Uncertainty Assessment of CMAQ Dry Deposition Predictions

Robin L. Dennis
Atmospheric Modeling Division

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Annapolis, MD

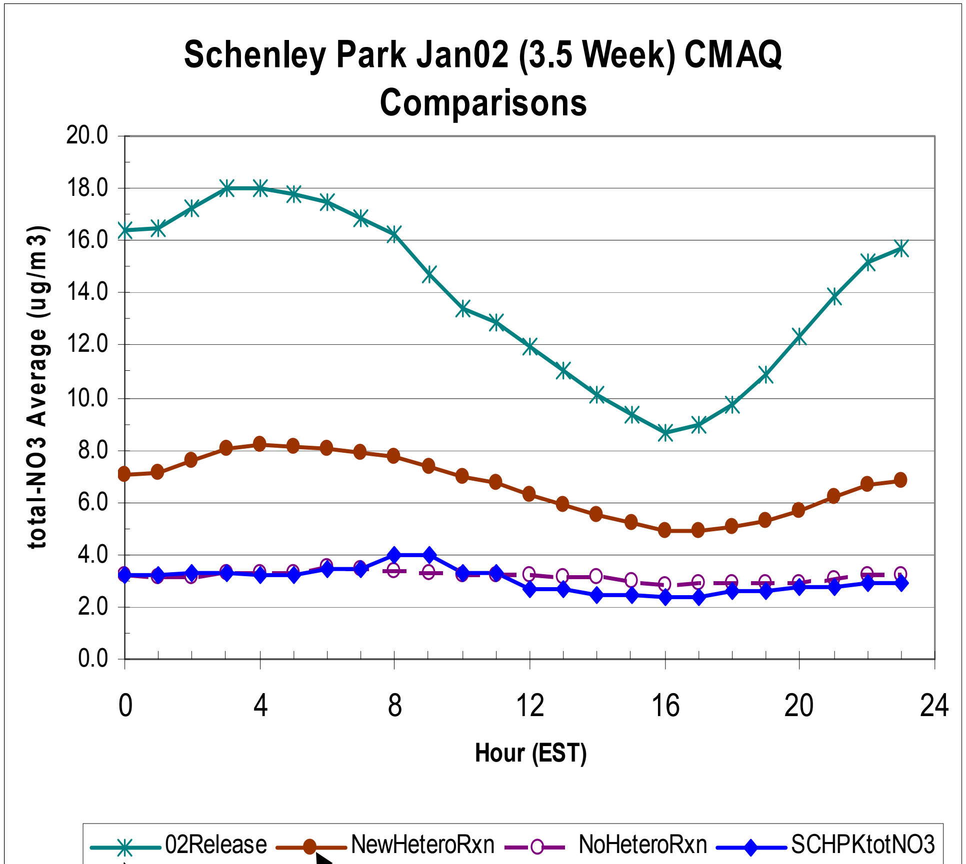
Uncertainty Assessment of CMAQ Dry Deposition

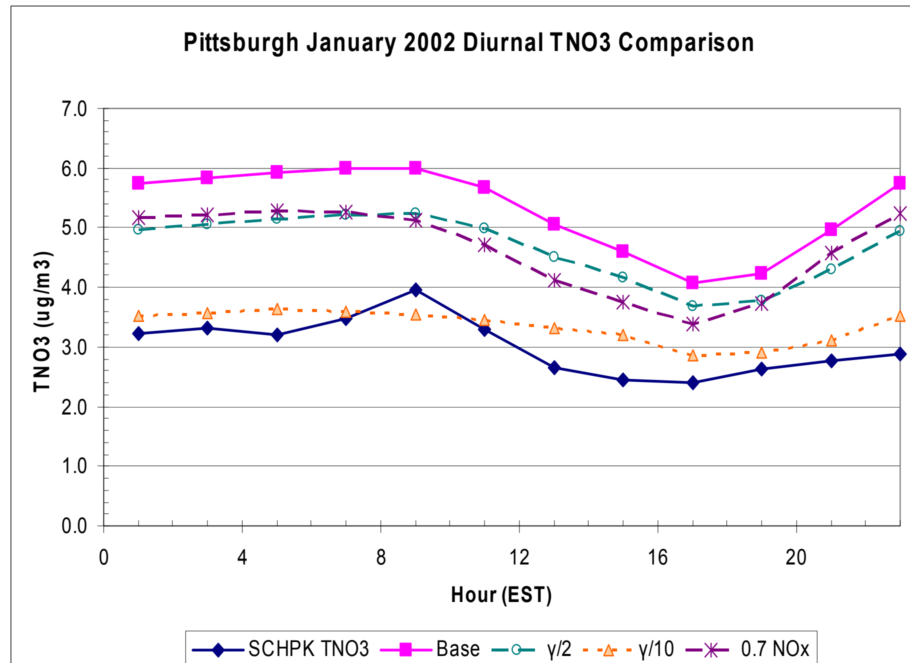
- We decided that directly providing dry deposition from CMAQ is the approach with the least introduction of error.
- We are taking advantage of an opening in the schedule to better understand uncertainties in the modeled dry deposition we are passing to the watershed model.
- Emission uncertainties (inputs uncertainties) affect the model output predictions. Here, I am interested in process-level uncertainties that have the potential to create a bias in the values handed off to the Bay models.

- There are two process-level uncertainties that we are aware of (parameterizations in CMAQ) that will affect dry deposition predictions.
  - Heterogeneous conversion of NO_2 to HNO_3 (affects Ox-N)
    - Tied to parameterization of the reaction probability, γ, for the heterogeneous production of HNO_3 from N_2O_5. Not well known.
    - We use the most recent (lowest) literature values for γ. Recent field experiments are consistent with model sensitivity analyses to suggest γ should be even lower.
  - Dry deposition flux of NH_3 (affects Red-N)
    - Tied to uncertainty about the ammonia deposition flux due to lack of measurements (very hard to measure flux) and recognition that there is a bi-directional flux from vegetation and also emissions from soils that confound interpretation of data.
    - Almost no reliable North American data. The judgment is that our latest parameterizations in CMAQ result in NH_3 fluxes that are too high. We don’t know where the truth is, but have some judgments, based on experiments, about the ballpark of a closer bound.

Starting Point for the Heterogeneous Production of HNO_3 Issue or (what we call) the N_2O_5 Issue

Pittsburgh Total-NO3 January 2002





CMAQ 4.2

CMAQ 4.3

CMAQ 4.4

γ/10

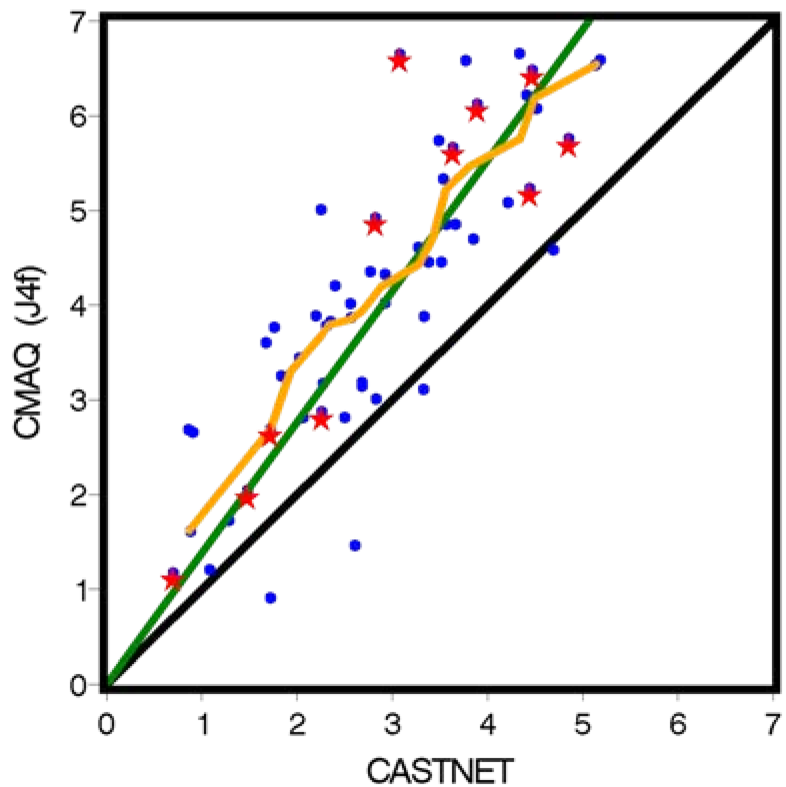
γ = reaction probability

- Sensitivity studies with CMAQ indicated reducing γ by a factor of 10 produced marked improvement in the simulation of total nitrate (compared to CASTNet measurements). But a factor of 10 seemed to go too far.

- We defined a sensitivity for Chesapeake Bay where we reduced γ by a factor of 7 (γ/7 Sensitivity).
    - **Base = J4f**
    - **Sensitivity = J4g**

- There is a clear improvement in CMAQ's total-nitrate predictions, in every season.

