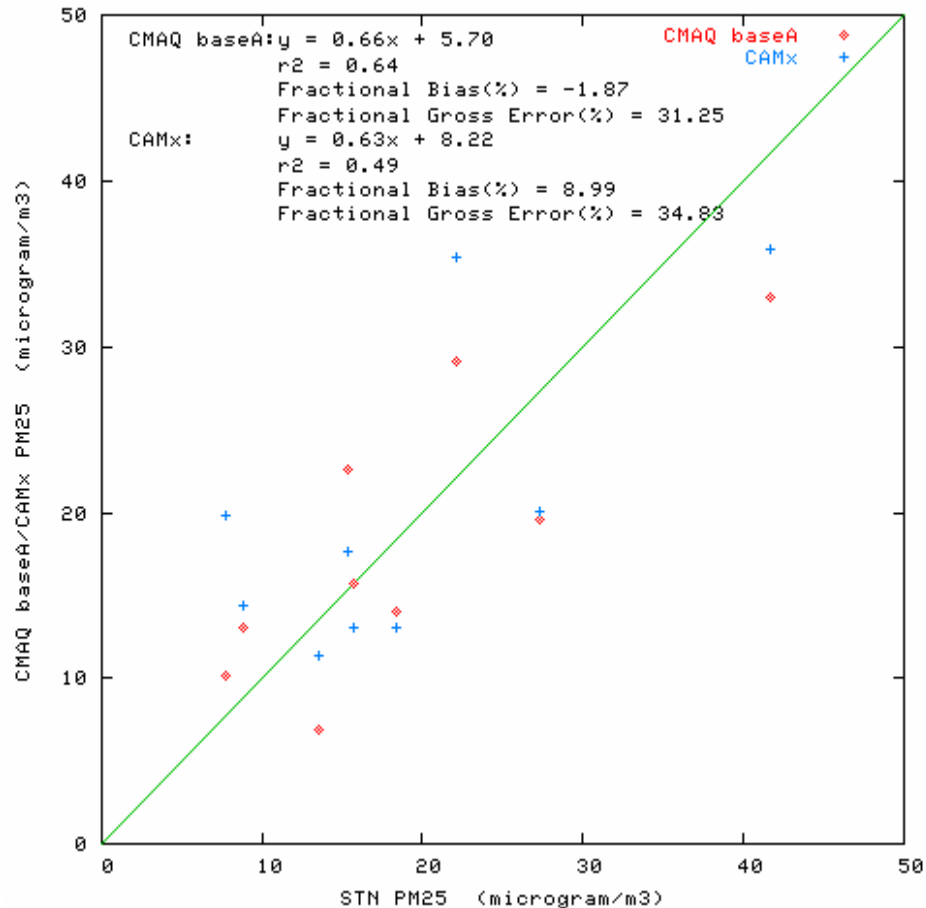
Blair St.

STN vs. CMAQ baseA/CAMx PM25 at station 29 510 0085 on 2002152-2002181



Grant

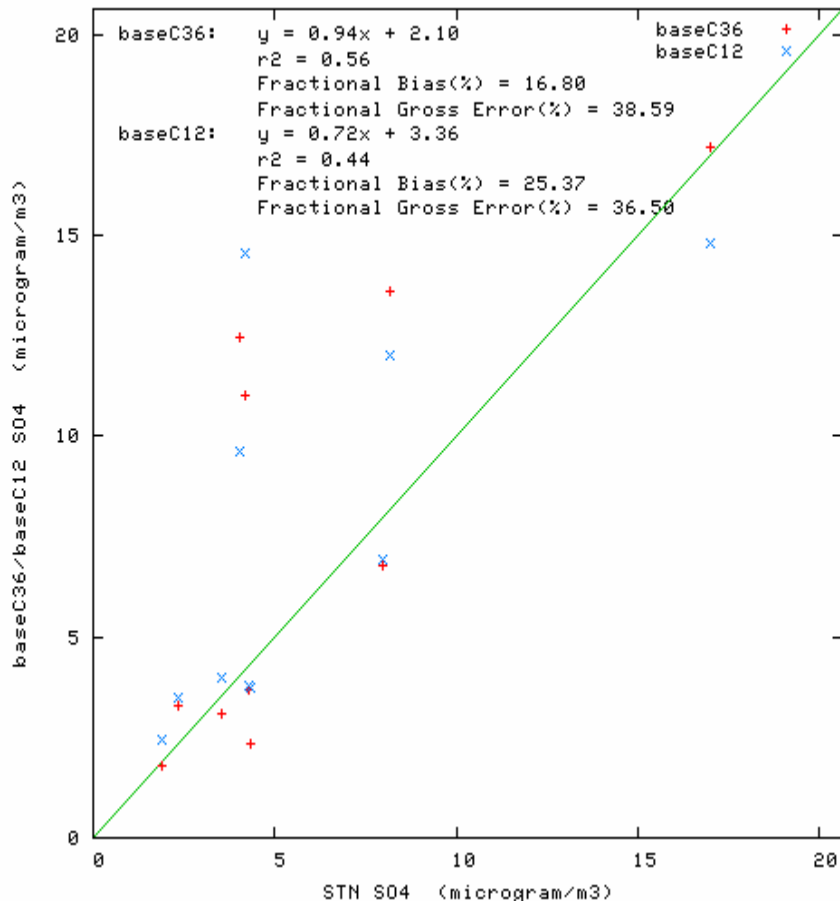
STN vs. CMAQ baseA/CAMx PM25 at station 29 510 0089 on 2002152-2002181



Sulfate- VISTAS 36/12 km June 02 Episode

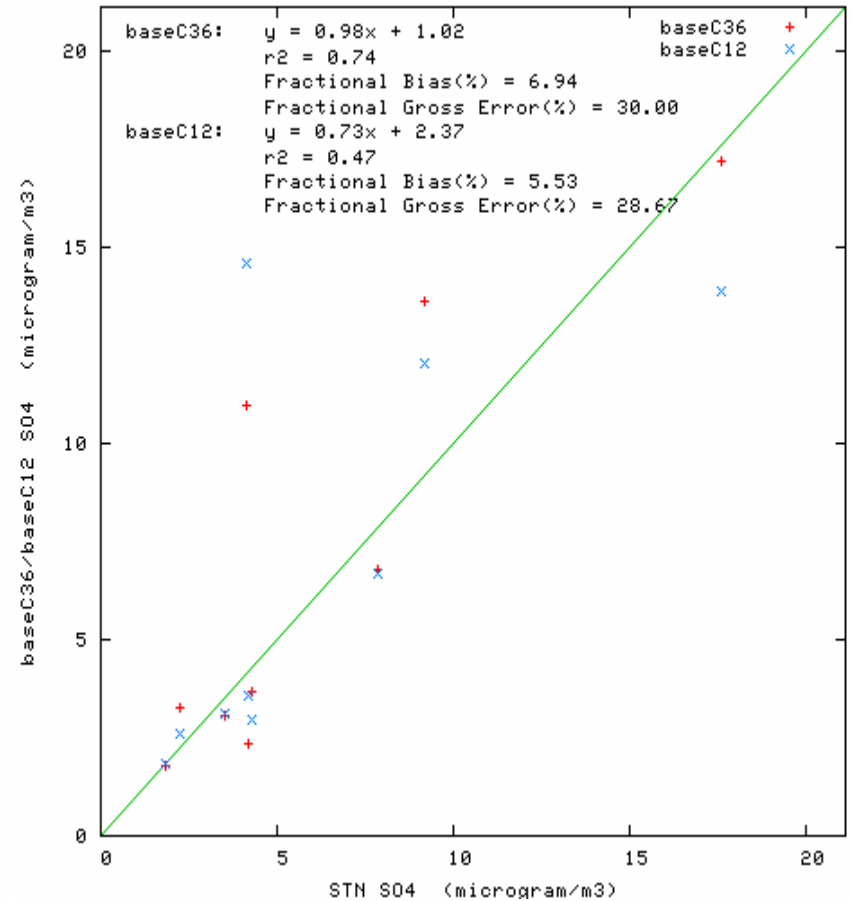
Blair St.

