A Model Assessment of Atmospheric Nitrogen Deposition Response to EGU Pollution Controls for the Escambia Bay, Florida Watershed

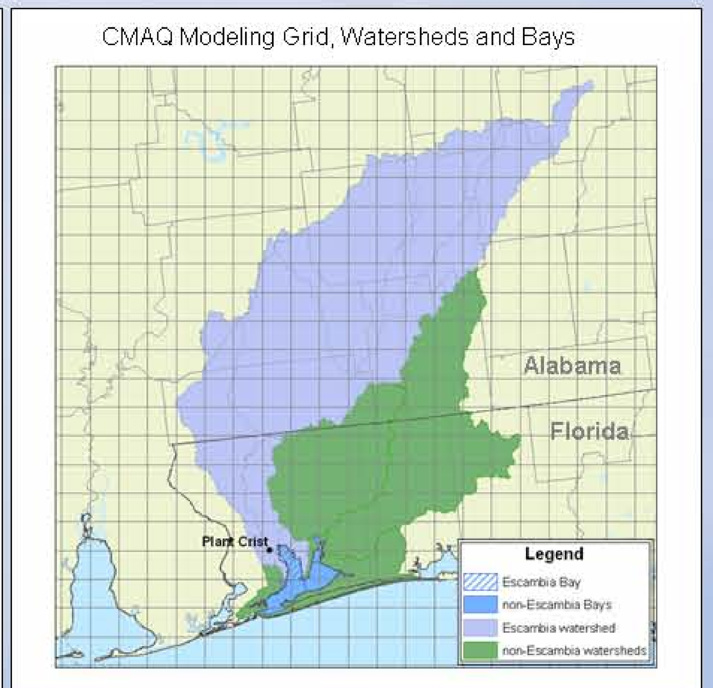
Justin Walters[1], Krish Vijayaraghavan[2], Jay L. Haney[3], Rochelle Balmori[2], Shu-Yun Chen[2], Sharon G. Douglas[3], Tom C. Myers[3], John J. Jansen[1], Eladio M. Knipping[4], and Christian Seigneur[2]

[1] Southern Company, Birmingham, AL
[2] Atmospheric & Environmental Research, Inc., San Ramon, CA
[3] ICF International, San Rafael, CA
[4] Electric Power Research Institute, Palo Alto, CA

1. Introduction

Atmospheric deposition is an important pathway for the input of nitrogen species to watersheds and water bodies. Atmospheric nitrogen deposition can cause acidification of soils and water bodies, as well as leaching of nitrogen to surface and ground waters, resulting in eutrophication and degradation in water quality.

Here we summarize findings from an air quality modeling study conducted to estimate the decrease in nitrogen deposition to Escambia Bay and watershed due to planned emissions controls of nitrogen oxides (NO_x) and sulfur dioxide (SO_2) at coal-fired Plant Crist. Three Eulerian chemical transport models and one puff model were applied as part of a larger study to estimate the net reduction in total nitrogen loading to Escambia Bay for the year 2002.