(NO3 + HNO3) AIR CONCENTRATION (UG/M3)
CMAQ (J4f)
VS. CASTNET (2001–2003 AVERAGED)
LIMITED TO SITES IN THE EASTERN U.S.
ANNUAL



LEGEND

REGRESSION THROUGH ORIGIN

RUNNING MEDIAN SMOOTH LINE

CASTNET SITES IN CHESAPEAKE BAY ★

(NO3 + HNO3) AIR CONCENTRATION (UG/M3)
CMAQ (J4g)
VS. CASTNET (2001–2003 AVERAGED)
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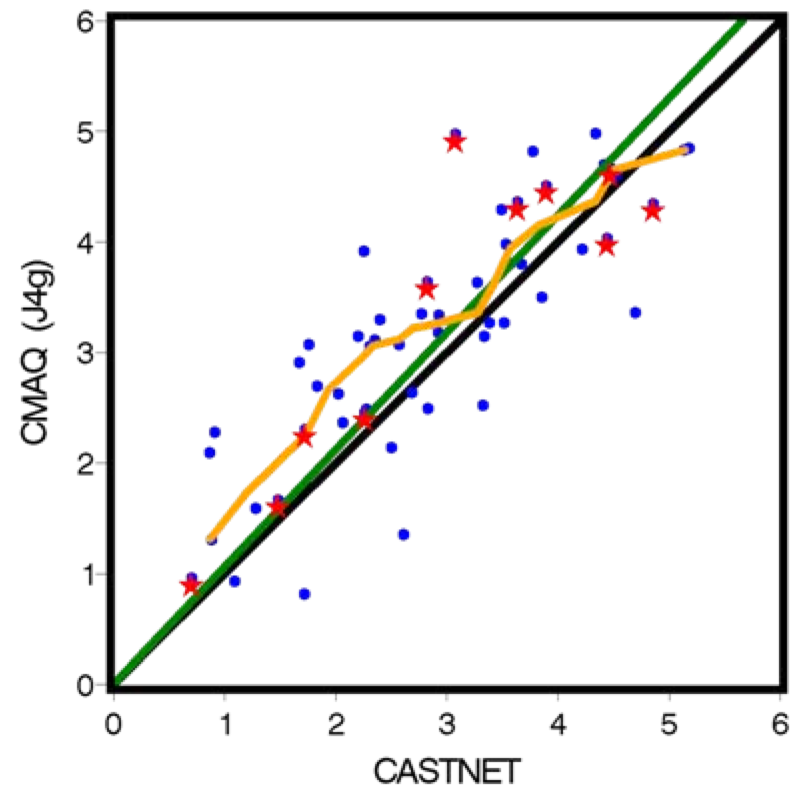
ANNUAL



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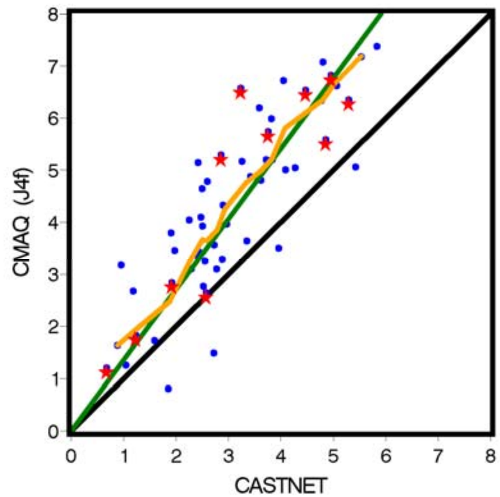
SPRING



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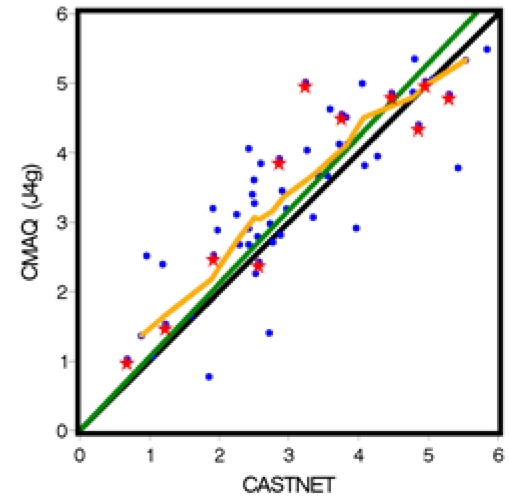
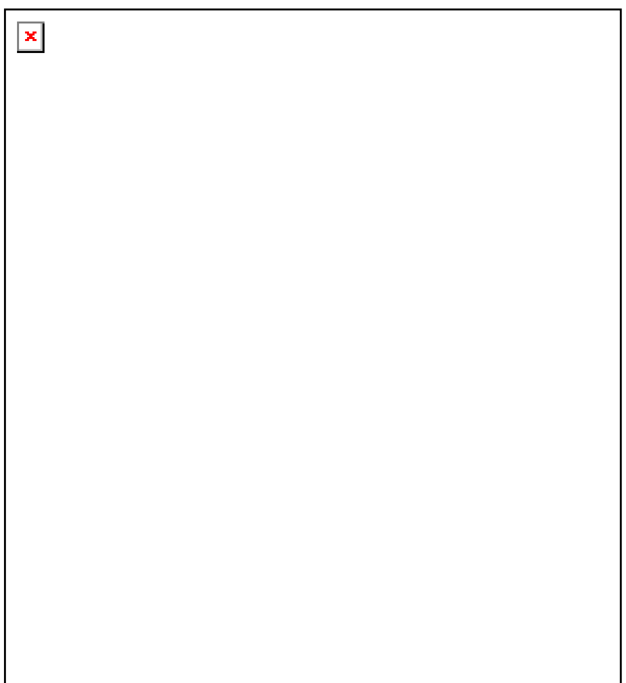
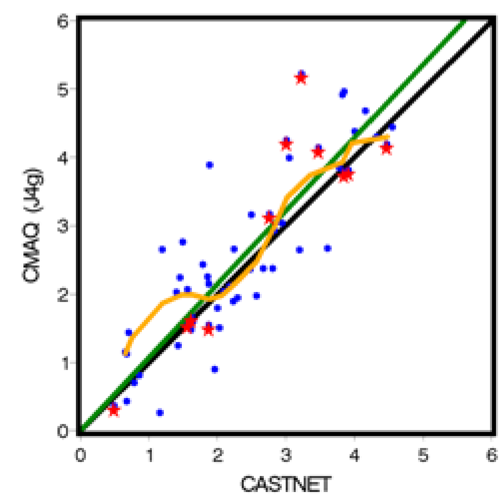




SUMMER



LEGEND
REGRESSION THROUGH ORIGIN
RUNNING MEDIAN SMOOTH LINE
CASTNET SITES IN CHESAPEAKE BAY ★

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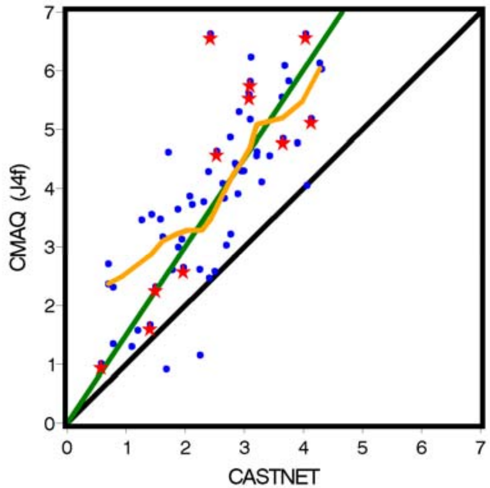
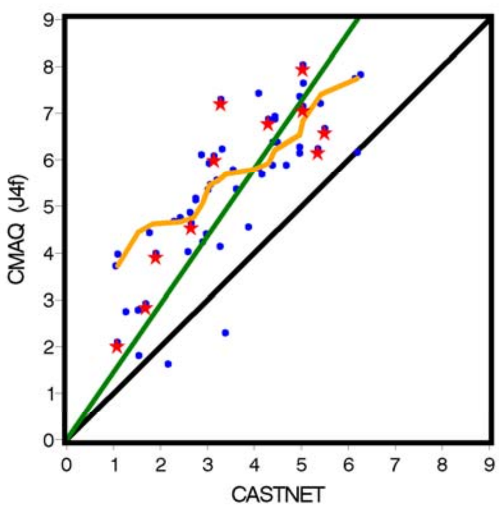
LIMITED TO SITES IN THE EASTERN U.S.
AUTUMN



WINTER



LEGEND
REGRESSION THROUGH ORIGIN
RUNNING MEDIAN SMOOTH LINE
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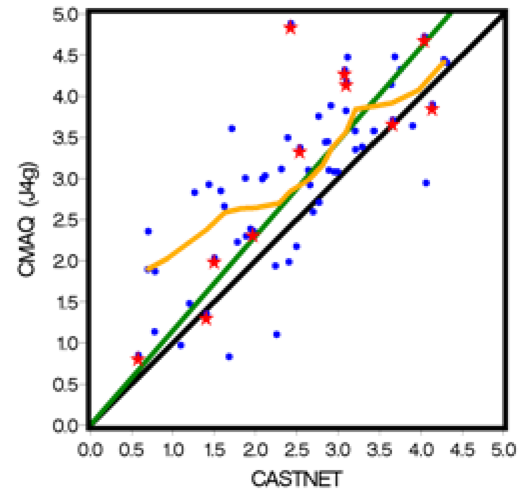
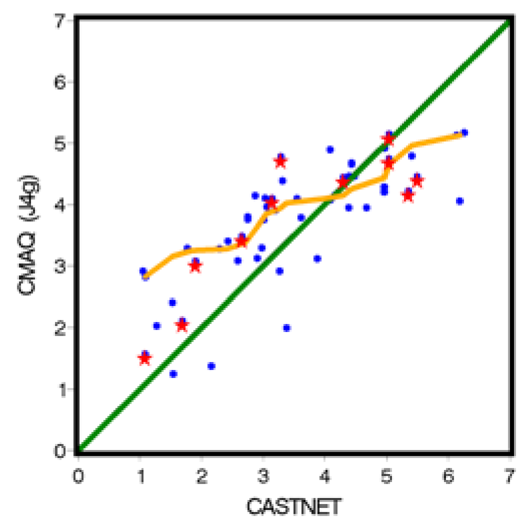


WINTER



LEGEND
REGRESSION THROUGH ORIGIN
RUNNING MEDIAN SMOOTH LINE
CASTNET SITES IN CHESAPEAKE BAY ★

Comparison of Total-Nitrate Concentrations: Model vs. Obs

	CMAQ Regressed Against CASTNet: Base (slope)	CMAQ Regressed Against CASTNet: γ/7 Sensitivity (slope)
Annual	1.38	1.06
Spring	1.35	1.06
Summer	1.21	1.07
Autumn	1.50	1.15
Winter	1.45	1.00

Dry deposition of Ox-N did not change as much as might be expected by considering Total-nitrate alone.

