Application of a Lagrangian stochastic dispersion model to forward and inverse air quality modeling

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Lagrangian stochastic dispersion modeling within complex modeling systems

1. Forward modeling

A hybrid model for ozone forecasting

- Meteorological model MM5 (Grell et al. 1994, NCAR)
- Lagrangian stochastic dispersion model (Koracin et al. 2007, Atm. Envir.)
- Eulerian chemical model with RACM (Stockwell et al. 1997, JGR)

* Supported by the DOD-SERDP (Strategic Environmental Research and Development Program)

Lagrangian stochastic dispersion modeling within complex modeling systems

2. Inverse modeling

Evaluation of receptor modeling & assessment of regional emission sources (eastern U.S.)

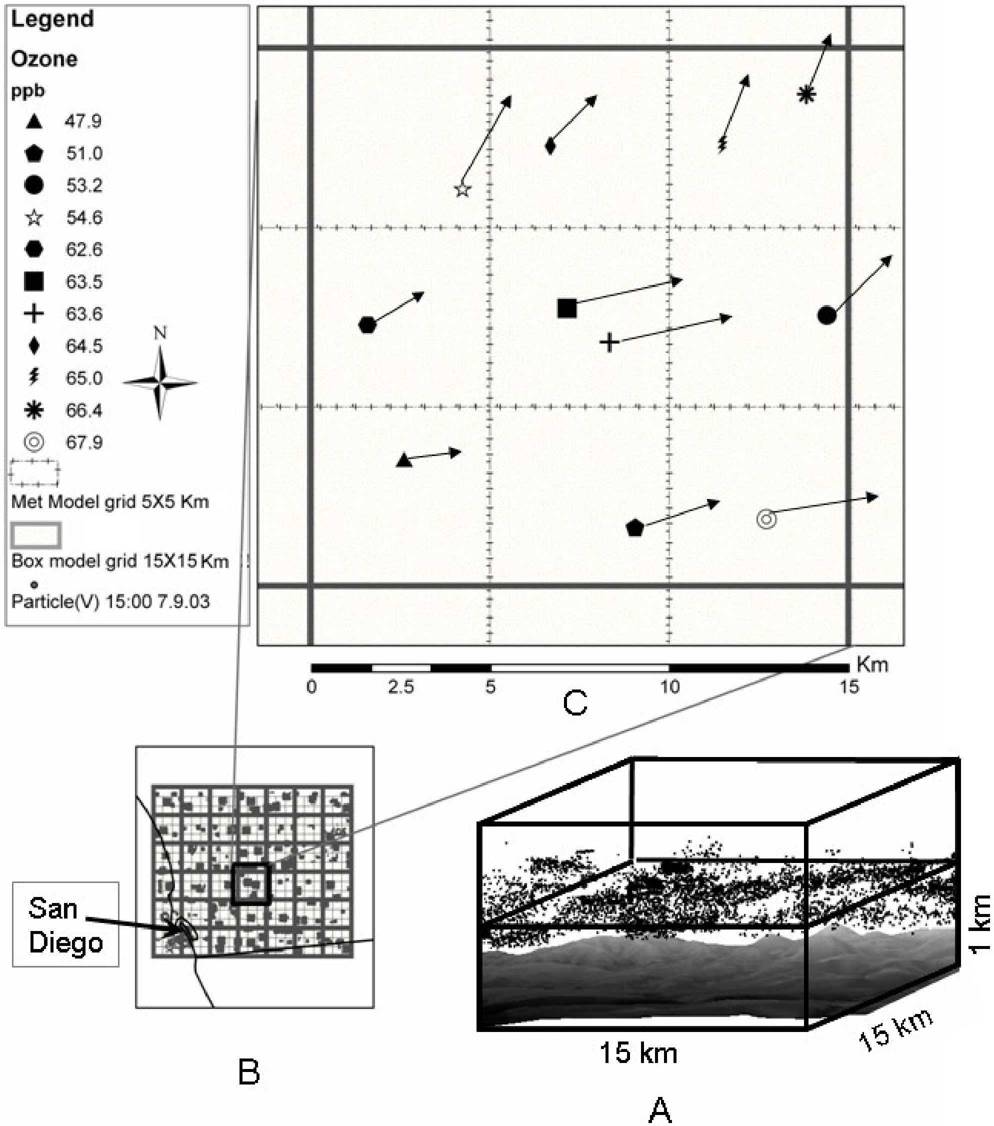
- EPA generated Meteorological model MM5 (Grell et al. 1994, NCAR) fields
- CMAQ baseline simulations (synthetic data set)
- HYSPLIT and EDAS trajectory computations
- Lagrangian stochastic dispersion model (Koracin et al. 2007, Atm. Environ.)