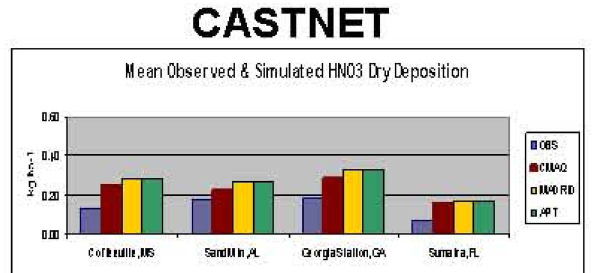
2. Air Quality Models

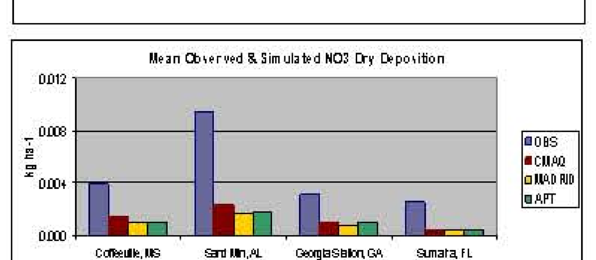
- **CMAQ-VISTAS**
  - CMAQ v. 4.5.1 with modifications to the secondary organic aerosol algorithm by VISTAS RPO
  - Carbon Bond IV (CB-IV) chemical mechanism
  - AERO4 aerosol module (with modal size distribution of aerosols)
    - Includes sea salt emissions, does not account for coarse sodium nitrate formation (sea-salt/HNO_3 interactions)
- **CMAQ-MADRID**
  - Model of Aerosol Dynamics, Reaction, Ionization, and Dissolution (MADRID)
  - Based on CMAQ 4.5.1 and also utilizes the CB-IV chemical mechanism
  - Uses a sectional representation of the particle size distribution instead modal size distribution
  - Includes heterogeneous formation of nitrate in the aqueous and particulate phase
  - Accounts for comprehensive sea-salt/HNO_3 chemistry
- **CMAQ-MADRID-APT**
  - Builds upon CMAQ-MADRID described above
  - Includes Advanced Plume Treatment (APT), a plume-in-grid algorithm based on SCICHEM
  - 40 point sources, including Plant Crist, were treated with APT
- **CALPUFF**
  - Grid-based puff model—uses the first-order chemical mechanism MESOPUFF II
  - Regulatory model to assess environmental impacts from one to several emission sources

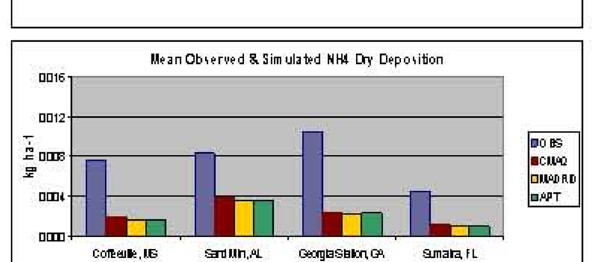
3. Model Performance Evaluation

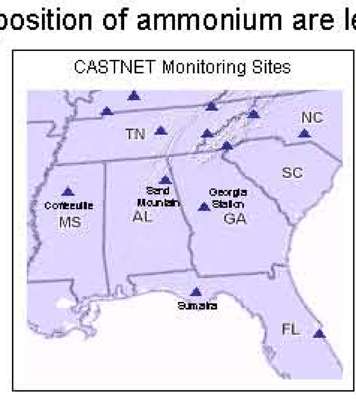
- Evaluation of the three Eulerian models showed similar overall performance
- The models consistently overestimate observed concentrations of HNO_3 in the region, with biases in the range of 40 to 120%.
- Nitrate air concentrations are consistently underestimated, but with MADRID and APT doing much better than CMAQ with lower biases and errors in the vicinity of Escambia Bay.
- The models consistently underestimate dry deposition of sulfate, nitrate, and ammonium, with biases in the range of -120 to -140% and errors in the range of 120 to 140%.
- The models generally underestimate wet deposition of sulfate, nitrate, and ammonium
- Precipitation is important! All three models overestimate the dry deposition of nitric acid and underestimate the wet deposition of nitrate, suggesting that precipitation input to these models may be underestimated or incorrectly distributed.
- The greatest contributors to nitrogen deposition are dry deposition of nitric acid followed by wet deposition of nitrate (in all forms).
- Dry deposition of nitrate and wet and dry deposition of ammonium are lesser contributors to nitrogen deposition.