STN vs. baseC36/baseC12 S04 at station 29 510 0085 on 2002152-2002181



Grant

STN vs. baseC36/baseC12 S04 at station 29 510 0089 on 2002152-2002181



Sulfate - CENRAP 36 km

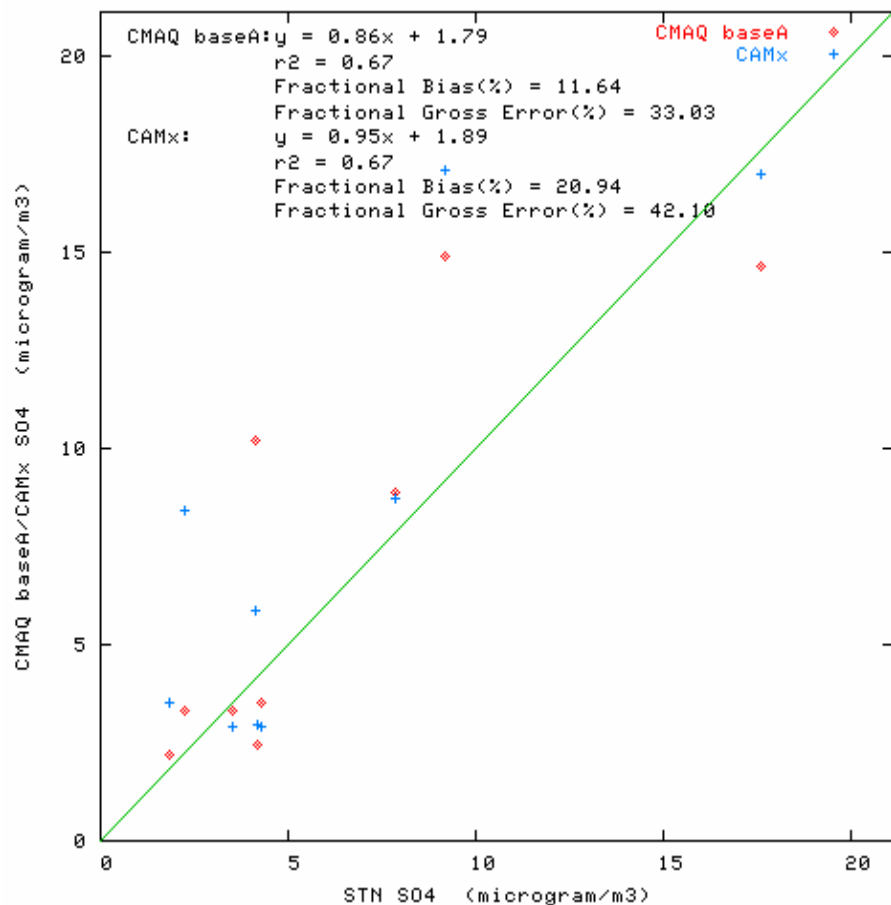
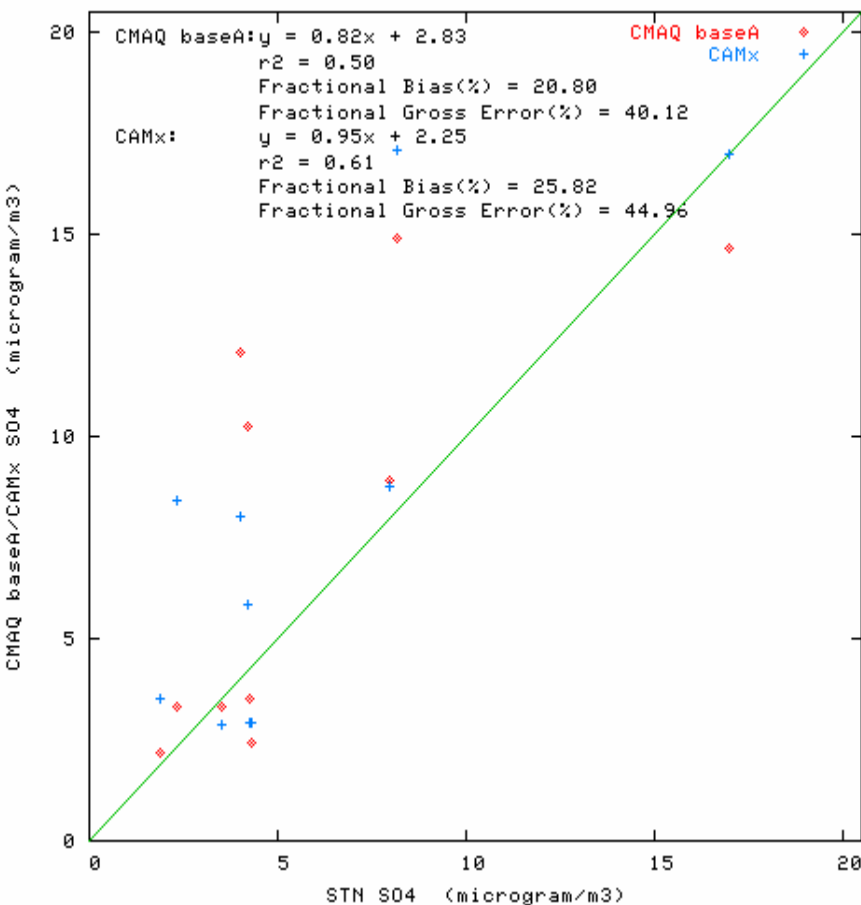
June 02 Episode

Blair St.

Grant

STN vs. CMAQ baseA/CAMx S04 at station 29 510 0085 on 2002152-2002181

STN vs. CMAQ baseA/CAMx S04 at station 29 510 0089 on 2002152-2002181



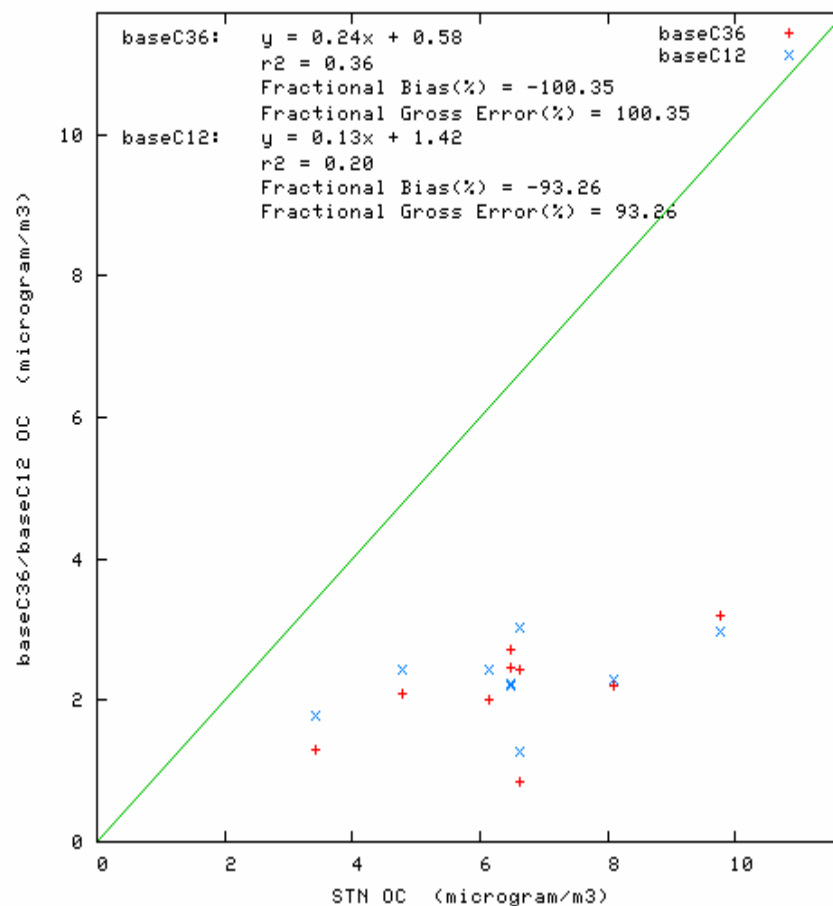
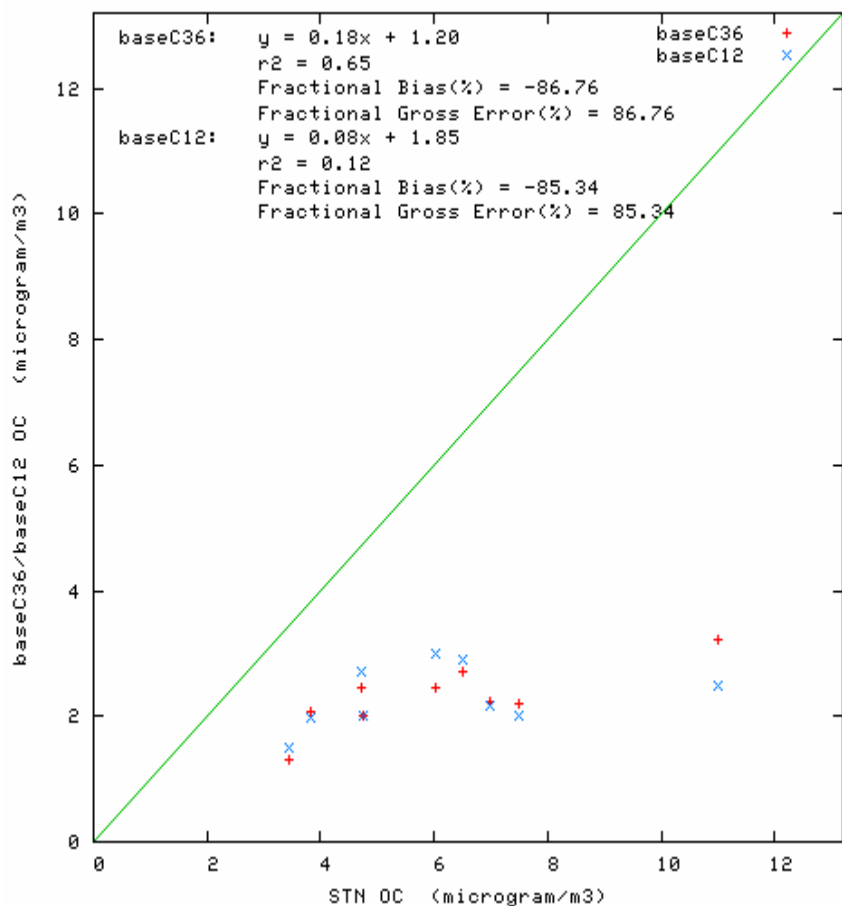
Organic Carbon - VISTAS 36/12 km June 02 Episode

