

3D Air Quality and the Clean Air Interstate Rule: Lagrangian Sampling of CMAQ Model Results to Aid Regional Pollution Accountability Metrics.

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#### Advanced Monitoring Initiative: 3D Air Quality and the Clean Air Interstate Rule (AMI-CAIR)

#### Background: The Clean Air Interstate Rule (CAIR)

is expected to reduce transport of air pollutants (e.g. fine sulfate particles) in non-attainment areas in Eastern. U.S. SIPs for particulate matter (PM) are due from MDE in April 08. CAIR highlights the need for an integrated air quality observational and modeling system to understand sulfate as it moves in multiple dimensions, both spatially and temporally. We need "air transport-related" accountability metrics.



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AMI-CAIR project goals: Demonstrate how air quality model results can be combined with a 3-d monitoring network to provide decision makers with a tool to help quantify the impact of CAIR reductions in SO2 emissions on regional transport contributions to sulfate concentrations at surface monitors in the Baltimore area, and help improve decision making for strategic implementation

plans (SIPs)

#### Partners:





Mid-Atlantic Regional



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#### Approach:

•Sample CMAQ model results using ensemble back trajectories computed with the LaRC trajectory model; provide Lagrangian time series and vertical profile information; compare with NASA satellite (MODIS), EPA surface, and lidar measurements.

•Use trajectory-sampled mean sulfate and SO2 to assess the regional transport contribution to surface SO4 measurements in the Baltimore MSA.

•Characterize dominant source regions for low, medium, and high SO4 episodes.



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quality model results can be combined with a 3-d

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monitoring network to provide decision makers

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**Benefit to partner(s):** EPA gain a tool that can be used to monitor impact of CAIR reductions in SO2 nationwide. MDE gain quantitative information to guide PM SIP (due 04/2008).

•Benefit to NASA Earth science: Improved understanding of regional air pollution transport.

•Benefit to NASA Applied science: Build collaboration with state and federal government agencies;

#### **Milestones**

•Complete demonstration capability for 2004 summer, and pass to EPA (09/07).

•Incorporate and handoff tool to EPA's RSIG for national applications and CAIR monitoring (09/07)



## Trajectory calculations for AMI CAIR





## Lagrangian back trajectory simulations:

- Air parcel clusters are initialized at various altitudes over Baltimore (20, 60, 100, 500, 1000m)
- Trajectories are computed using the 3-d Met./ Chem. Interface Processor (MCIP) wind fields (MM5) used to drive CMAQ.
- 3-day back trajectories are computed (5-minute, 4th order Runge Kutta time stepping)
- Daily back trajectory simulations sample chemical and aerosol fields from a 3-month CMAQ simulation for June-August 2004.
- MCIP and CMAQ data are provided on a 12 km regional-scale grid with 14 vertical levels at 1-hour intervals
- Trajectory output provided every hour



# 3-day ensemble back trajectories initialized at 20,100,500,1000m at 00Z, 20040825



PM2.5 reached almost 60 ug/m<sup>3</sup> at Baltimore on August 24th

Lagrangian timeseries: sampling CMAQ along backtrajectories 500m CMAQ\_backtraject 2004082500 39.3 N, 283. E



Significant vertical divergence of ensemble altitudes after 60hrs.



X-axes show back trajectory time: -72 hrs .....0 hrs





Parcels descending into daytime boundary Layer during previous 60hrs Significant vertical divergence of ensemble altitudes after 60hrs.

X-axes show back trajectory time: -72 hrs .....0 hrs





### Lagrangian curtains constructed following mean parcel location

CMAQ 500m Lagrangian (Baltimore) 202004082500



Solid line shows mean parcel altitude; vertical lines show range from Baltimore, 80km intervals



3-day back trajectories, 20040825 35 20m 100m 500m 1000m PM2.525 Bext Bext Î Î 3 Attitu -20-20-80-40-40 Time (hours) Time (hours) 25.0 ug/m3 2.5010.0 17,5 32.5 0.20 0.26 0.02

Lagrangian curtains show the vertical profiles of PM2.5 and aerosol extinction following the mean parcel location.

km='

#### **Advanced Monitoring Initiative: 3D Air Quality and the Clean Air Interstate Rule** (AMI-CAIR)



Optical depths from CMAQ may now be compared with MODIS and LIDAR observations. Mean air parcel location links observed and simulated AOD.