* Supported by the EPA-STAR Program

1. Forward modeling

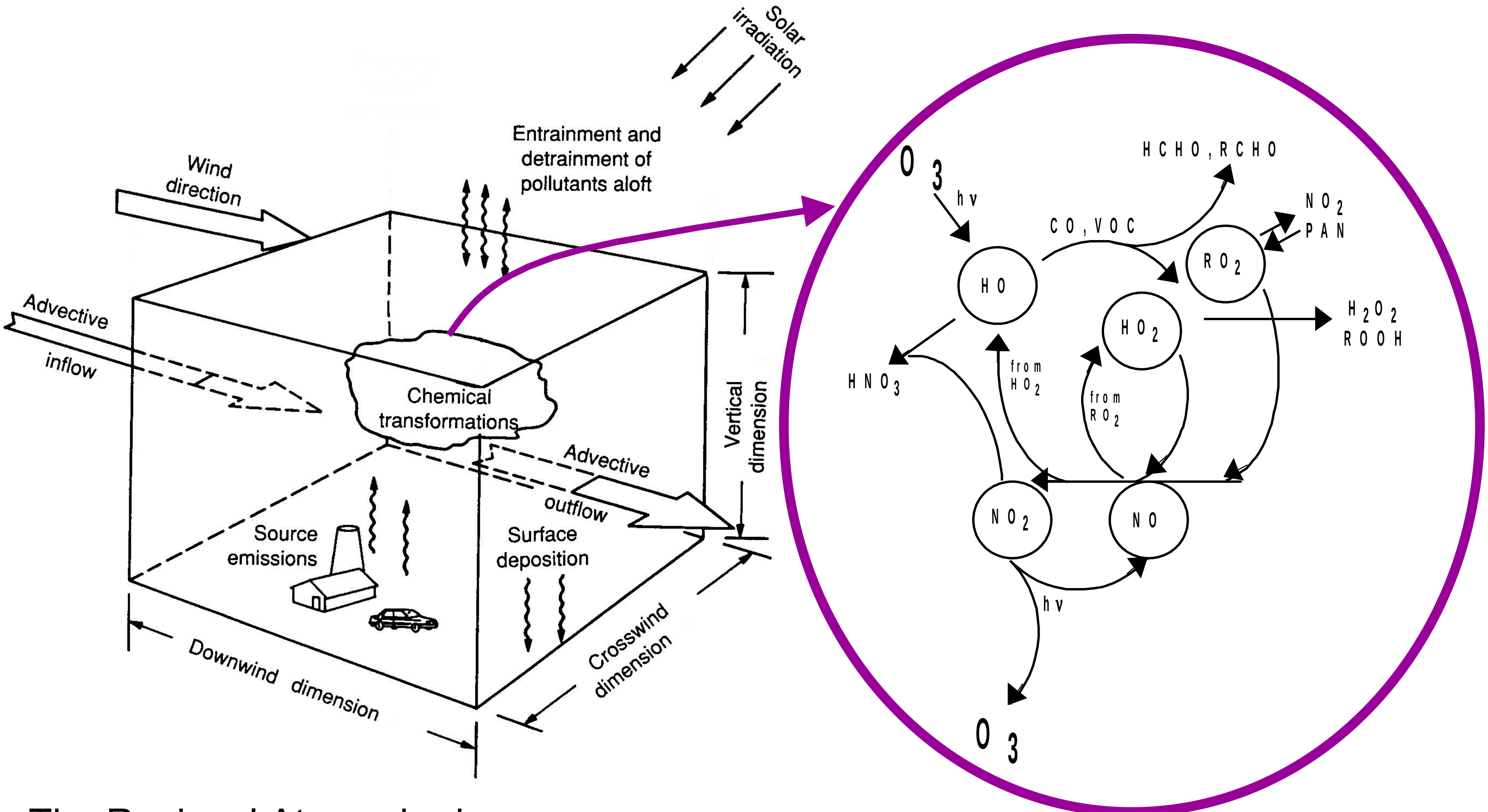
A hybrid model for ozone forecasting

- MM5: Regional meteorological fields (wind, pressure, temperature), grid cell 5X5 km
- Emissions (stationary, mobile)
- Lagrangian stochastic model – transport and dispersion
- Eulerian box chemistry model - RACM chemistry mechanism
- Hybrid model – Linkage of all these components: Simulates physical and chemical processes in the troposphere



Model domains
Grid resolution
- MM5: 5x5 km2
- Box chemistry model: 15x15 km2
Each particle is apportioned by the emissions and carries “chemical dimensions”

SBOX (Eulerian chemical model)



The Regional Atmospheric Chemistry Mechanism, RACM, [Stockwell et al., 1997] was used.

Chemistry - Box model

- The Regional Atmospheric Chemistry Mechanism, RACM, [Stockwell et al., 1997] was used. The RACM mechanism is a revised version of the RADM2 mechanism [Stockwell et al., 1990]
- A total of 17 stable inorganic species and 4 inorganic intermediates. Organic species are aggregated into 32 stable organic species and 24 organic intermediates.
- There are a total of 237 reactions in the RACM mechanism.
- Photolysis rate coefficients for the 23 photochemical reactions according to Madronich [1987] with an actinic flux computed by a radiative transfer model that is based on the delta-Eddington technique [Joseph and Wiscombe, 1976].