Blair St.

Grant

STN vs. baseC36/baseC12 OC at station 29 510 0085 on 2002152-2002181

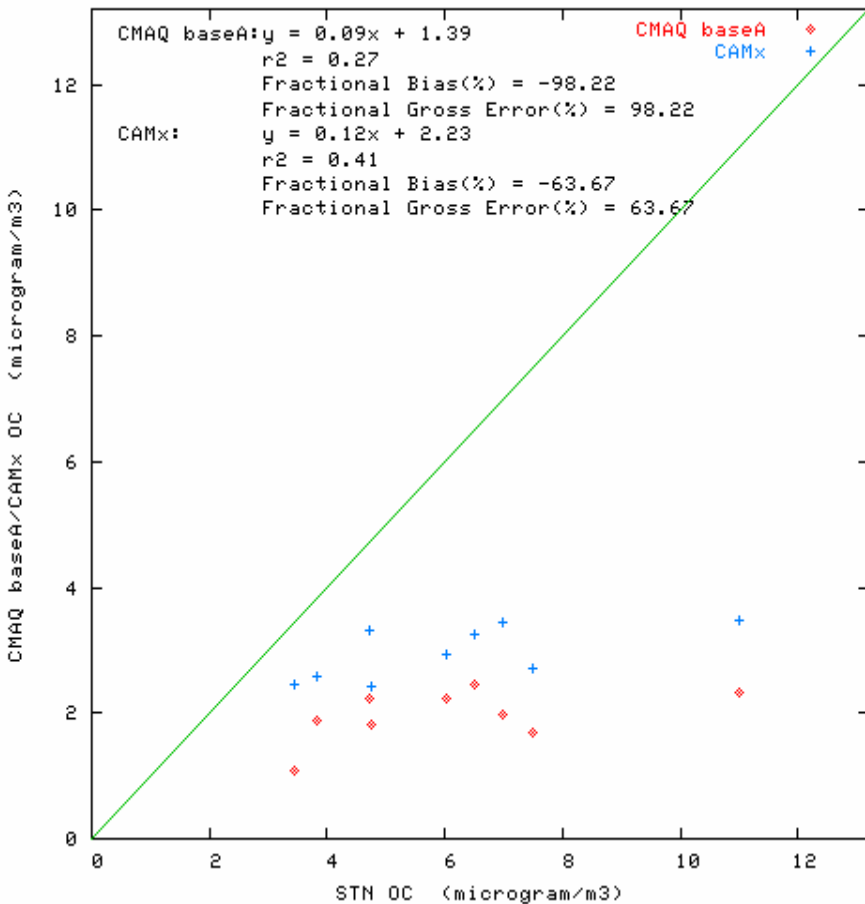
STN vs. baseC36/baseC12 OC at station 29 510 0089 on 2002152-2002181



Organic Carbon - CENRAP 36 km June 02 Episode

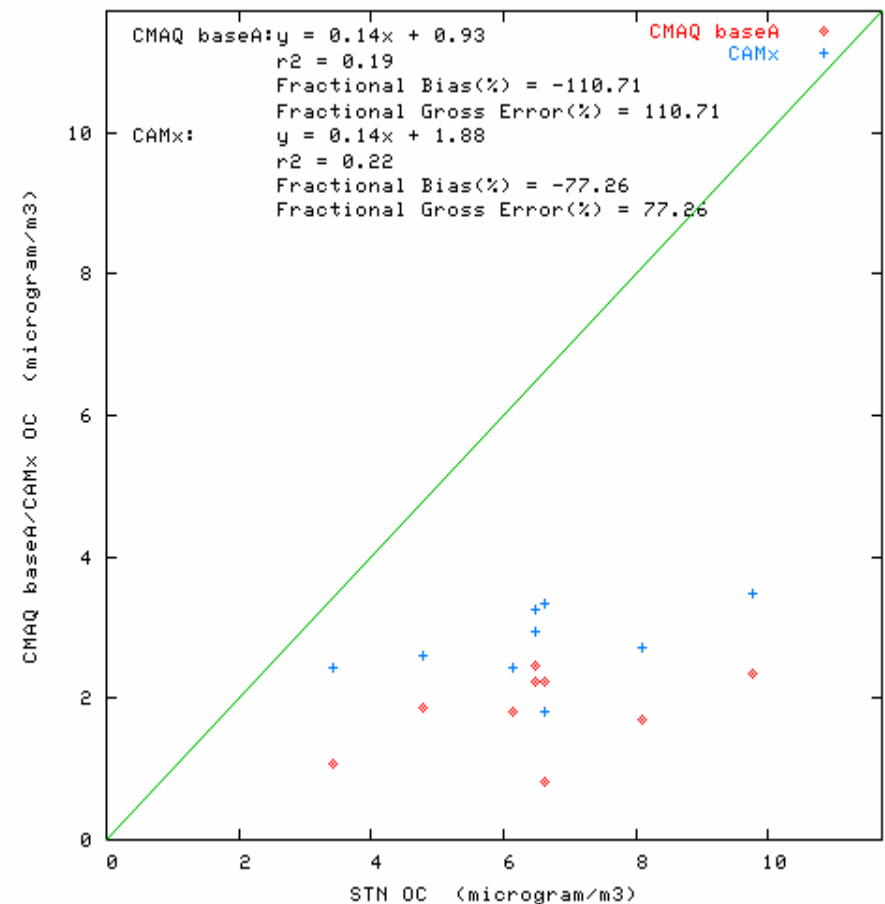
Blair St.