NITROGEN DEPOSITION TO THE CHESAPEAKE BAY (LAND + WATER)
CMAQ 36km - J4f and J4g
NO BIAS ADJUSTMENTS
ANNUAL

MAIN	SPECIES	Base J4f (lbs)	Sensitivity J4g (lbs)
1) DRYOX_N	DRYNO2_N	31,967,088	34,243,019
	DRYNO_N	9,273,265	9,597,669
	DRYN2O5_N	8,671,448	16,414,557
	DRYHNO3_N	121,266,418	99,518,580
	DRYHONO_N	262,290	271,378
	DRYNO3T_N	3,577,350	2,652,012
	DRYORGNO3T_N	3,627,020	3,713,229
	DRYPANT_N	11,920,777	12,189,141
	-------------	--------------	--------------
1) DRYOX_N		190,565,657	178,599,585
2) WETOX_N	WETN2O5_N	6,803	11,798
	WETNO3T_N	108,311,822	105,550,661
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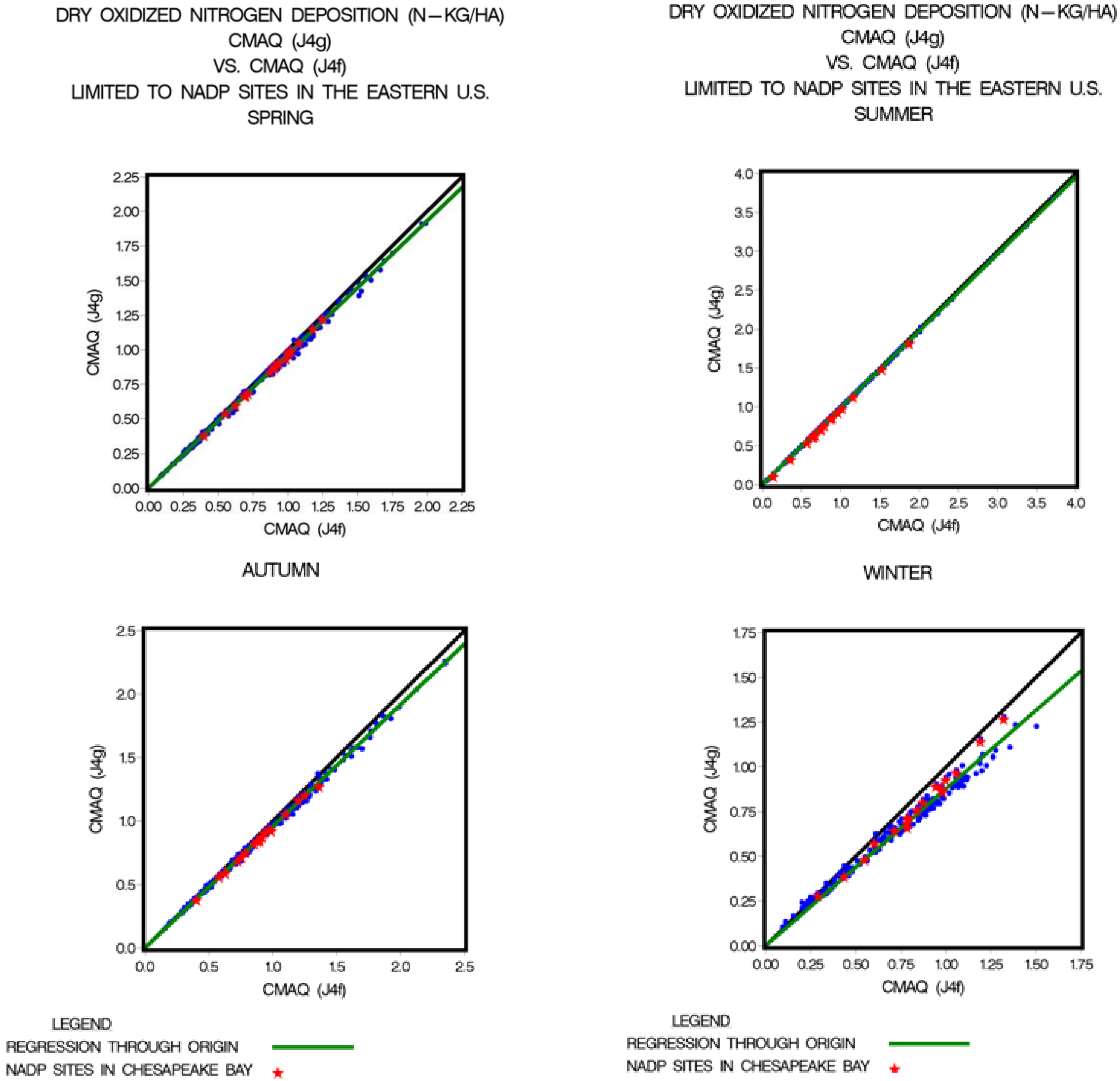
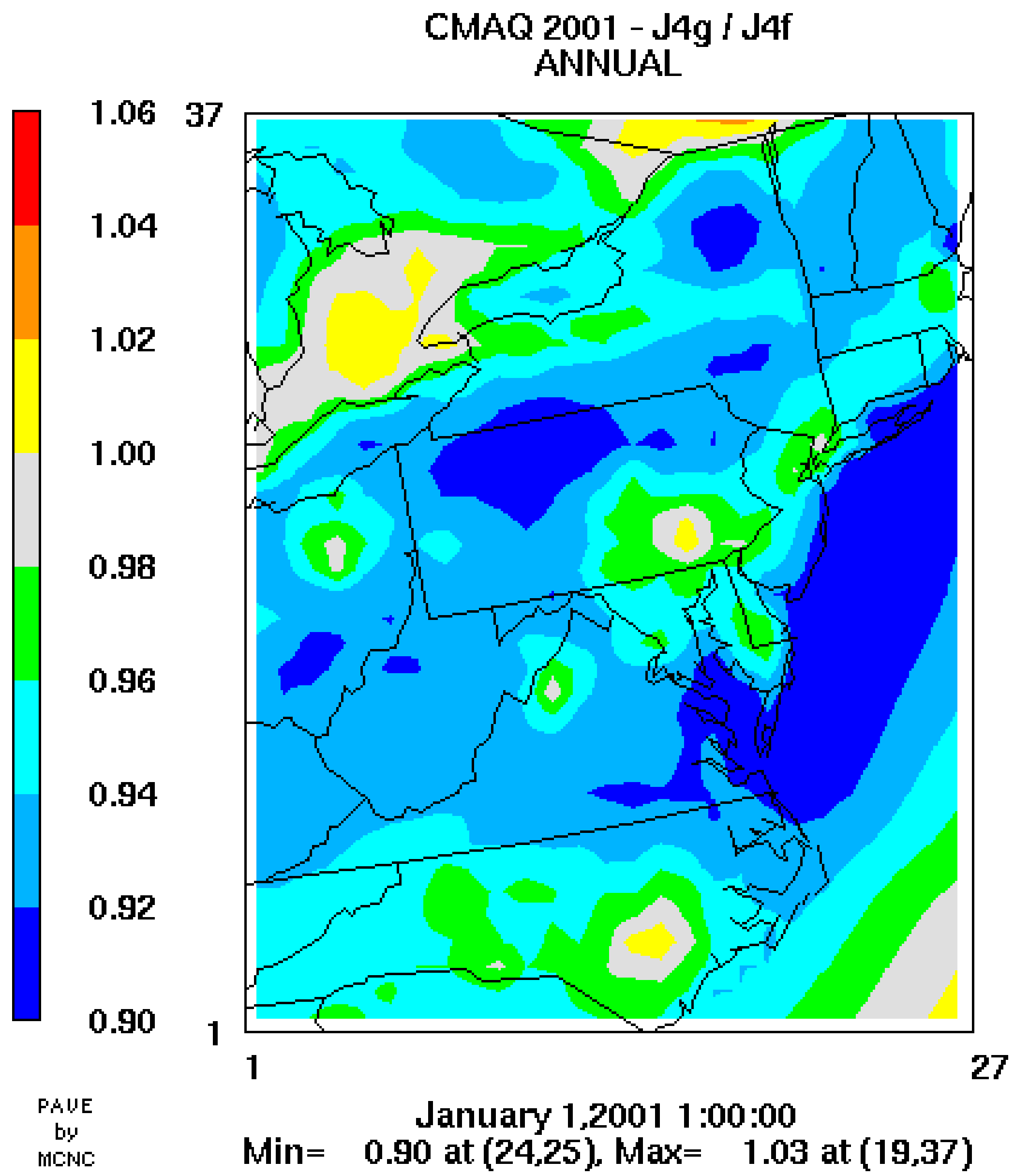
2) WETOX_N		108,318,625	105,562,458
3) TOTALOX_N	TOTALOX_N	298,884,282	284,162,044