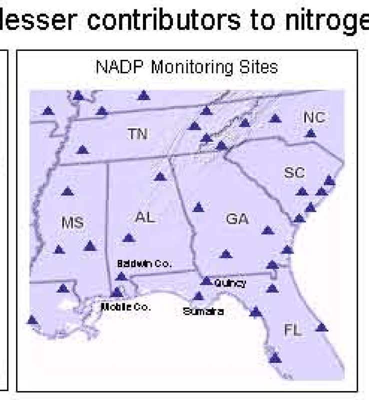
CASTNET



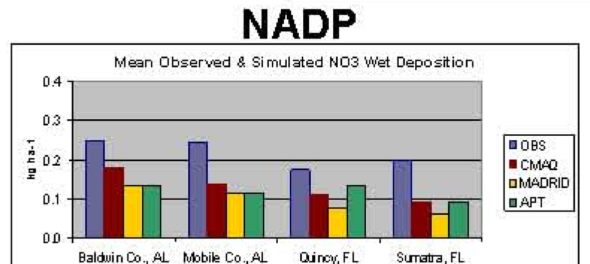


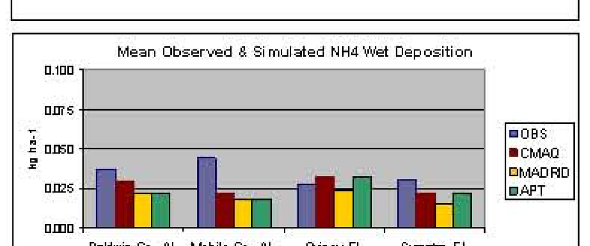


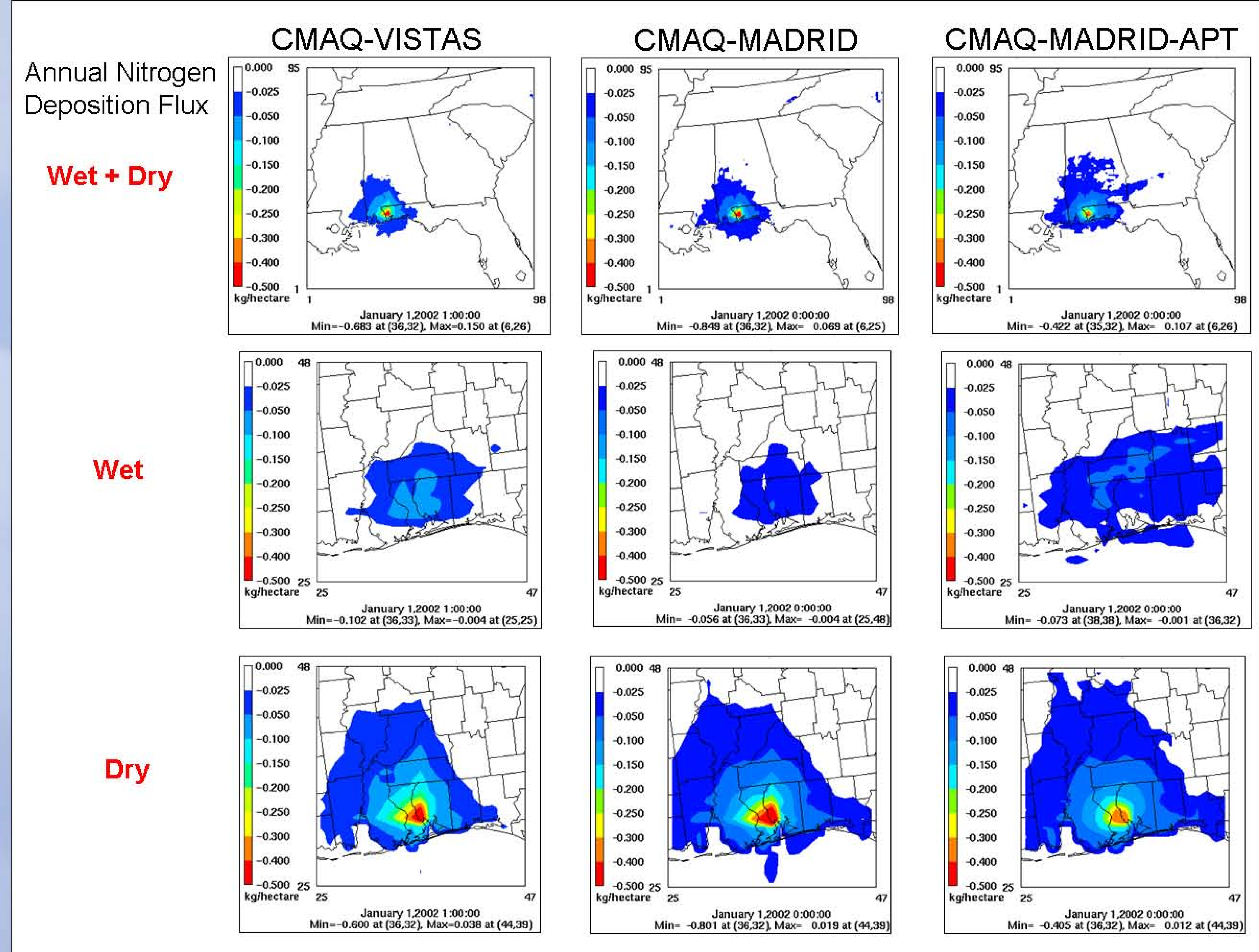


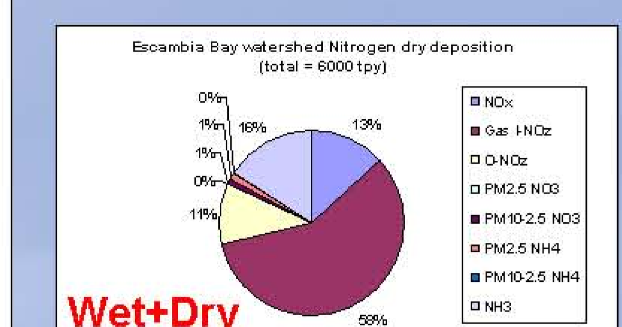


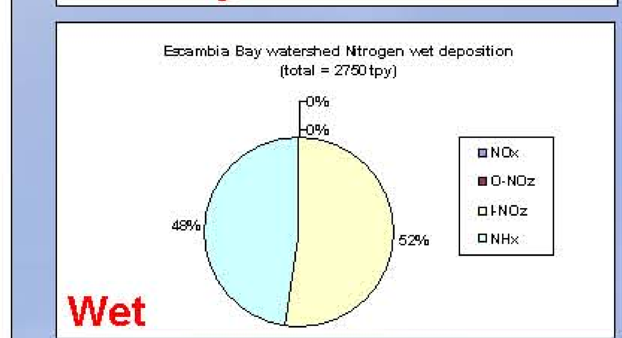
NADP

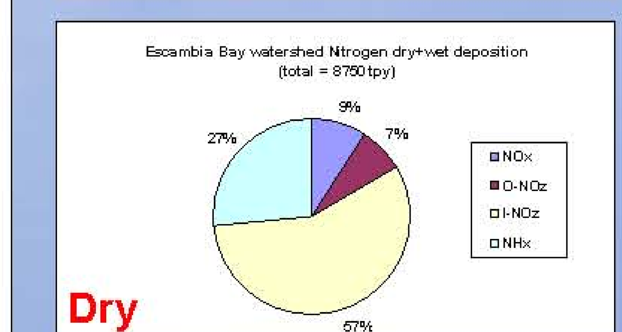












Nitrogen Wet Deposition to Escambia Bay Watershed

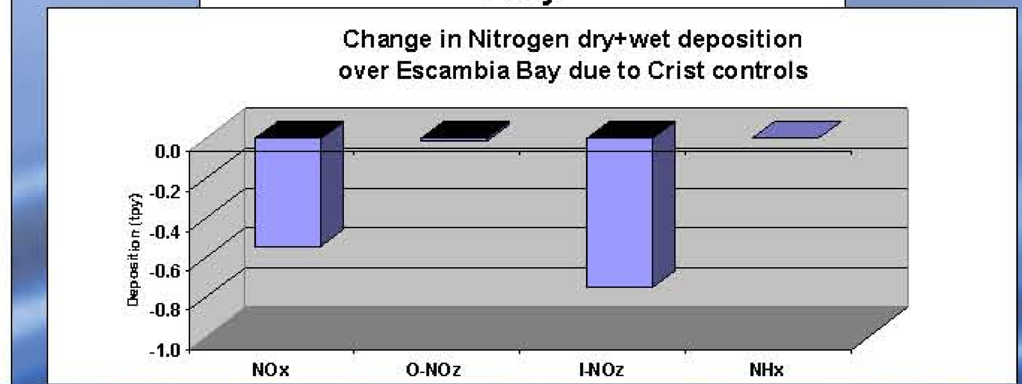
Species grouping	CMAQ base	MADRID base	APT base	CMAQ control	MADRID control	APT control	CMAQ control-base	MADRID control-base	APT control-base
NO_x	0.9	0.0	0.0	0.9	0.0	0.0	0.0	0.0	0.0
O - NO_z	1.1	0.4	0.4	1.0	0.4	0.4	0.0	0.0	0.0
I - NOz	1804.1	1367.7	1434.0	1773.3	1344.3	1400.8	-30.8	-23.4	-33.2
NH_x	1610.0	1287.6	1315.1	1606.2	1285.0	1309.6	-3.8	-2.6	-5.5
TOTAL	**3416**	**2656**	**2750**	**3381**	**2630**	**2711**	**-35**	**-26**	**-39**