STN vs. CMAQ baseA/CAMx OC at station 29 510 0085 on 2002152-2002181



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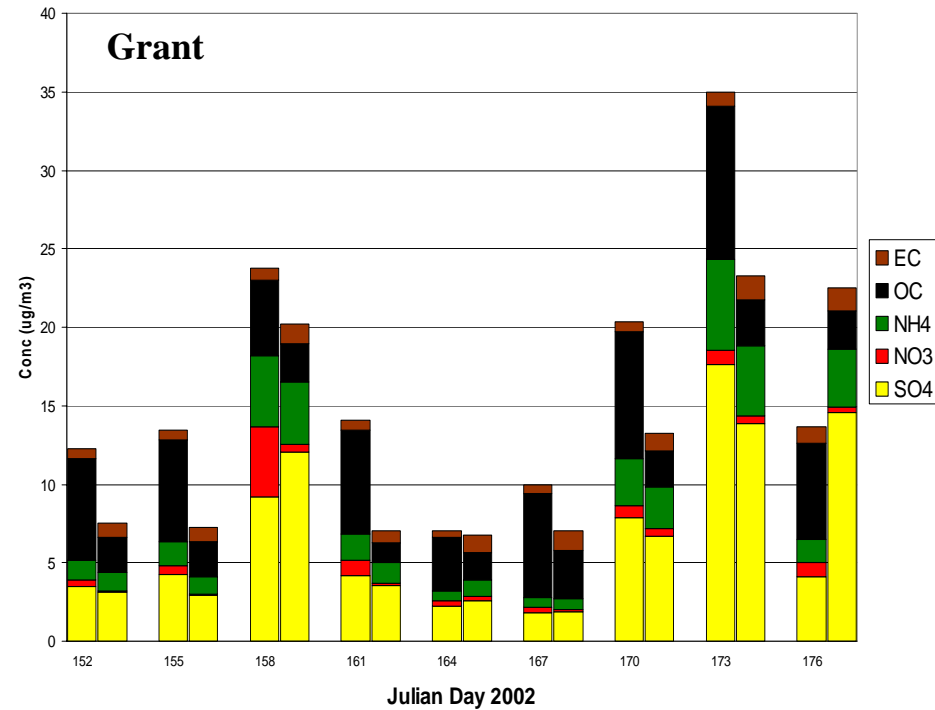
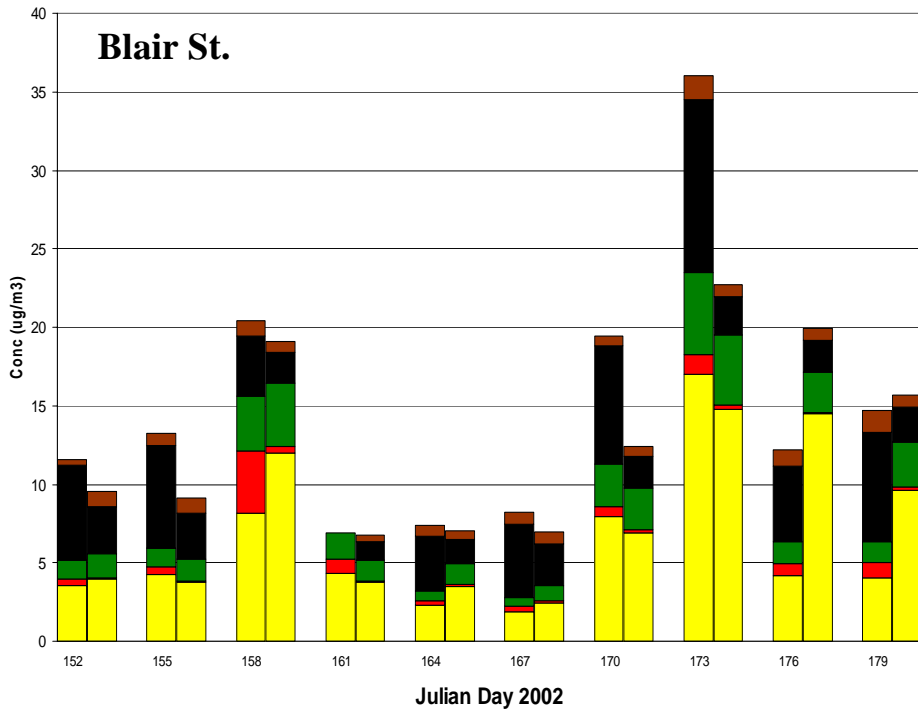
STN vs. CMAQ baseA/CAMx OC at station 29 510 0089 on 2002152-2002181



St. Louis PM2.5 - CENRAP

June Obs vs 36km CMAQ at 29-510-0085

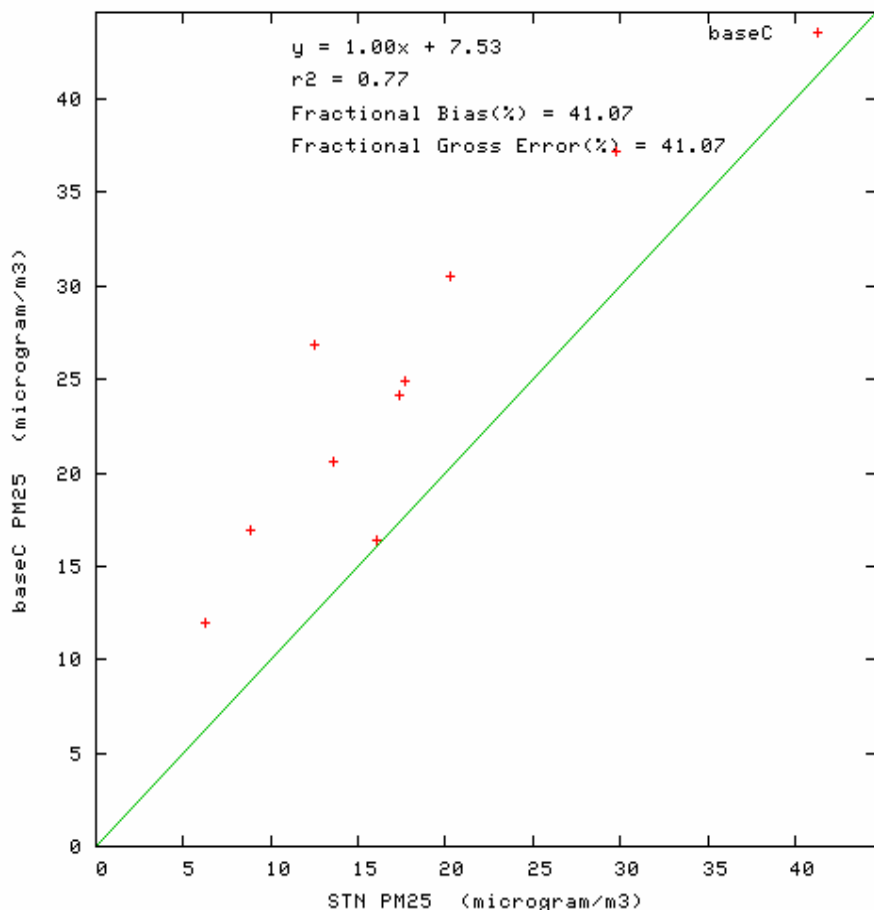
June Obs vs 36km CMAQ at 29-510-0089



PM2.5 - VISTAS 12 km January 02 Episode

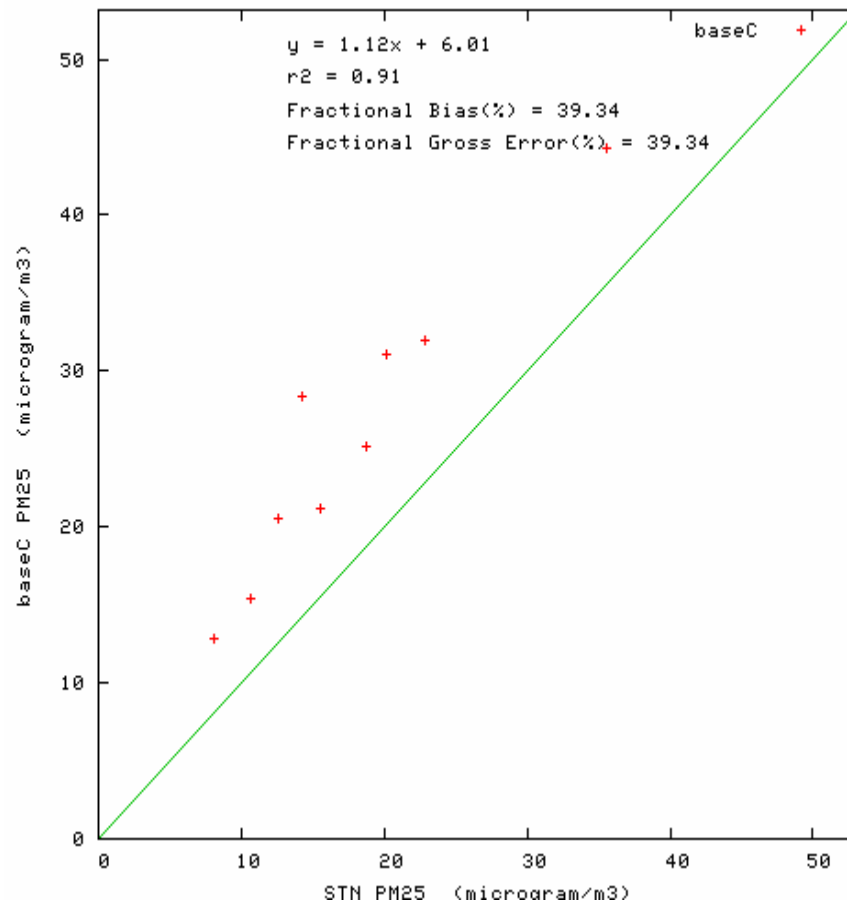
Blair St.