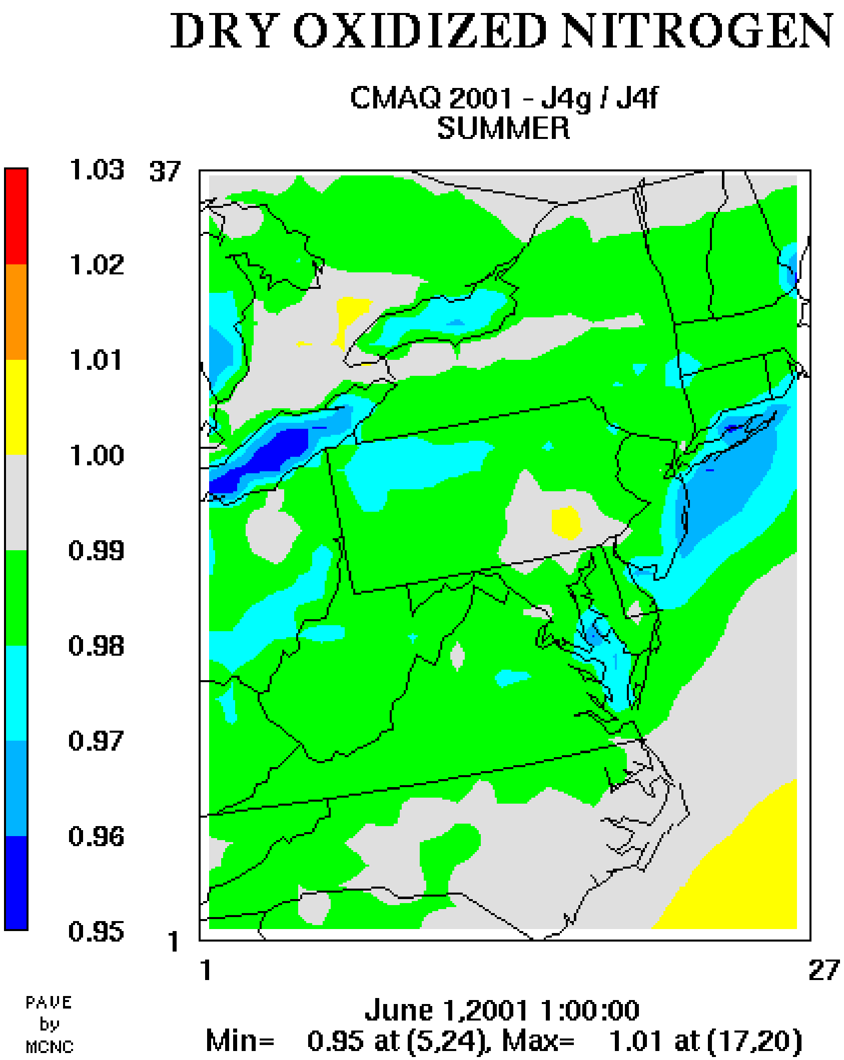

DRY OXIDIZED NITROGEN DEPOSITION (N—KG/HA)
CMAQ (J4g)
VS. CMAQ (J4f)
LIMITED TO NADP SITES IN THE EASTERN U.S.
SPRING
CMAQ (J4g)
CMAQ (J4f)
DRY OXIDIZED NITROGEN DEPOSITION (N—KG/HA)
CMAQ (J4g)
VS. CMAQ (J4f)
LIMITED TO NADP SITES IN THE EASTERN U.S.
SUMMER
CMAQ (J4g)
CMAQ (J4f)
AUTUMN
CMAQ (J4g)
CMAQ (J4f)
WINTER
CMAQ (J4g)
CMAQ (J4f)
LEGEND
REGRESSION THROUGH ORIGIN
NADP SITES IN CHESAPEAKE BAY
LEGEND
REGRESSION THROUGH ORIGIN
NADP SITES IN CHESAPEAKE BAY

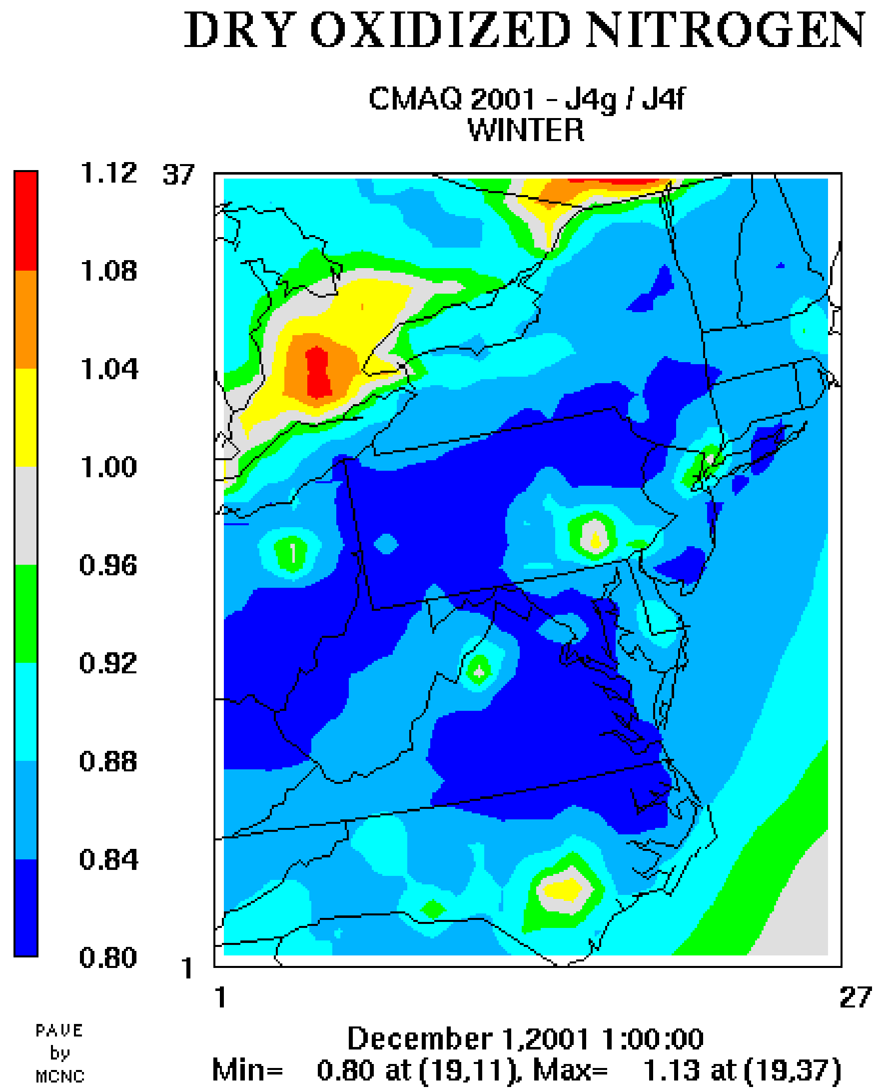
Change in Dry Deposition Associated with γ/7 Sensitivity

	Ox-N Dry Deposition	Red-N Dry Deposition
Annual	-6.3%	3.8%
Spring	-5.1%	3.8%
Summer	-1.4%	0.3%
Autumn	-5.6%	5.5%
Winter	-16.0%	13.2%

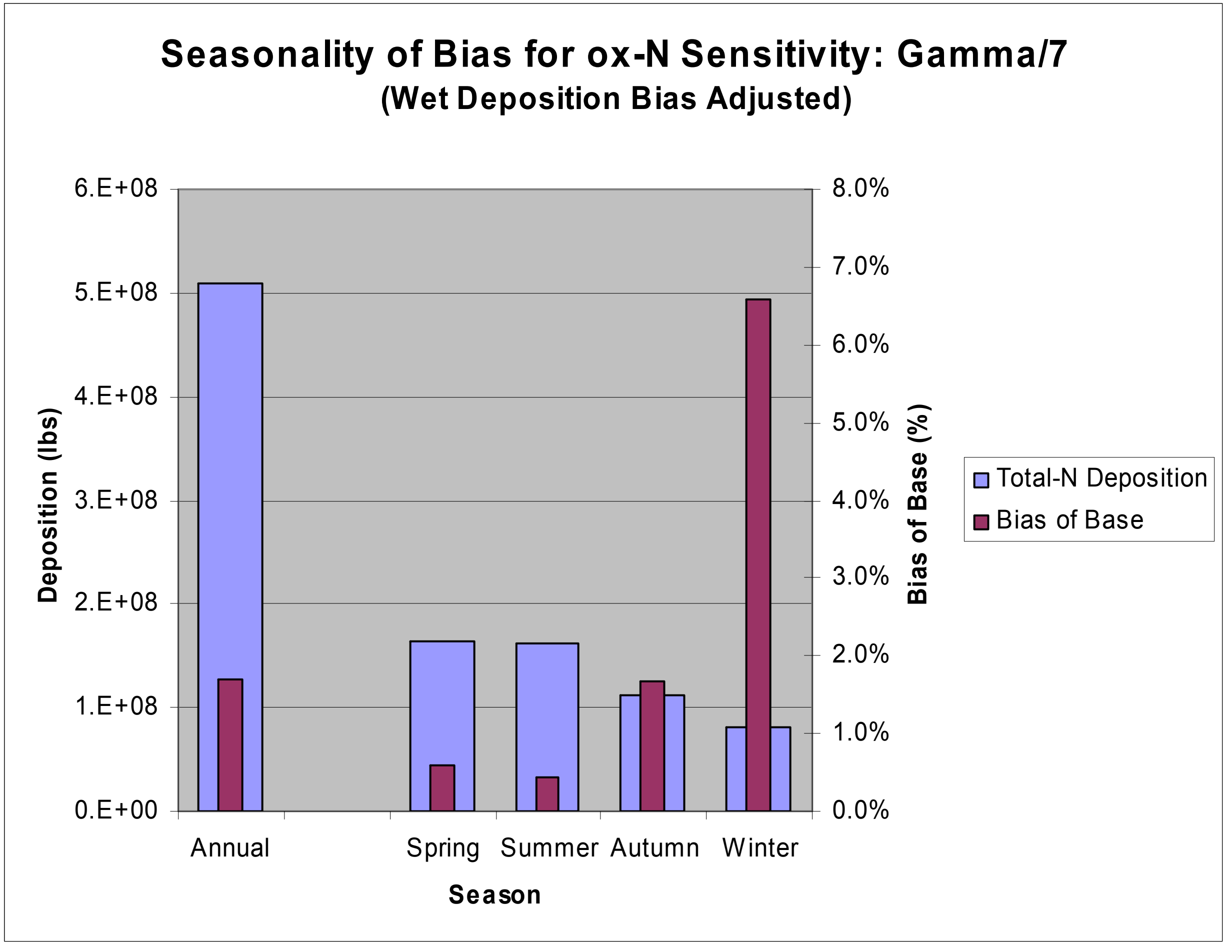
DRY OXIDIZED NITROGEN




DRY OXIDIZED NITROGEN
CMAQ 2001 - J4g / J4f
SUMMER
1.03
1.02
1.01
1.00
0.99
0.98
0.97
0.96
0.95
37
1
1
27
PAVE
by
MCNC
June 1,2001 1:00:00
Min= 0.95 at (5,24), Max= 1.01 at (17,20)


DRY OXIDIZED NITROGEN
CMAQ 2001 - J4g / J4f
WINTER
1.12
1.08
1.04
1.00
0.96
0.92
0.88
0.84
0.80
37
1
1
27
PAVE
by
MCNC
December 1,2001 1:00:00
Min= 0.80 at (19,11), Max= 1.13 at (19,37)

In terms of the total nitrogen deposition to the Chesapeake Bay watershed, the uncertainty in the heterogeneous production of HNO_3 does not contribute a significant degree of uncertainty to the input of total N.