Each Lagrangian particle has multi-dimensional identifiers (spatial, ambient meteorology, chemical components, ID number, time)

$\text{Particle}_k(x,y,z,T,RH,p,chm_i \ldots chm_j,ID,t)$

For each time step Δt, there are k particles in a grid cell

Each particle (m^{th}) is disaggregated into n chemical species

$P_{m,n}$ – mass of particle m of chemical species n

$P_{T(n)}$ – the total mass of chemical n from all particles in the grid cell is converted into concentration for this species

Chemical computation is then performed for each species and each grid cell

The predicted concentrations are converted back into the new total mass

$$P_{Tot(n)} \downarrow_{t+\Delta t}$$

The mass is then apportioned back to each particle by a weighted average:

$$P_{(m,n)} \downarrow_{t+\Delta t} = \frac{P_{(m,n)} \downarrow_{t}}{P_{Tot(n)} \downarrow_{t}} P_{Tot(n)} \downarrow_{t+\Delta t}$$

Each Lagrangian particle has multi-dimensional identifiers (spatial, ambient meteorology, chemical components, ID number, time)

$\text{Particle}_k(x,y,z,T,RH,p,chm_i....chm_j,ID,t)$

<u>Correction of the new computed mass</u> $P_{Tot(n)}(t+\Delta t)$:

Distribution of newly formed species is based on a factor <u>*f* - intermixing efficiency</u> as a function of diffusion, time scale, mixing height, and turbulence intensity (Song et al. 2003)