STN vs. baseC PM25 at station 29 510 0085 on 2002001-2002031



Grant

STN vs. baseC PM25 at station 29 510 0089 on 2002001-2002031



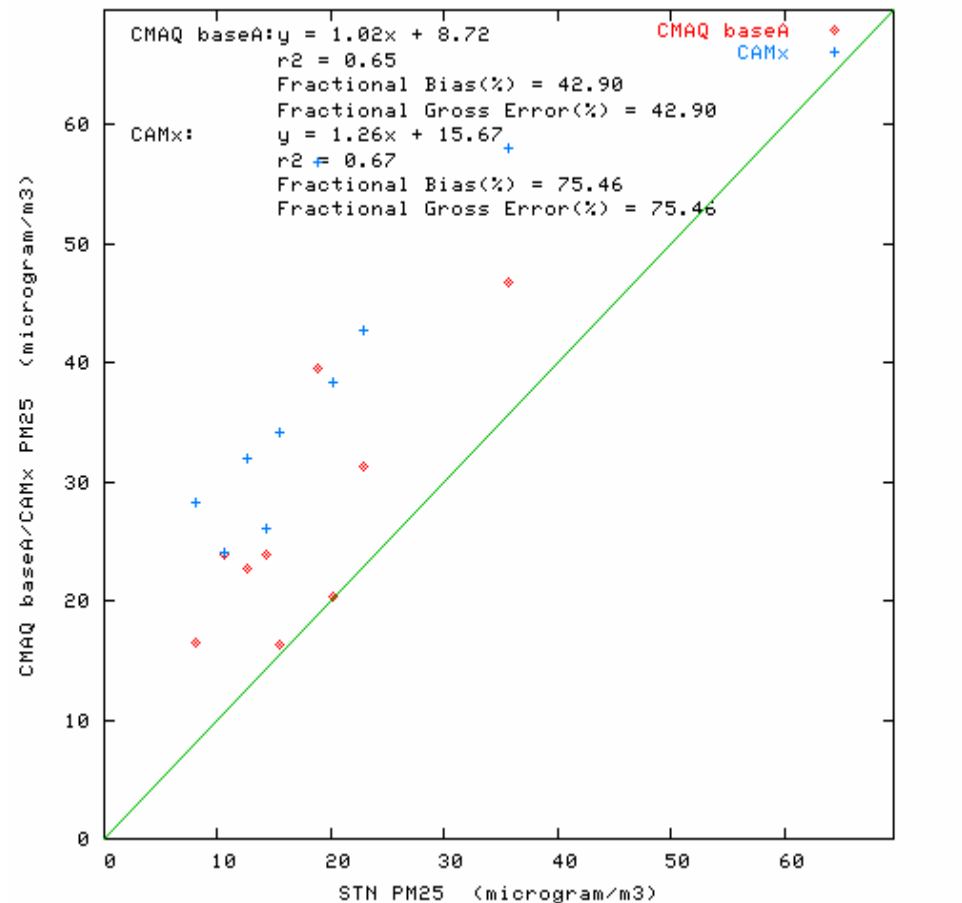
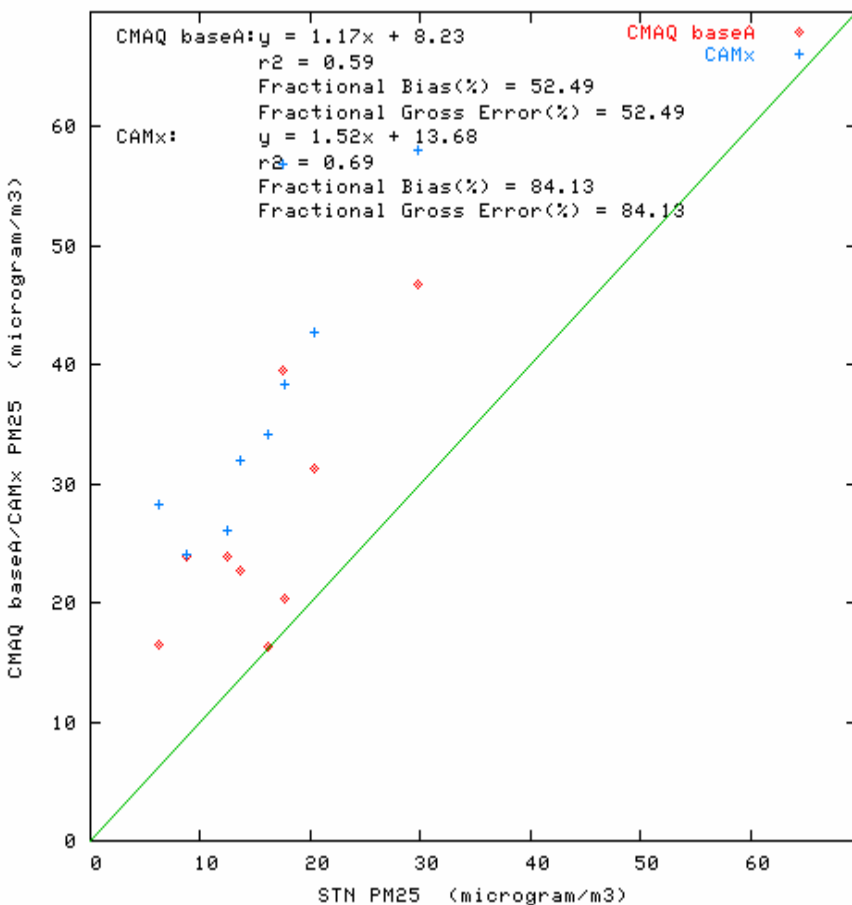
PM2.5 - CENRAP 36 km January 02 Episode

Blair St.

Grant

STN vs. CMAQ baseA/CAMx PM25 at station 29 510 0085 on 2002001-2002031

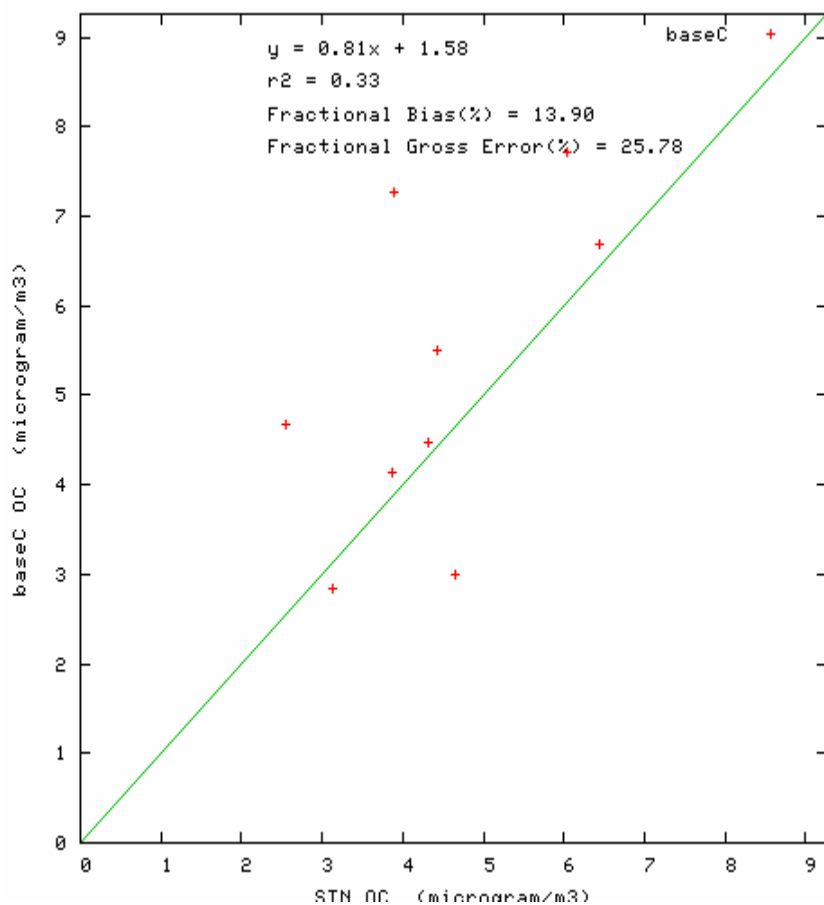
STN vs. CMAQ baseA/CAMx PM25 at station 29 510 0089 on 2002001-2002031