Uncertainty: Heterogeneous conversion of NO_2 to HNO_3

(affects Ox-N)

- This uncertainty is not a serous source of ox-N deposition uncertainty.
- This uncertainty/bias is much smaller than the estimated spatially-associated uncertainty in NOx emissions of roughly ±40-45%.
- We expect CMAQ to update over time to move in the direction represented by this sensitivity.
- The impact of the expected improvements to CMAQ deposition predictions passed to the Chesapeake Bay Program are expected to be small.

2. Dry deposition flux of NH_3

- Deposition Flux is conceptually represented as:

  Flux = [Concentration] x Vd,

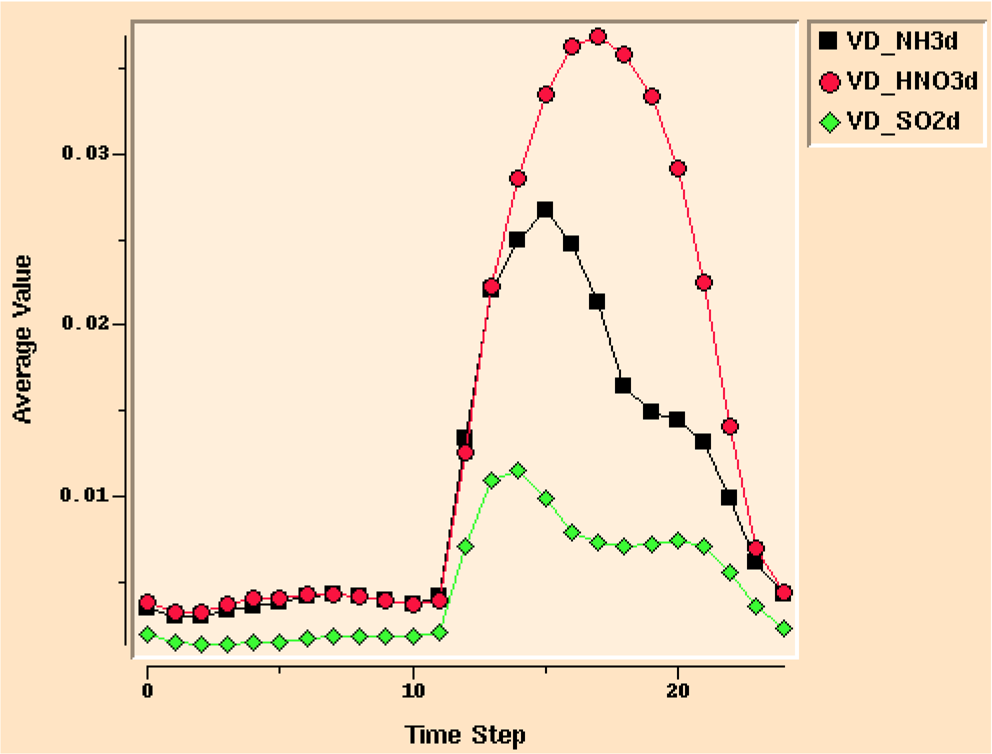
  where Vd is a derived deposition velocity based on a resistance-to-uptake paradigm

- The Extended RADM NH_3 Vd had been boosted to get it closer to the published European values.

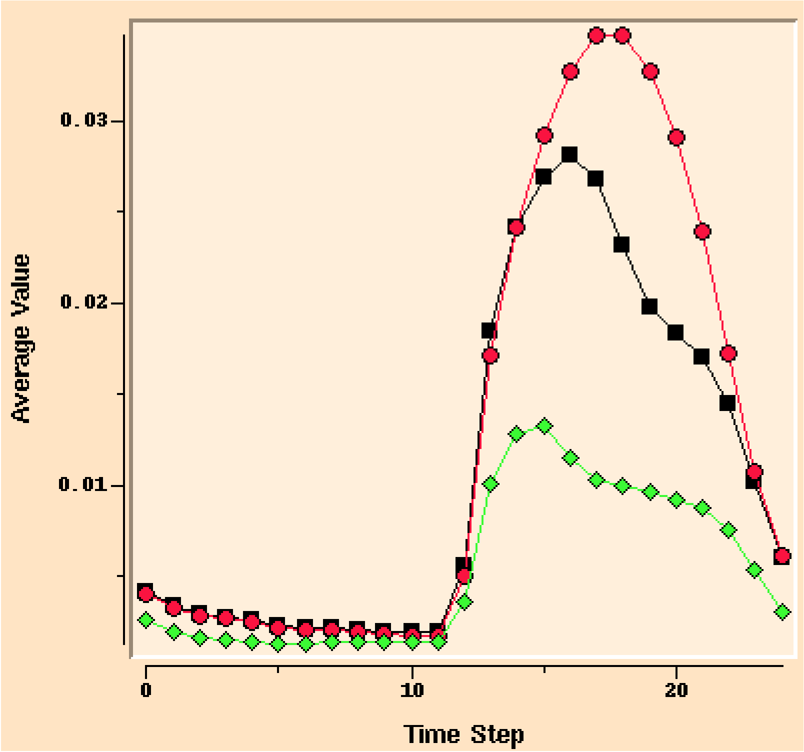
- The CMAQ NH_3 Vd was updated to address the earlier RADM issues and to now include the effects of water/dew on surfaces. This boosted the CMAQ NH_3 Vd significantly. Many average NH_3 Vd's now look high relative to European averages.

Average Deposition Velocity Across Spatial Domain
June 25, 2002

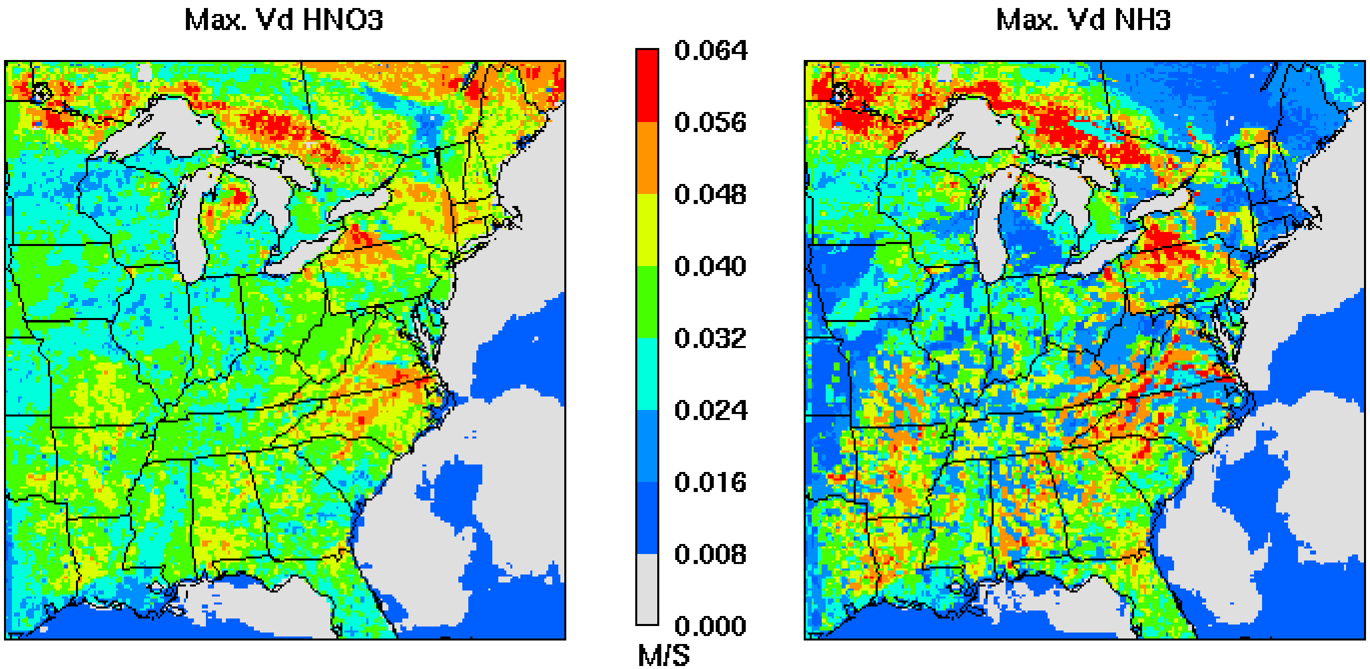
Chesapeake Watershed domain



Larger Eastern domain

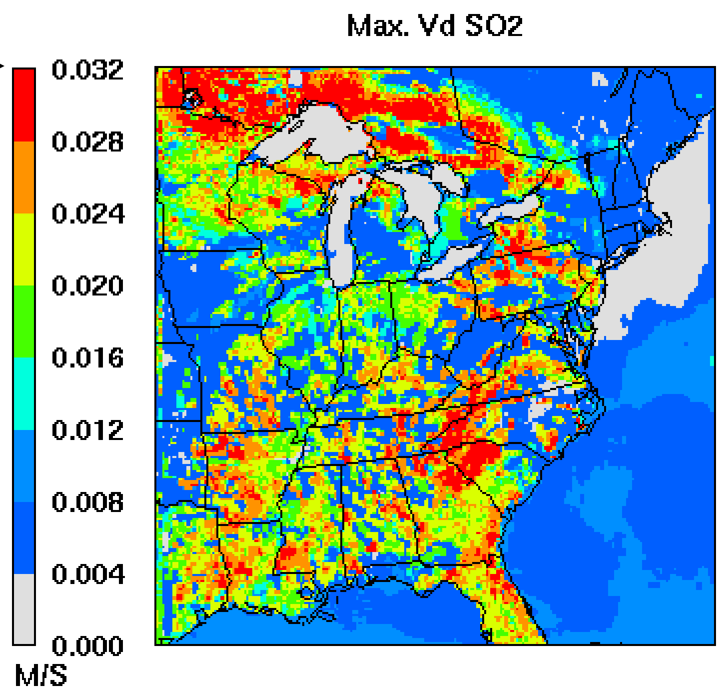


The CMAQ NH_3 Vd is now between that of HNO_3 and SO_2 in agreement with conventional wisdom.