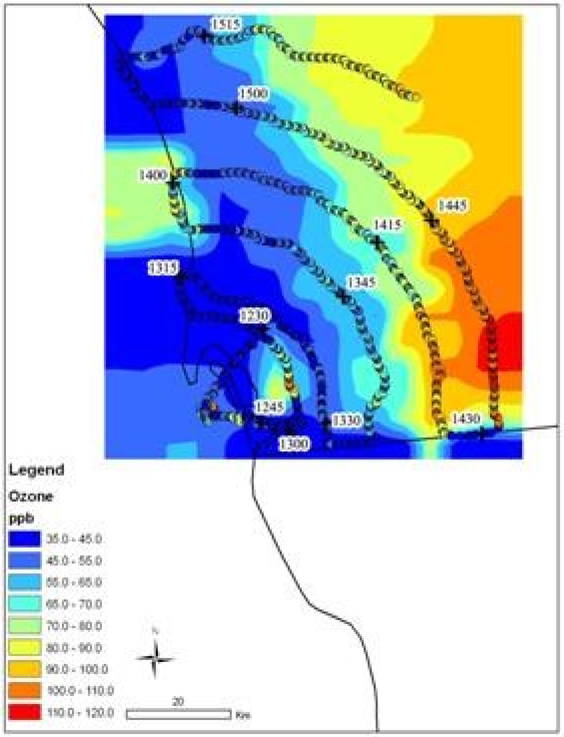
In that case, the apportionment is updated by:

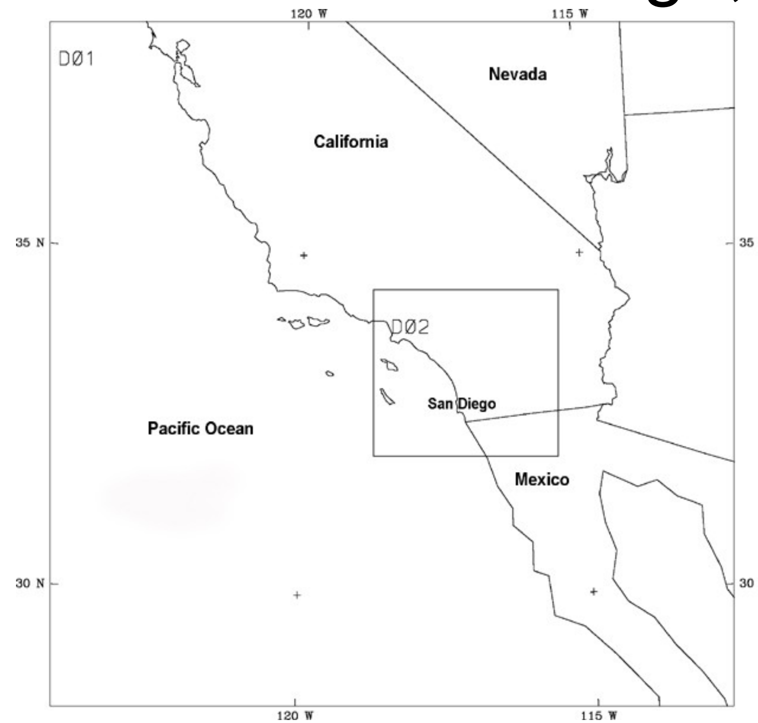
$$P_{(m,n)}\downarrow_{t+\Delta t} = \frac{P_{(m,n)}\downarrow_{t}}{P_{Tot(n)}\downarrow_{t}}\left[P_{Tot(n)}\downarrow_{t+\Delta t} - B_{(n)}f\right]$$

Where $B_{(n)}$ is the production result between time steps t and $t+\Delta t$ for the particles that had the new chemical species