Organic Carbon - VISTAS 36/12 km January 02 Episode

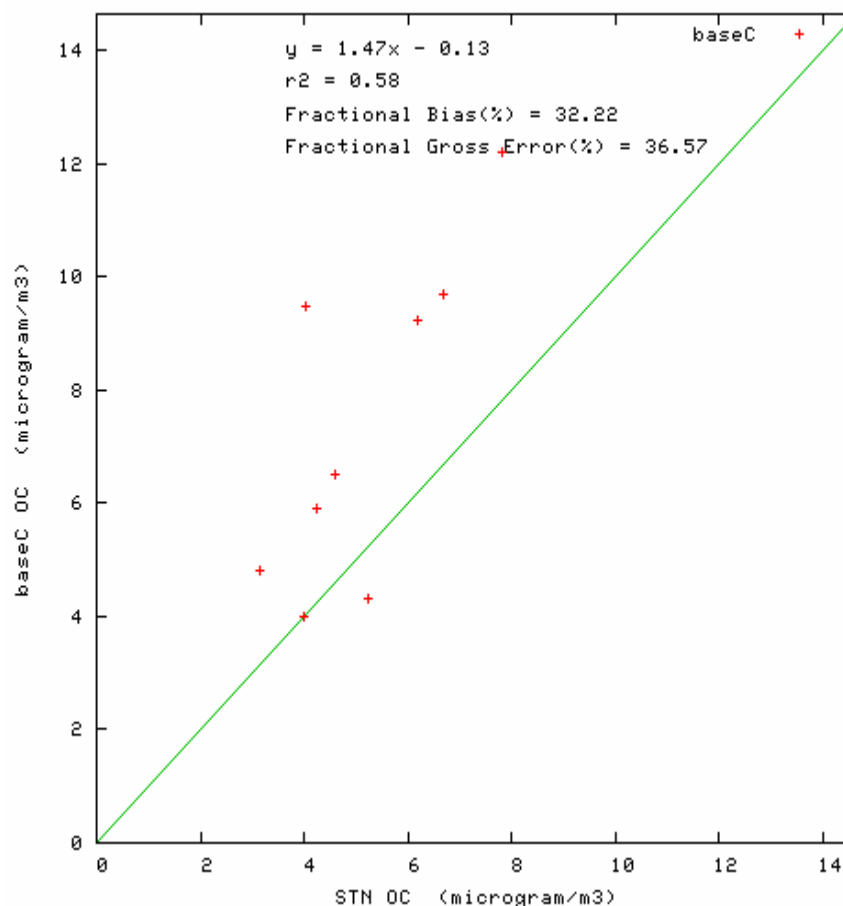
Blair St.

STN vs. baseC OC at station 29 510 0085 on 2002001-2002031



Grant

STN vs. baseC OC at station 29 510 0089 on 2002001-2002031

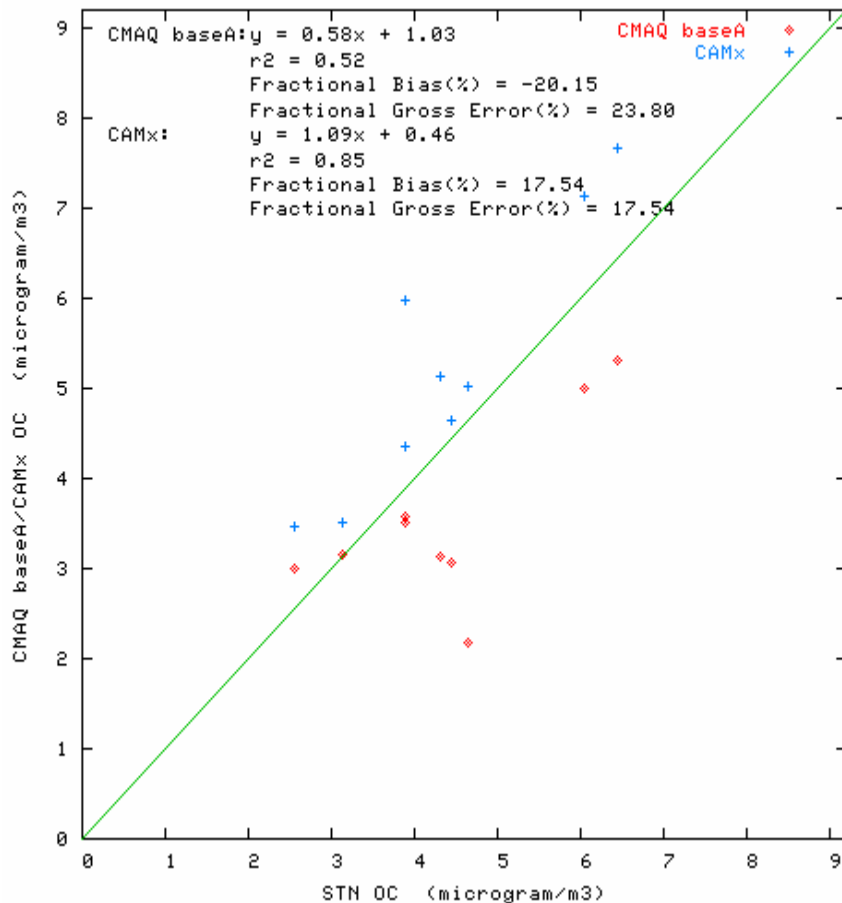


Organic Carbon - CENRAP 36 km

January 02 Episode

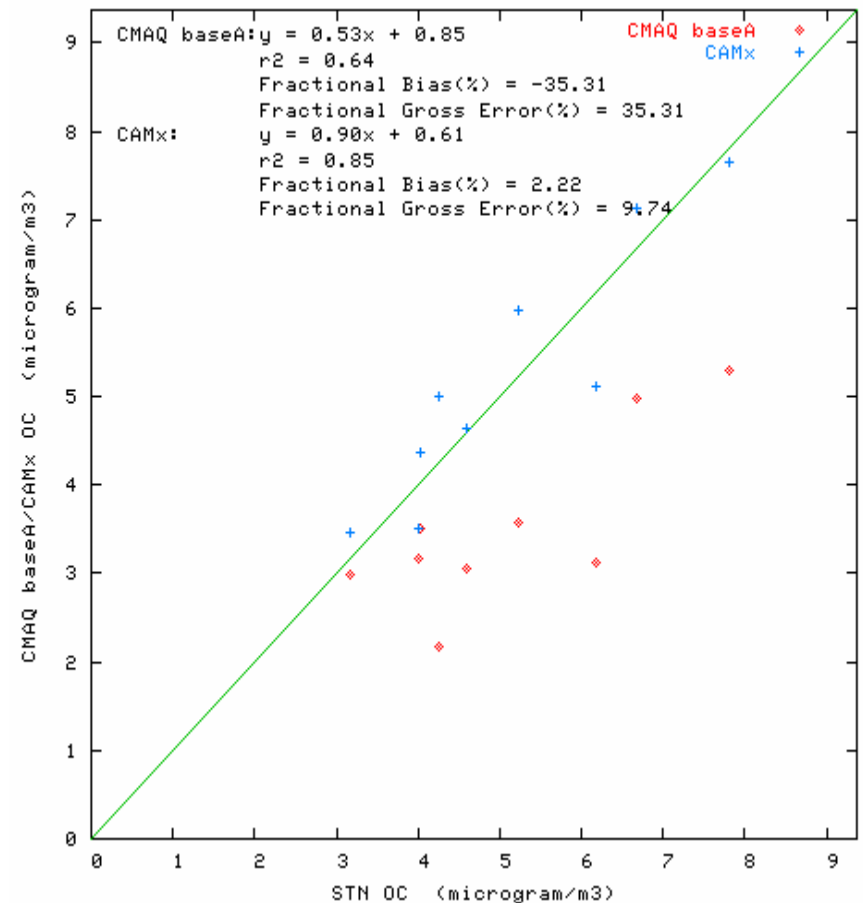
Blair St.

STN vs. CMAQ baseA/CAMx OC at station 29 510 0085 on 2002001-2002031



Grant

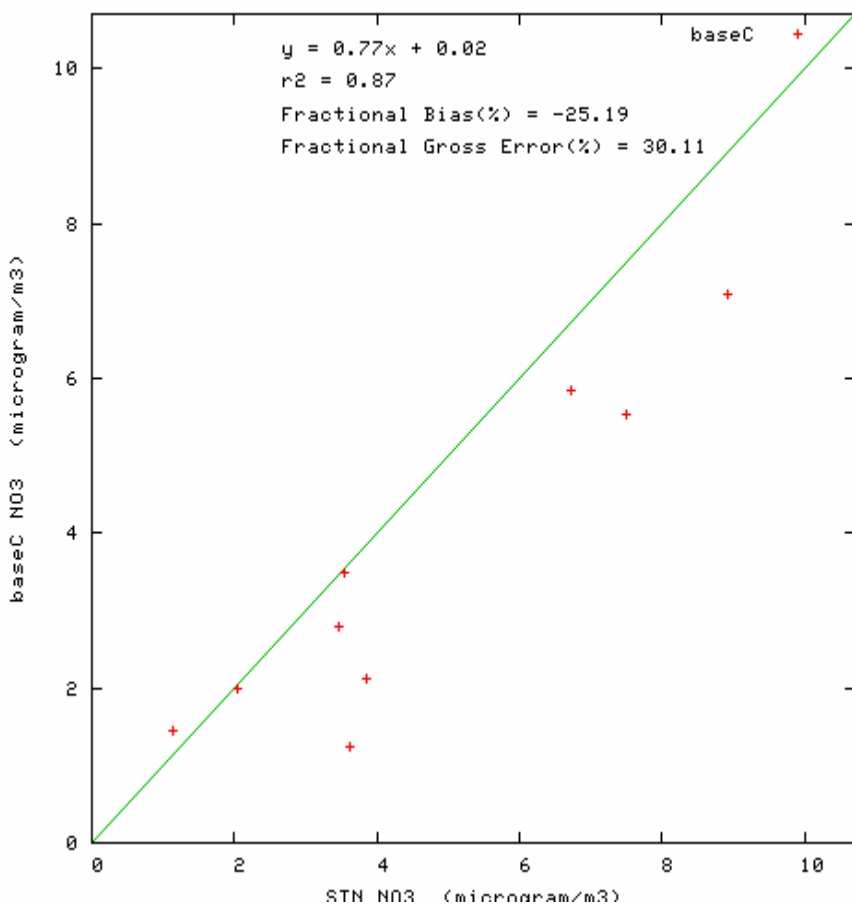
STN vs. CMAQ baseA/CAMx OC at station 29 510 0089 on 2002001-2002031