The maximum Vd for NH_3 can equal that for HNO_3. That is pretty high.

Scale ½ of above



June 25, 2002

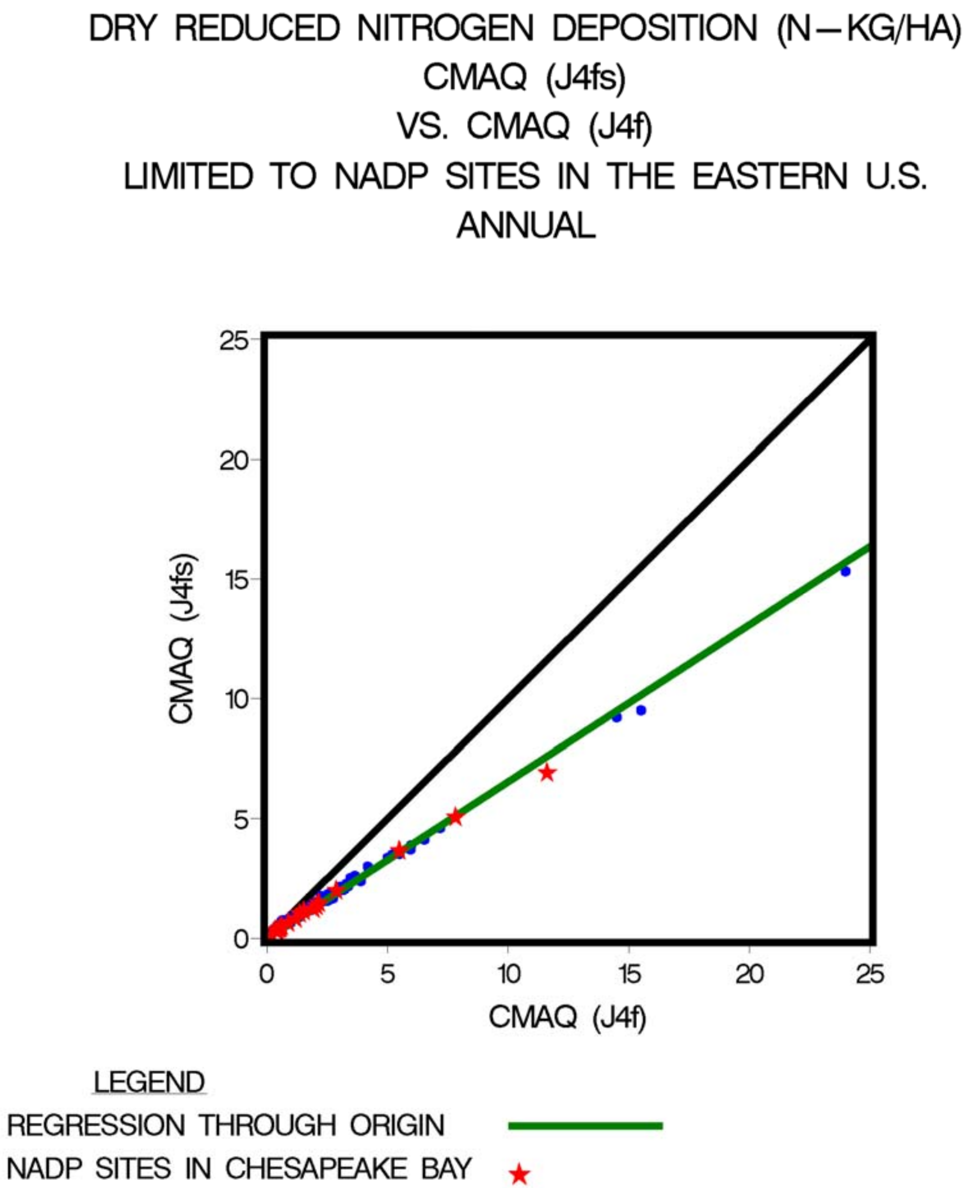
The pattern of maximum Vd is similar for SO_2 and NH_3.

- Recent North American flux measurements and greater understanding about the bi-directionality of ammonia air-surface exchange, suggests the NH_3 flux should be closer to SO_2 and could be even lower over some agricultural areas.

- What the ammonia flux should be is not well established and is an area of investigation. What we can do is make an educated guess as to a definable lower bound for our work as a sensitivity study to bring us closer to what we think is the truth. But truth still eludes us.

- We defined a sensitivity in which the current CMAQ NH_3 Vd was made equal to the SO_2 Vd. The spatial pattern remains close to what it was.
    - **Base = J4f**
    - **NH_3 Sensitivity = J4fs**

Dry deposition of Red-N did change significantly.



NITROGEN DEPOSITION TO THE CHESAPEAKE BAY (LAND + WATER)
CMAQ 36km - J4f and J4fs
NO BIAS ADJUSTMENTS
ANNUAL

MAIN	SPECIES	J4f (lbs)	J4fs (lbs)
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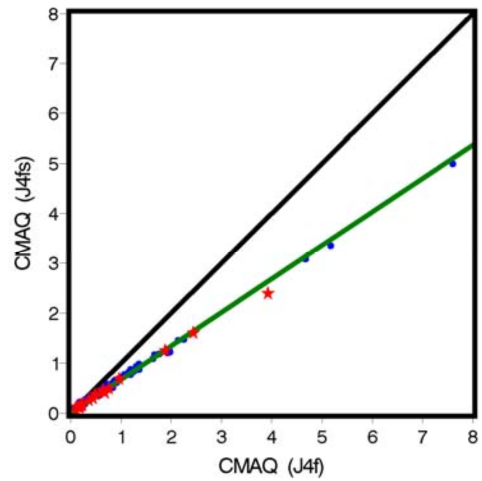
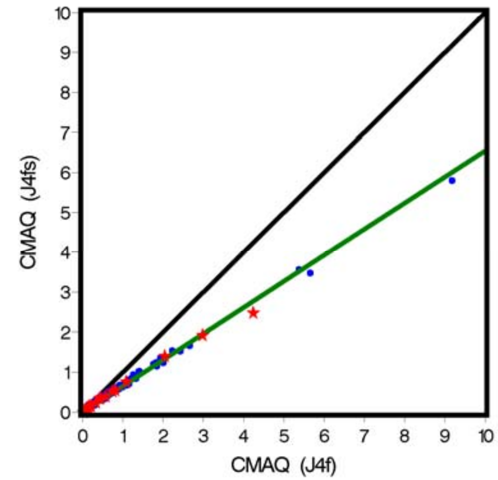
	DRYHNO3_N	121,266,418	115,857,579
	DRYNO3T_N	3,577,350	4,382,215
	-------------	------------	------------
1) DRYOX_N		190,565,657	186,050,956
2) WETOX_N		108,318,625	109,603,205
3) TOTALOX_N	TOTALOX_N	298,884,282	295,654,161
4) DRYRED_N	DRYNH3_N	76,448,294	47,658,106
	DRYNH4T_N	16,539,245	18,793,707
	-------------	------------	------------
4) DRYRED_N		92,987,539	66,451,812
5) WETRED_N	WETNH4T_N	101,750,572	113,825,595
6) TOTALRED_N	TOTALRED_N	194,738,111	180,277,407

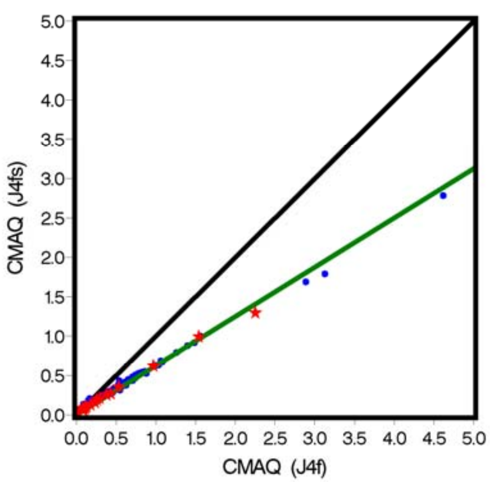
DRY REDUCED NITROGEN DEPOSITION (N-KG/HA)
CMAQ (J4fs)
VS. CMAQ (J4f)
LIMITED TO NADP SITES IN THE EASTERN U.S.
SPRING



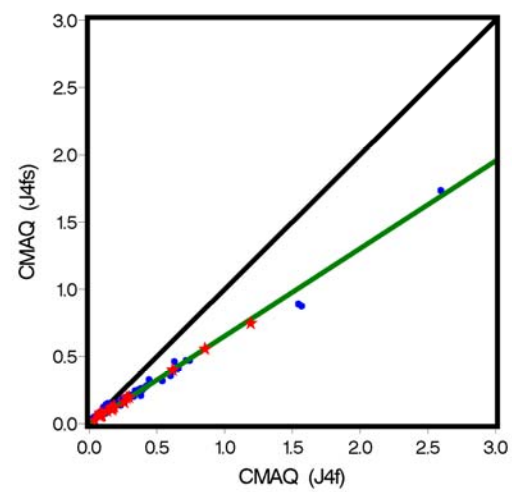
DRY REDUCED NITROGEN DEPOSITION (N-KG/HA)
CMAQ (J4fs)
VS. CMAQ (J4f)
LIMITED TO NADP SITES IN THE EASTERN U.S.
SUMMER