Aircraft measurements

Comparison: Hybrid & CAMx models vs. aircraft data – San Diego, CA



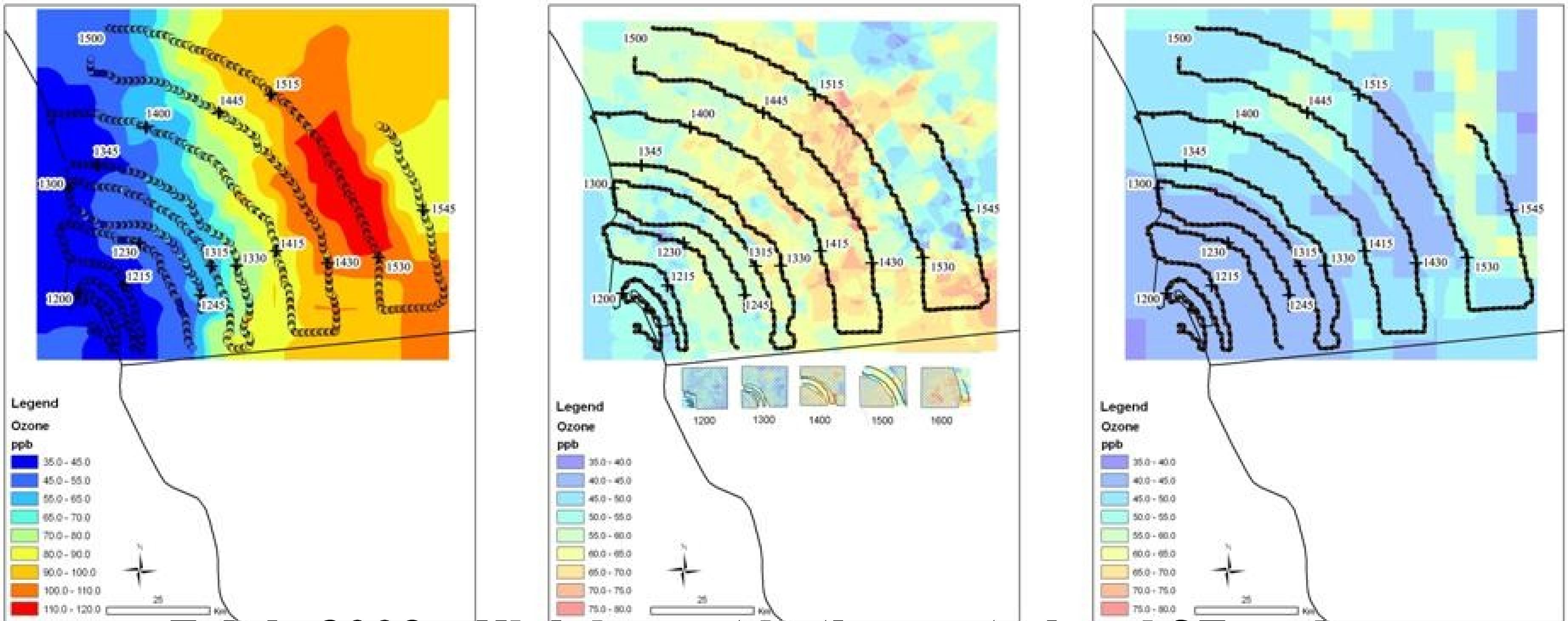


Dots represent aircraft measurements of ozone (ppbv) with spatial interpolation using Kriging.

Mapped hourly predictions of ozone by the Hybrid and CAMx models were cut in hourly sections corresponding to the aircraft flight time and locations.

A mosaic from the hourly sections was assembled to match the aircraft flight information