Mean parcel positions



following the mean parcel location.

# Air Quality Applications Quality and the Clean Air Interstate Rule (AMI-CAIR) 3-day back trajectories, 20040825 (AMI-CAIR)

**Advanced Monitoring Initiative: 3D Air** 



Engel-Cox et al. (2006)



Trajectory cluster classification: How best to characterize regional vs. local contributions?

• Define a "local domain," 80 km circle centered on Baltimore, and a "regional domain," outside of 80 km. We characterize the "regional" contribution to SO4 at Baltimore in terms of the mean rate of change of SO4 in the regional domain. i.e.  $\varphi$  = mean d(SO4)/dt in the regional domain. For air parcels initialized at 500m altitude at Baltimore

•Define classes: (1):  $\phi > 0.12$  ug m<sup>-3</sup> hr<sup>-1</sup> (strong regional influence)





### Class 1: regional d(ASO4)/dt > 0.12 ug m<sup>-3</sup> hr<sup>-1</sup> (strong regional impact)

Frequency of cases, and background concentrations for class 1 cases.



Figure shows the trajectory paths for strong regional influence, and the mean concentrations from CMAQ along the trajectory paths



Lagrangian sampling of CMAQ: Time series of classifications (colors), SO4 at BMA, and SO4 at regional boundary

GREEN: strong regional SO4 increase; Blue: regional SO4 decrease



Dashed: CMAQ SO4 at regional boundary

For elevated SO4 events at BMA, the dashed line approaching the solid line indicates a strong regional contribution; when the dashed line is well below the solid line, we interpret local (within 80km) sources to be most important



- We're demonstrating a prototype tool here. Observations help us assess the fidelity of the. The 2004 simulation has limitations, e.g. ambient boundary conditions, no separation of SO4 production/ loss estimates.
- The kind of statement we're aiming for here is "our results show that d(SO4)/dt > 3 ug m<sup>-3</sup> day<sup>-1</sup>, with SO4 in the range 3 - 9 ug m<sup>-3</sup>, is associated with the principal regional transport routes, for SO4 reaching Baltimore daytime BL."
- Trajectory/ CMAQ sampling products are being used and evaluated vs. satellite and surface data by Batelle (Weber, Engel-Cox), as part of their analysis.
- We continue to explore different clustering criteria that may provide a cleaner separation of regional and local influences, and tailor products to best suit EPA and MDE metrics.



Deliverables: AMI-CAIR project:

- 9/06: Configure NASA LaRC trajectory model for MCIP meteorology and CMAQ model output (completed)
- 12/06: Transfer 2004 CMAQ and MCIP data from EPA RTP to NASA (completed)
- 03/07: Complete Lagrangian sampling of CMAQ aerosol predictions; handoff trajectory calculations to EPA, Battelle colleagues (completed).
- 09/07 Transition code to RSIG at RTP (code transferred).
- 09/07: Complete NASA Benchmark report, transfer results to EPA colleagues.



End





Top panels are for initial, final and regional boundary concentrations

Bottom panels: Orange: local domain average Blue: regional domain average

delimiter: d(SO4)/dt = 0.12 in regional domain



Class 3: regional d(ASO4)/dt < 0.0 ug m<sup>-3</sup> hr<sup>-1</sup> (negative)

Frequency of cases, and background concentrations for class 3 cases.



Figure shows the trajectory paths for this class, and the mean concentrations from CMAQ along the trajectory paths



Engal Coviet al (Atmos Env. 2006)

500m CMAQ\_backtraject 2004082500 39.3 N, 283. E



500m CMAQ\_backtraject 2004082500 39.3 N, 283. E







August 24th 2004

## Trajectory cluster classification (20m parcels):



delimiter: d(SO4)/dt = 0.08 in regional domain



Class 1: regional d(ASO4)/dt > 0.06 ug m<sup>-3</sup> hr<sup>-1</sup> (strong regional impact)

Frequency of cases, and background concentrations for class 1 cases.



Figure shows the trajectory paths for this class, and the mean concentrations from CMAQ along the trajectory paths



Class 3: regional d(ASO4)/dt < 0.0 ug m<sup>-3</sup> hr<sup>-1</sup> (negative)

Frequency of cases, and background concentrations for class 3 cases.



Figure shows the trajectory paths for this class, and the mean concentrations from CMAQ along the trajectory paths