AUTUMN



WINTER



LEGEND
REGRESSION THROUGH ORIGIN
NADP SITES IN CHESAPEAKE BAY

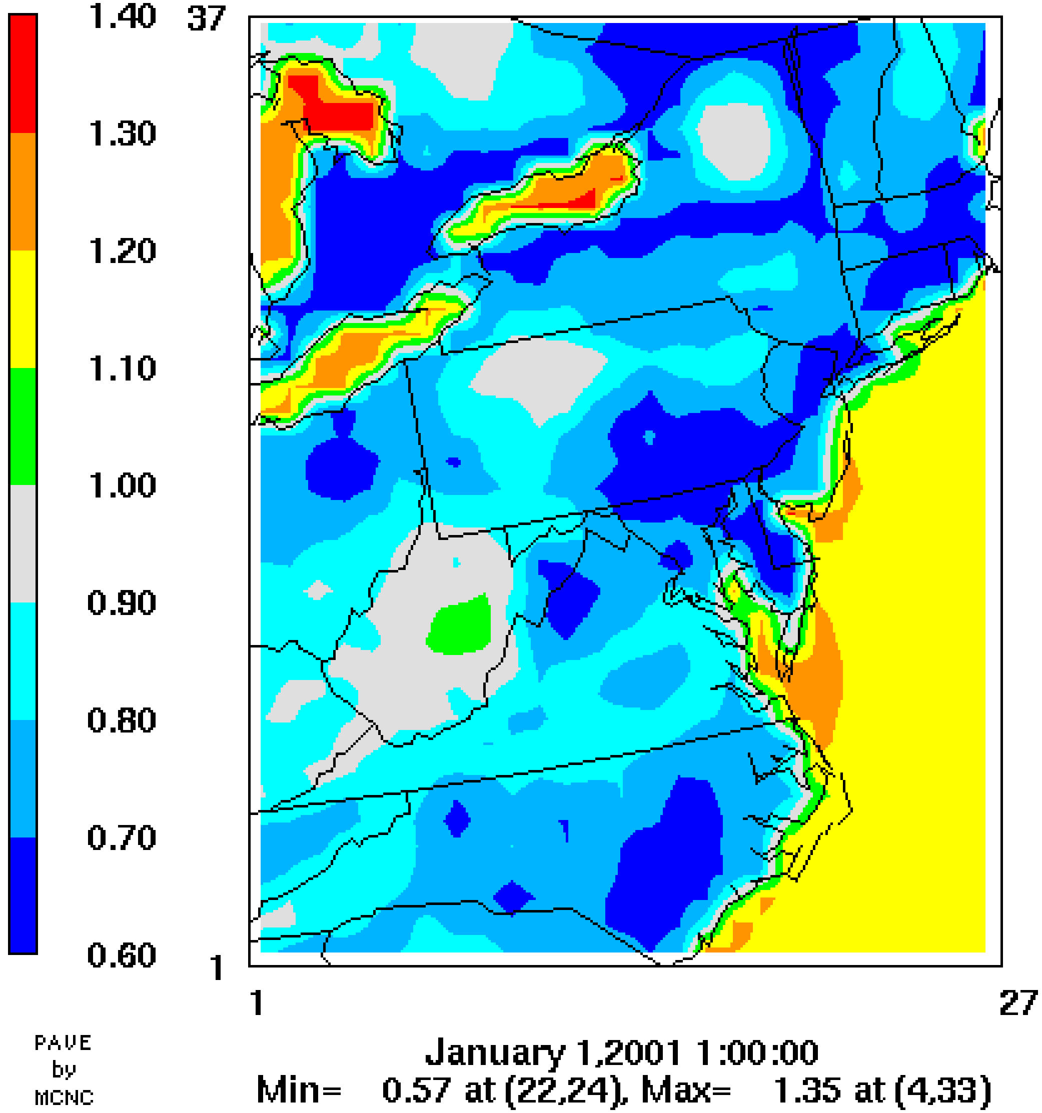
LEGEND
REGRESSION THROUGH ORIGIN
NADP SITES IN CHESAPEAKE BAY

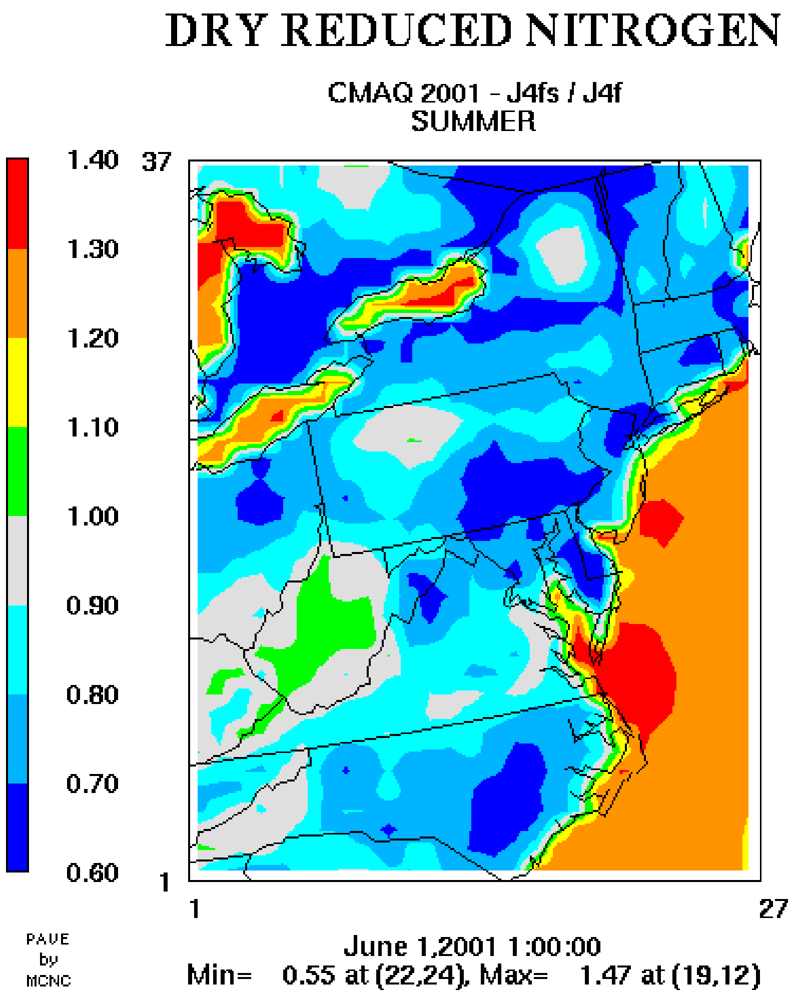
Change in Dry Deposition Associated with SO_2 Vd Sensitivity

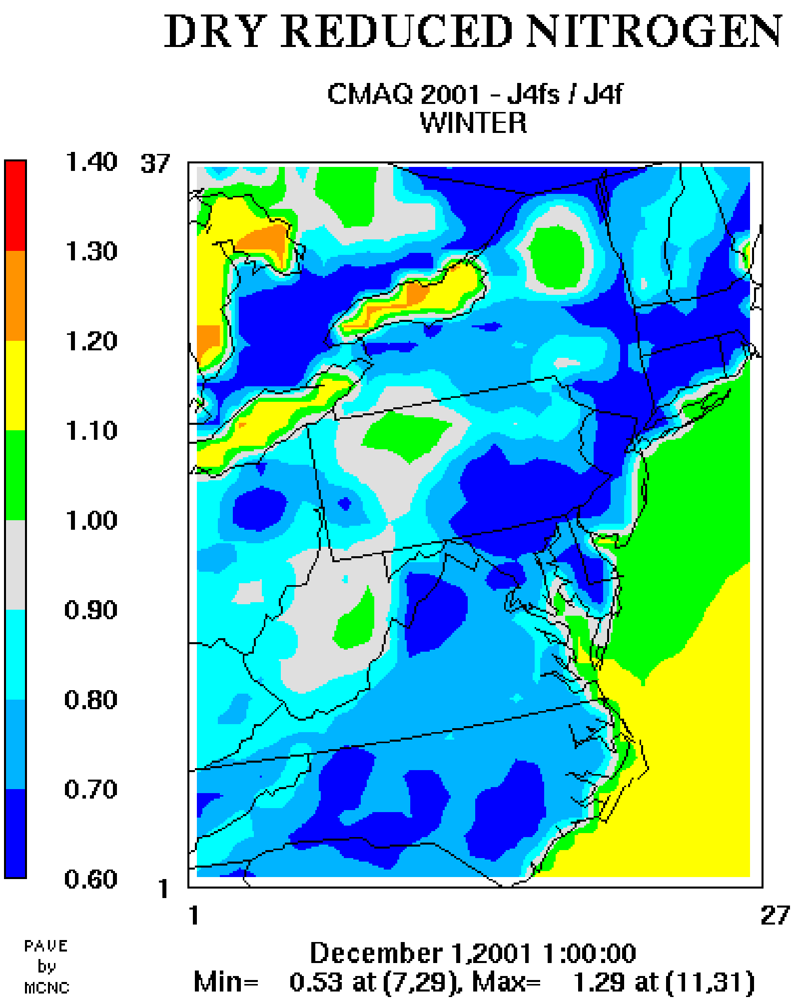
	Red-N Dry Deposition	Ox-N Dry Deposition
Annual	-28.5%	-2.4%
Spring	-27.1%	-3.6%
Summer	-27.8%	-0.7%
Autumn	-31.7%	-2.7%
Winter	-30.3%	-3.0%