a. Aircraft b. Hybrid model c. CAMx model



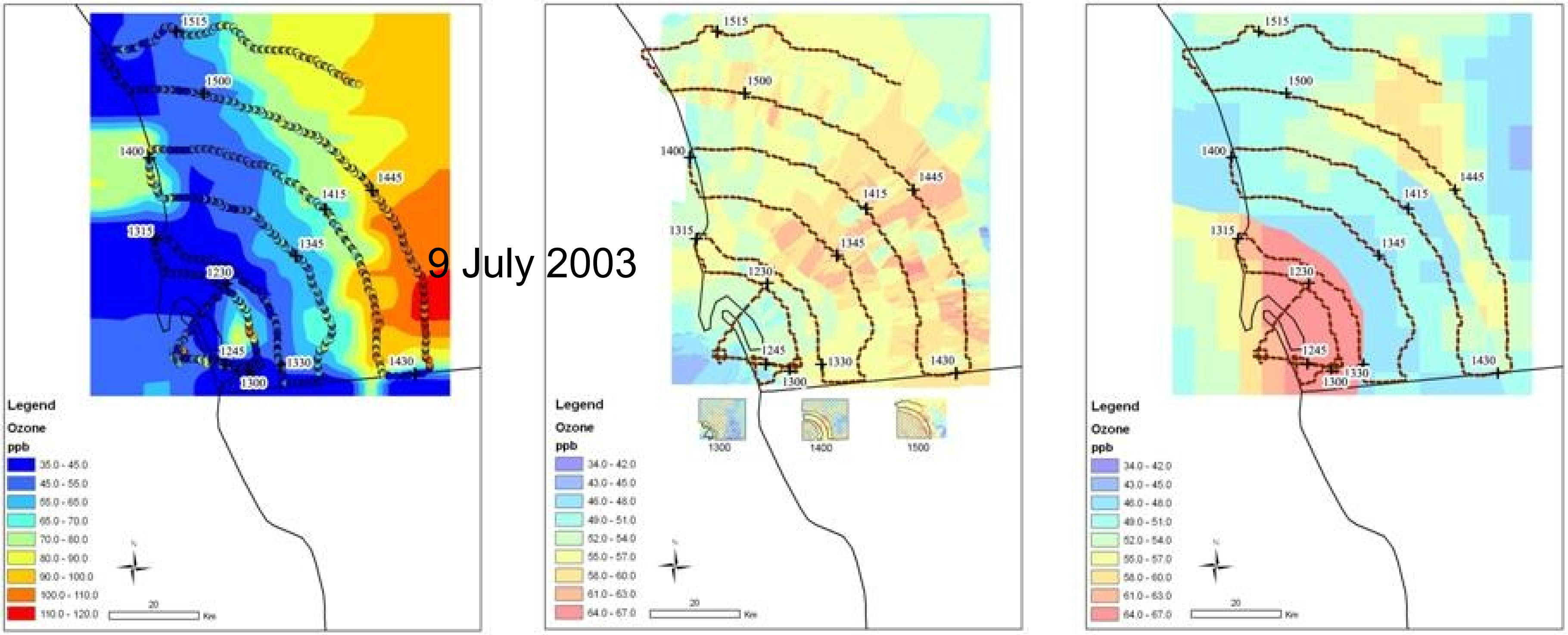
7 July 2003 – High impact in the central and SE regions

a. Ozone concentration (ppbv) at 300 m AGL from krigged aircraft observations (shaded colors) and aircraft observations (color dots) on 7 July 2003 at 1200-1600 LT.

b. Ozone concentration (ppbv) at 300 m AGL from HYBRID model (shaded colors) and aircraft observations path (dots) on 7 July 2003 at 1200-1600 LT

c. Ozone concentration (ppbv) at 300 m AGL from CAMx model (shaded colors) and aircraft observations path (dots) on 7 July 2003 at 1200-1600 LT

a. Aircraft b. Hybrid model c. CAMx model



9 July 2003 – High impact in the eastern and SE regions

a. Ozone concentration (ppbv) at 300 m AGL from krigged aircraft observations (shaded colors) and aircraft observations (color dots) on 9 July 2003 at 1300-1500 LT.

b. Ozone concentration (ppbv) at 300 m AGL from HYBRID model (shaded colors) and aircraft observations path (dots) on 9 July 2003 at 1300-1500 LT

c. Ozone concentration (ppbv) at 300 m AGL from CAMx model (shaded colors) and aircraft observations path (dots) on 9 July 2003 at 1300-1500 LT