Nitrate - VISTAS 12 km January 02 Episode

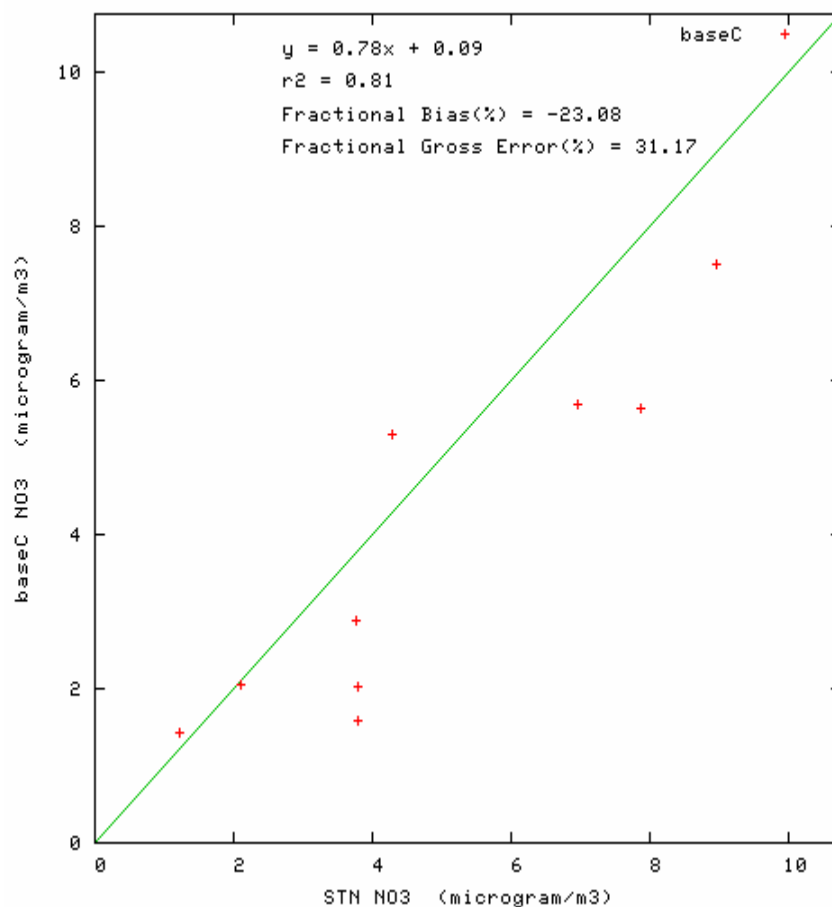
Blair St.

STN vs. baseC N03 at station 29 510 0085 on 2002001-2002031



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STN vs. baseC N03 at station 29 510 0089 on 2002001-2002031

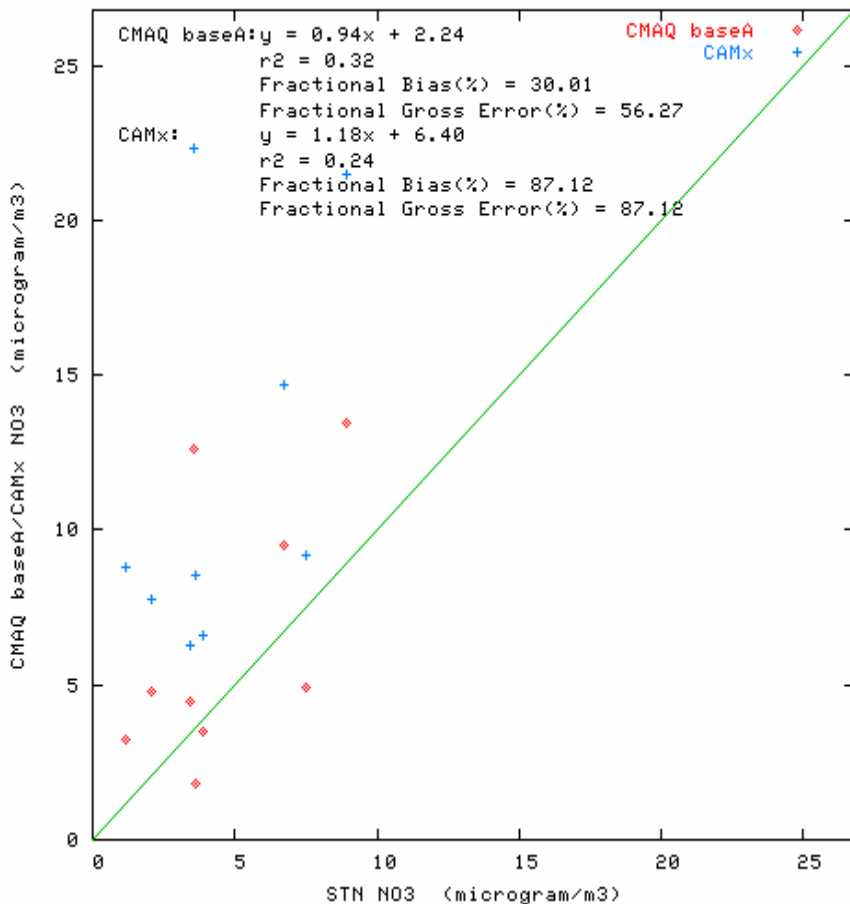


Nitrate - CENRAP 36 km

January 02 Episode

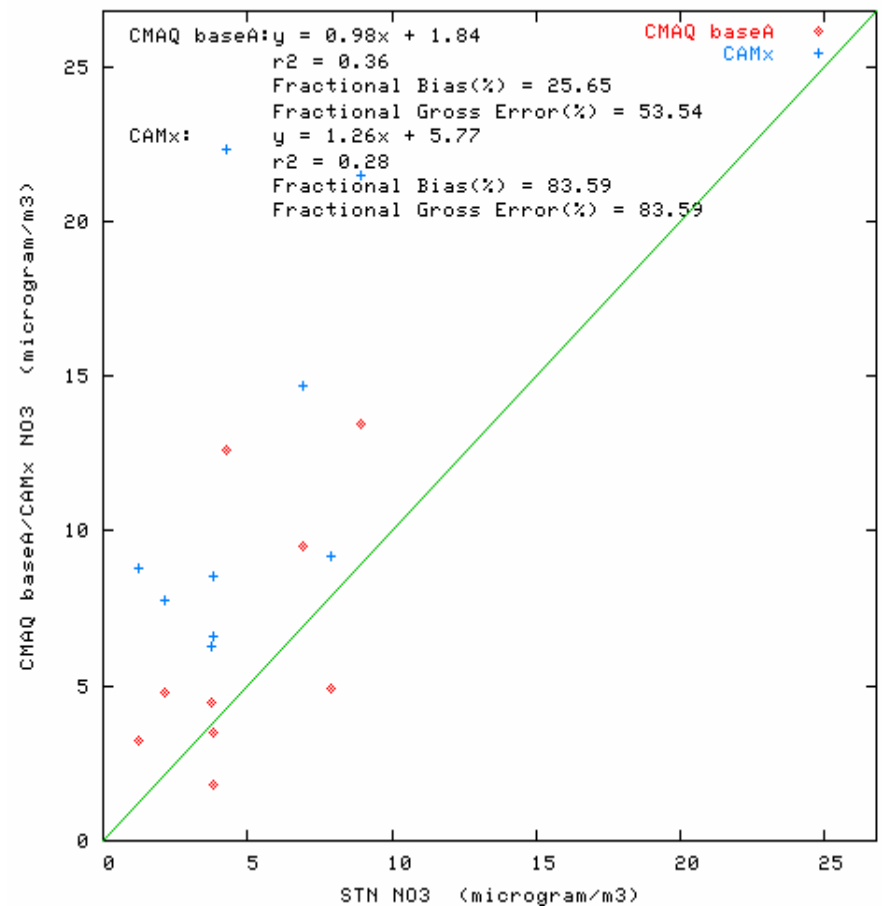
Blair St.