Nitrogen Dry Deposition to Escambia Bay Watershed

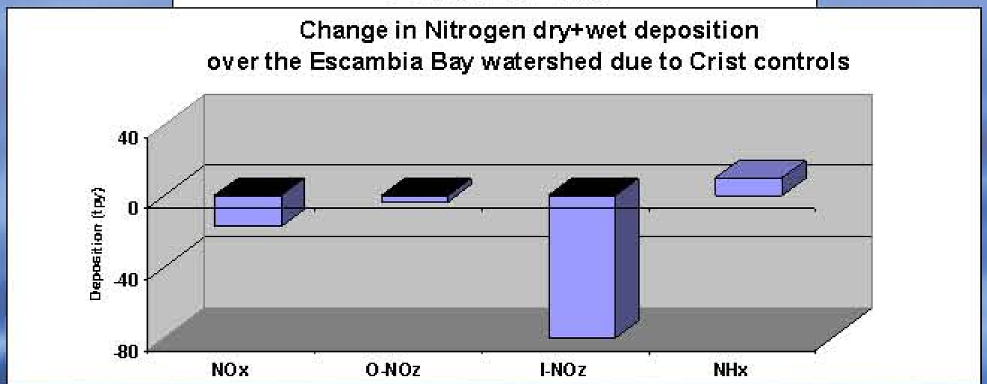
SPECIES GROUPING	CMAQ BASE	MADRID BASE	APT BASE	CMAQ CONTROL	MADRID CONTROL	APT CONTROL	CMAQ CONTROL-BASE	MADRID CONTROL-BASE	APT CONTROL-BASE
NO_x	694.6	797.4	793.0	674.4	770.7	775.6	-20.2	-26.6	-17.4
O - NO_z	612.5	651.3	653.0	610.0	649.2	649.6	-2.4	-2.2	-3.4
Gas I - NO_z **	3250.7	3490.5	3469.3	3195.5	3422.6	3406.4	-55.2	-67.9	-62.9
$PM_{2.5}$ NO_3	8.9	8.3	8.4	8.8	8.4	8.5	0.0	0.1	0.1
$PM_{10-2.5}$ NO_3	-	44.7	46.9	-	47.3	48.2	-	2.6	1.3
$PM_{2.5}$ NH_4	85.2	72.0	71.7	83.2	71.5	71.2	-1.9	-0.6	-0.4
$PM_{10-2.5}$ NH_4	-	14.6	15.3	-	14.7	15.3	-	0.1	0.0
NH_3	950.4	928.2	942.8	975.3	950.1	959.1	25.0	21.8	16.3
I - NO_z ***	3259.6	3543.4	3524.6	3204.4	3478.3	3463.1	-55.2	-65.1	-61.5
NH_x ***	1035.6	1014.9	1029.7	1058.6	1036.2	1045.6	23.0	21.3	15.9
TOTAL	**5602**	**6007**	**6000**	**5547**	**5934**	**5934**	**-55**	**-73**	**-66**

NO_x = NO + NO_2
Organic NO_z (O-NO_z) = PAN + NTR
Gas Inorganic NO_z (Gas I-NO_z) = NO_3 + N_2O_5 + HNO_3 + HONO + PNA
Gas NH_x = NH_3
PM NH_x = NH_4_1 + NH_4_2
PM I-NO_z = NO_3_1 + NO_3_2
I-NO_z = Gas I-NO_z + PM I-NO_z
Gas NO_y = NO_x + Gas I-NO_z + O-NO_z
PM NO_y = PM I-NO_z
NO_y = Gas NO_y + PM NO_y
NH_x = Gas NH_x + PM NH_x