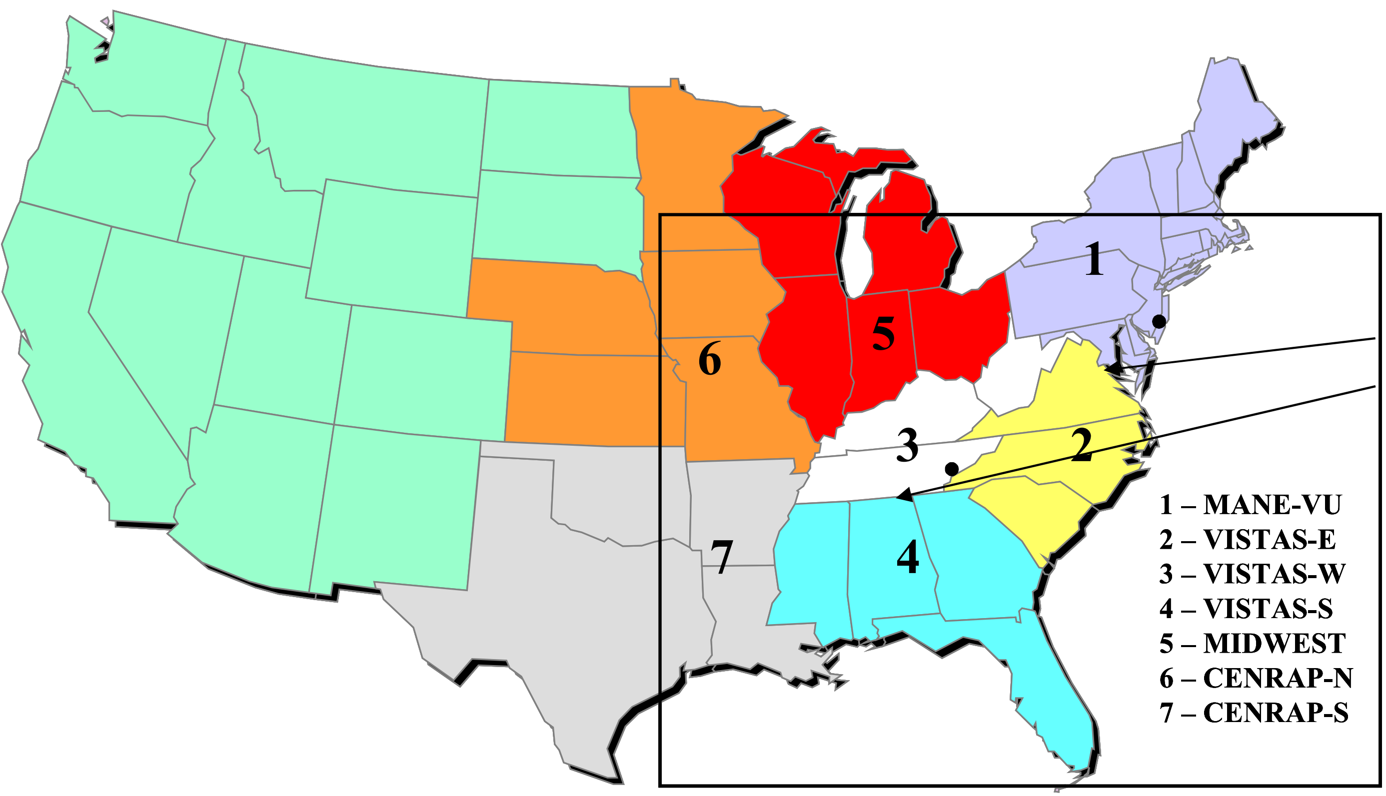
Summary - Forward Lagrangian stochastic modeling – Hybrid model

- Uncertainties present due to Mexico’s unknown emissions
- Uncertainties due to aircraft “mosaic” concentration patterns
- Hybrid model consisting of Lagrangian transport and dispersion with Eulerian chemistry can be used in complex environmental conditions
- Using aircraft data from the field program in southern California, the hybrid model results compared better than an Eulerian photochemical model (CAMx)

2. Inverse modeling

Lagrangian stochastic dispersion modeling

- Assessment of regional sources (eastern U.S.)