STN vs. CMAQ baseA/CAMx N03 at station 29 510 0085 on 2002001-2002031



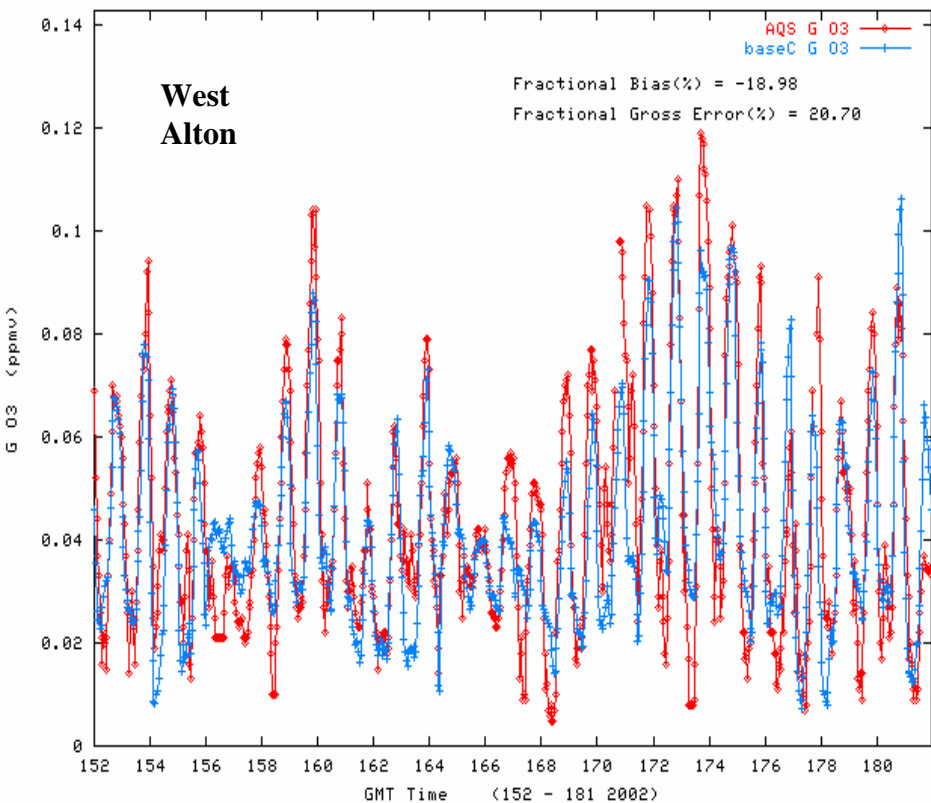
Grant

STN vs. CMAQ baseA/CAMx N03 at station 29 510 0089 on 2002001-2002031

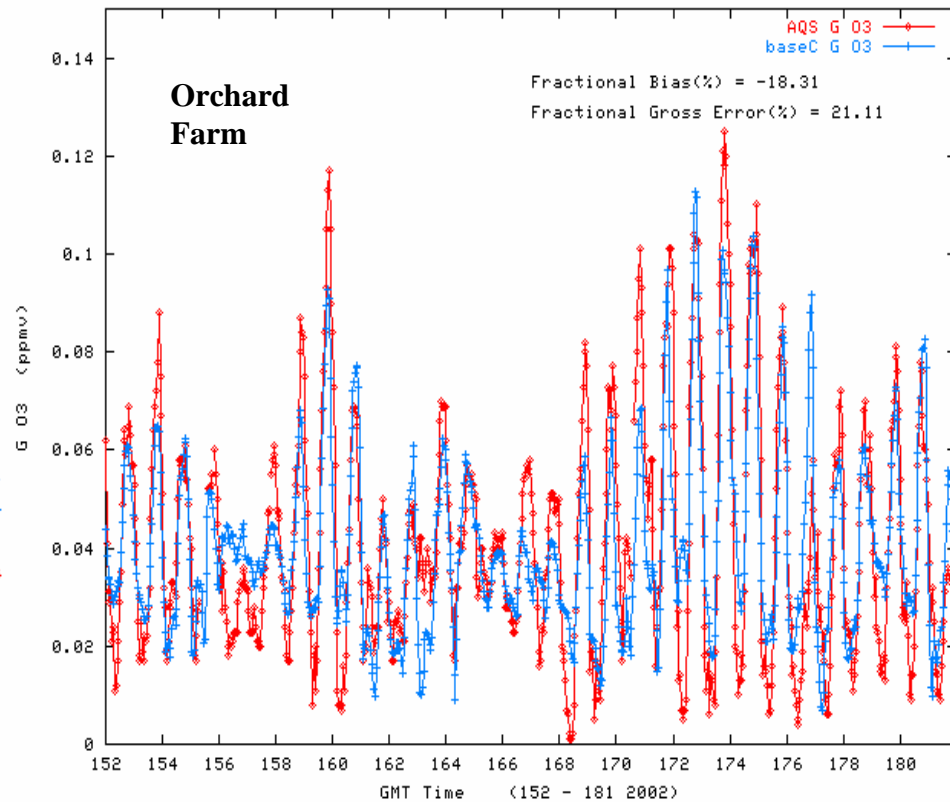


Ozone - VISTAS 12 km June 02 Episode

Time Series for AQS vs. baseC G 03 at station 29 183 1002

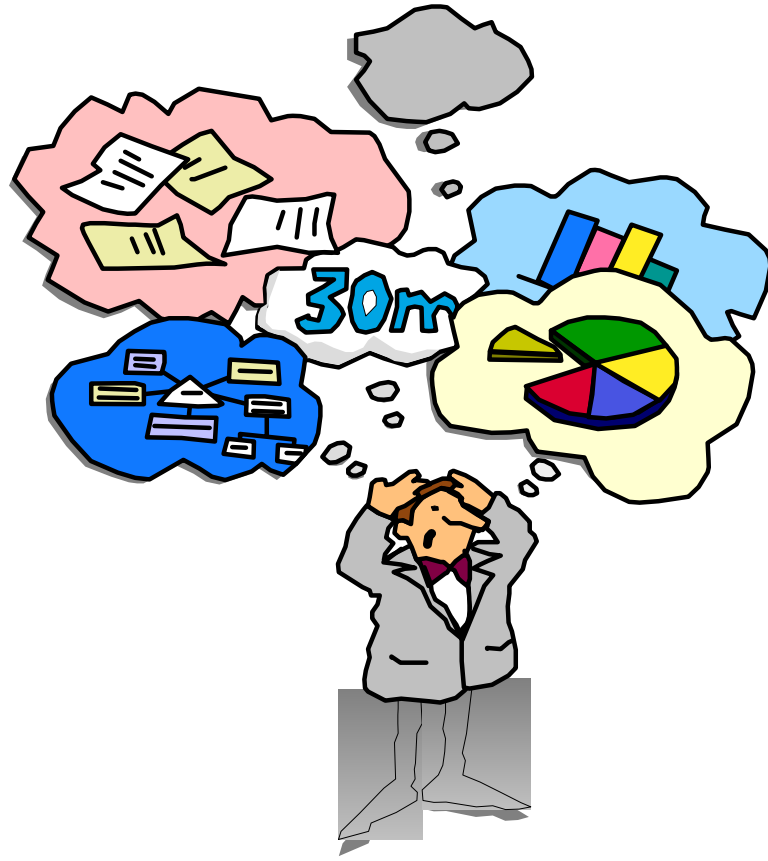


Time Series for AQS vs. baseC G 03 at station 29 183 1004



Summary of Model Performance

- For June, both VISTAS (36/12 km) and CENRAP (CMAQ/CAMx) results seem to agree fairly well with obs. for PM_{2.5}. However, performance varies by day and specie, good performance for sulfate, underprediction of organic carbon by both models.
- For January, both VISTAS and CENRAP model results overpredicted PM_{2.5} at both monitor sites. Performance for organic carbon & nitrate are acceptable except for CAMx nitrate. Overprediction for sulfate.
- For ozone, VISTAS 12 km results closely follow the diurnal profile at both monitoring sites, but miss the daily peak and valley.
- Further evaluation is needed, other months, sensitivities, 2009 modeling, etc.



Questions ???????