Bay



Watershed



4. CMAQ, MADRID and APT Results Discussion

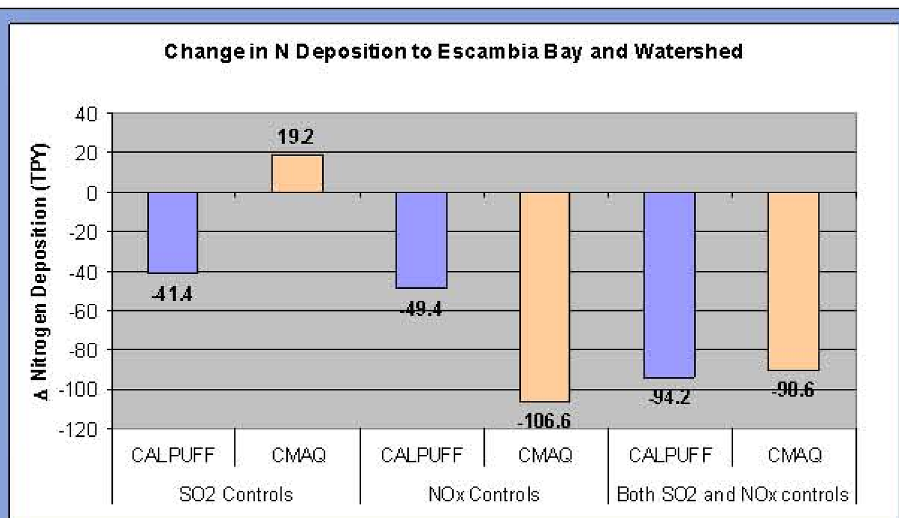
- Due to its high water solubility, HNO_3 is rapidly deposited on surfaces and absorbed into water droplets. Hence, it has very high dry and wet deposition rates.
- The coarse PM nitrate and ammonium species have significantly higher dry deposition rates than the corresponding $PM_{2.5}$ species.
- Most of the reductions in deposition are due to decreases in dry deposition, especially near Plant Crist.
- Purely grid-based models, such as CMAQ and MADRID, tend to overestimate the vertical dispersion and hence dry deposition of HNO_3 in the vicinity of the source.
- NO_x emission controls on Plant Crist result in reductions in atmospheric nitrogen deposition in the Escambia Bay watershed area while SO_2 emission controls cause an increase in nitrogen deposition due to an ammonia dis-benefit.

5. CALPUFF Modeling

Right answer for the wrong reason!

The bar graph below presents a comparison between CALPUFF and CMAQ-VISTAS, showing changes in nitrogen deposition resulting from three different scenarios at Plant Crist: 1) SO_2 controls only, 2) NO_x controls only and 3) both SO_2 and NO_x controls.

- Changes in total nitrogen deposition are similar for the "Both SO2 and NOx Controls" scenario for both models.
- For SO_2 controls alone, CALPUFF shows a **decrease** in total nitrogen deposition, while CMAQ shows an **increase**
- For NO_x controls alone, CMAQ shows a much greater decrease in total nitrogen deposition than CALPUFF
- CALPUFF does not simulate ammonia species explicitly—hence, it does not correctly account for the effect of SO_2 controls on nitrogen deposition.
- CMAQ uses more robust chemical processes and wet deposition algorithms than CALPUFF



6. Summary

- All models exhibit significant biases in dry and wet deposition
- HNO_3 has the largest contribution (~60%) to nitrogen dry deposition in all three Eulerian models
- Inorganic NO_z (gaseous + particulate) is the largest contributor (~52%) to wet deposition
- Over Escambia Bay and its watershed, CMAQ, MADRID and APT predict annual nitrogen deposition reductions of 91 tons, 100 tons and 106 tons, respectively, and show maximum gridded reductions in deposition fluxes of 0.68, 0.85 and 0.42 kg/ha/yr, respectively
- Differences in results between the models are attributable to differences in model formulation and configuration
- The Eulerian models show spatial differences in deposition (both magnitude and species) that may be significant for complex watershed modeling
- It is important to use a plume-in-grid treatment for emissions from large elevated point sources so that sulfur and nitrogen deposition can be correctly simulated
- The screening model CALPUFF does not provide robust results and is not a good tool for assessing nitrogen deposition
- The air quality model deposition results presented here were subsequently used in a watershed modeling study to estimate the net nitrogen loading to Escambia Bay after retention/transport in the watershed