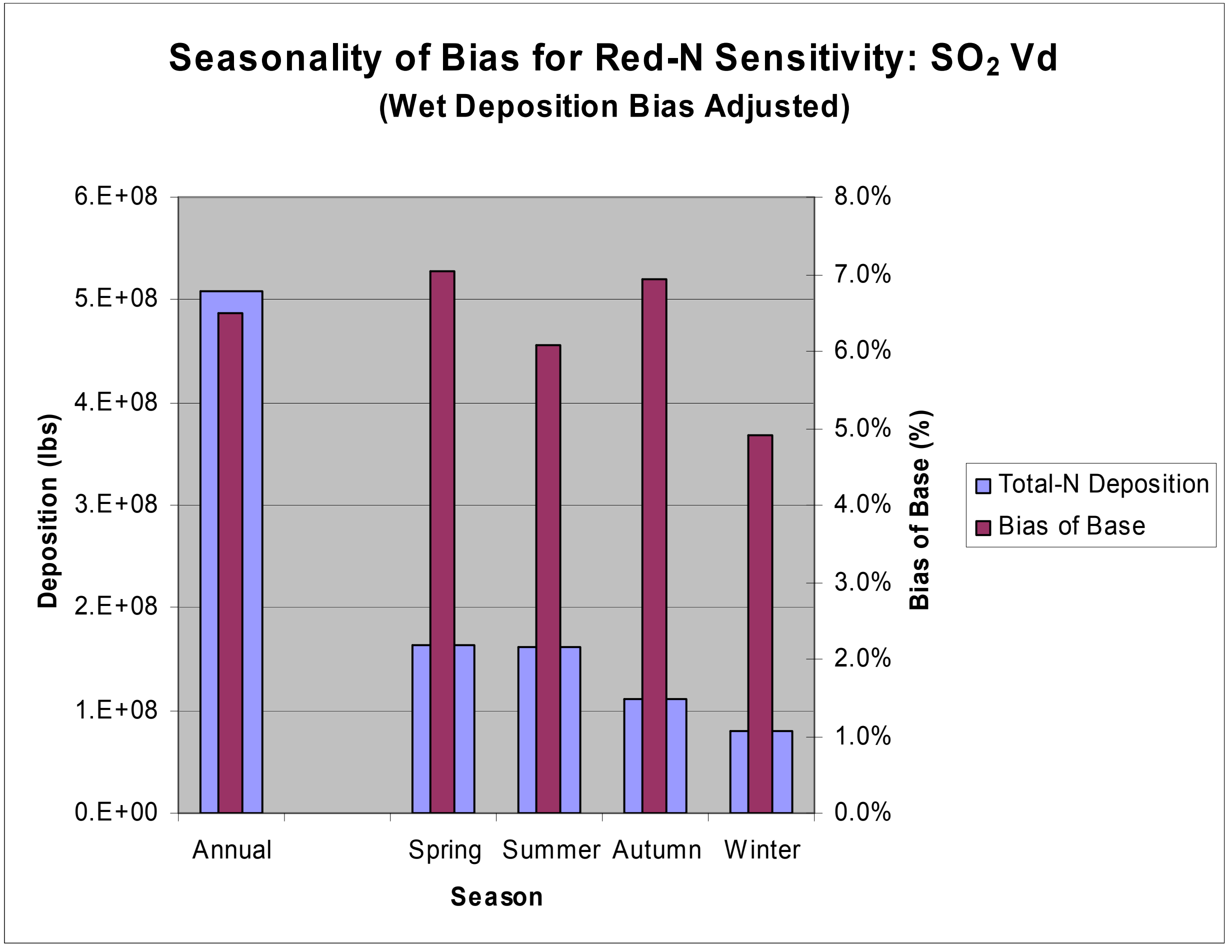
DRY REDUCED NITROGEN

CMAQ 2001 - J4fs / J4f
ANNUAL




DRY REDUCED NITROGEN
CMAQ 2001 - J4fs / J4f
SUMMER
1.40
1.30
1.20
1.10
1.00
0.90
0.80
0.70
0.60
37
1
1
27
PAVE
by
MCNC
June 1,2001 1:00:00
Min= 0.55 at (22,24), Max= 1.47 at (19,12)

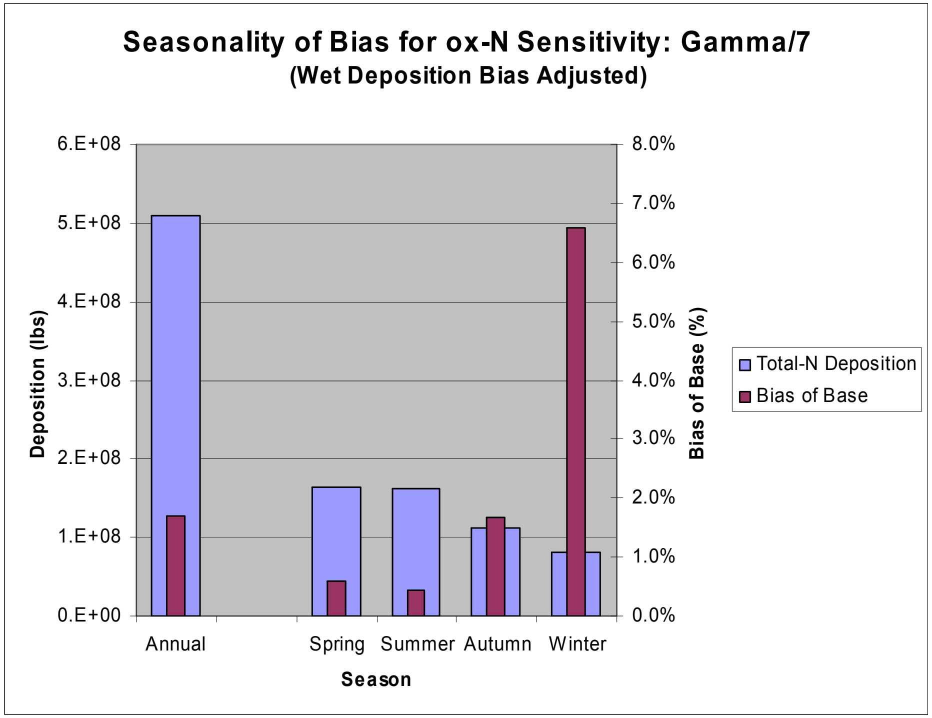

DRY REDUCED NITROGEN
CMAQ 2001 - J4fs / J4f
WINTER
1.40
1.30
1.20
1.10
1.00
0.90
0.80
0.70
0.60
37
1
1
27
PAVE
by
MCNC
December 1,2001 1:00:00
Min= 0.53 at (7,29), Max= 1.29 at (11,31)

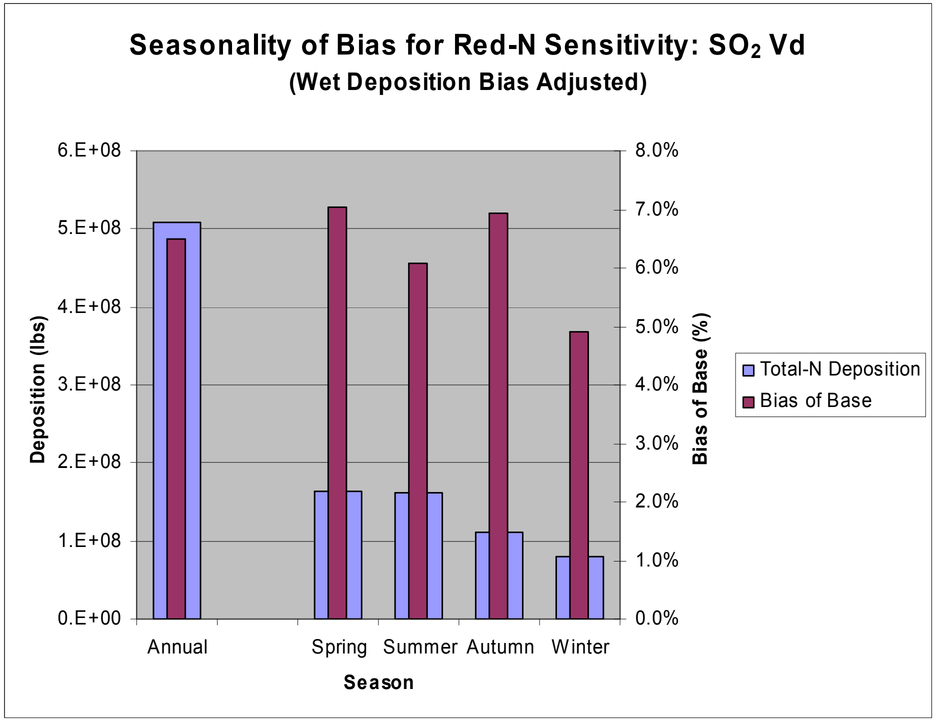


Seasonality of Bias for Red-N Sensitivity: SO2 Vd
(Wet Deposition Bias Adjusted)
6.E+08
5.E+08
4.E+08
3.E+08
2.E+08
1.E+08
0.E+00
Deposition (lbs)
8.0%
7.0%
6.0%
5.0%
4.0%
3.0%
2.0%
1.0%
0.0%
Bias of Base (%)
Annual
Spring
Summer
Autumn
Winter
Season
Total-N Deposition
Bias of Base

Uncertainty: Dry deposition flux of NH_3 (affects Red-N)

- The NH_3 deposition velocity uncertainty does create a modest uncertainty in red-N dry deposition, given our judgment of using the SO_2 deposition velocity as an indicator of the domain of truth.
- This uncertainty/bias is smaller than the estimated spatially-associated uncertainty in ammonia emissions/ deposition of roughly ±55% (±50% for deposition).
- We do not expect any upgrades to CMAQ in the next couple of years until we collect more field study data (starting this summer) and analyze it. This uncertainty or bias will stay with us for a while.





The two uncertainties will not combine linearly. The combined effect will be less. Thus the overall bias we are estimating here is roughly 7% of the total atmospheric N input into the Watershed model, with most of it coming from the ammonia Vd uncertainty, except in winter.

Establishing the Way Forward

- The potential biases are smaller than typical uncertainties. They appear tolerable. (Especially relative to total N dep.)
- We, in general, do not know where truth really is. We only have judgments about where it might be. Any bias adjustment would be a judgment call. The judgments do not have much literature support.
- CMAQ will be used for regulatory applications (most likely) without any bias adjustments. Consistency is desirable.
- The prudent approach seems to be to use the CMAQ results as is. We can perform sensitivity calculations later to see the effect on strategy delta changes.
- Recommendation: move forward with CMAQ scenarios with present system and outputs.

Planned CMAQ Scenarios

- 2010 CAIR+CAMR+BART
  - End of April
- 2020 CAIR+CAMR+BART (new growth projections to take into account)
  - End of May
- 2020 Allocation of State Responsibility
  - PA, VA, MD, WV, and NY
  - PA, VA, MD, WV, NY and DE as a single set
    - End of November
- 2020 Sector Responsibility
  - EGU, Mobile and Industry (other by subtraction)
    - End of January 2007

- - - - - may run into an issue of money by this point - - - - - -

- 2020 LOT (from OAQPS)
  - End of February 2007
- 2030 Long-Range Projection (from OAQPS)
  - End of March 2007