7 regions

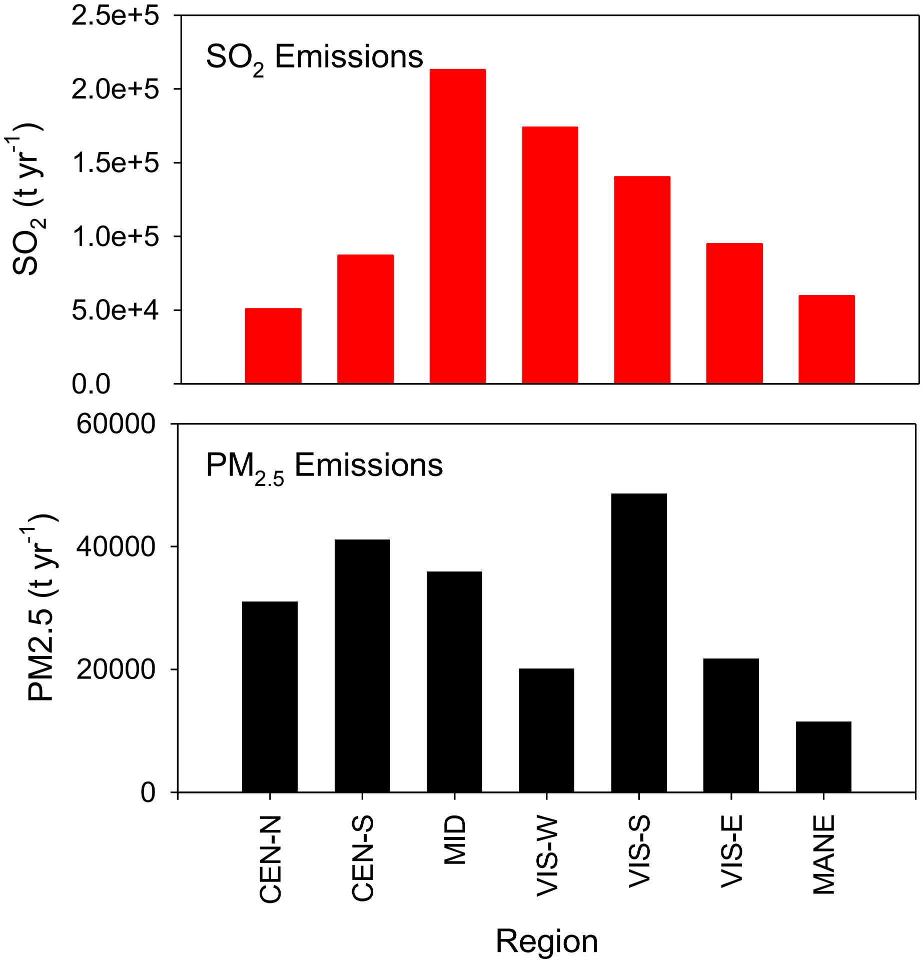
2 receptors:
- Brigantine NJ
- Great Smoky Mtn, TN

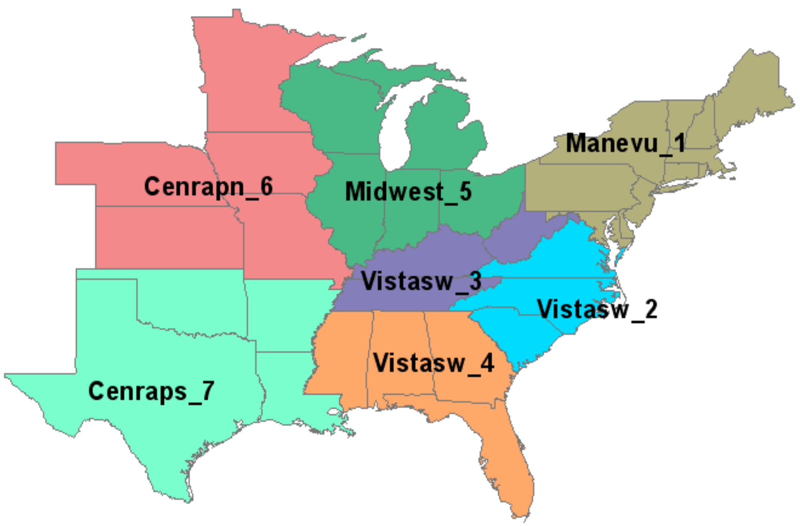
2. Inverse modeling

Lagrangian stochastic dispersion modeling

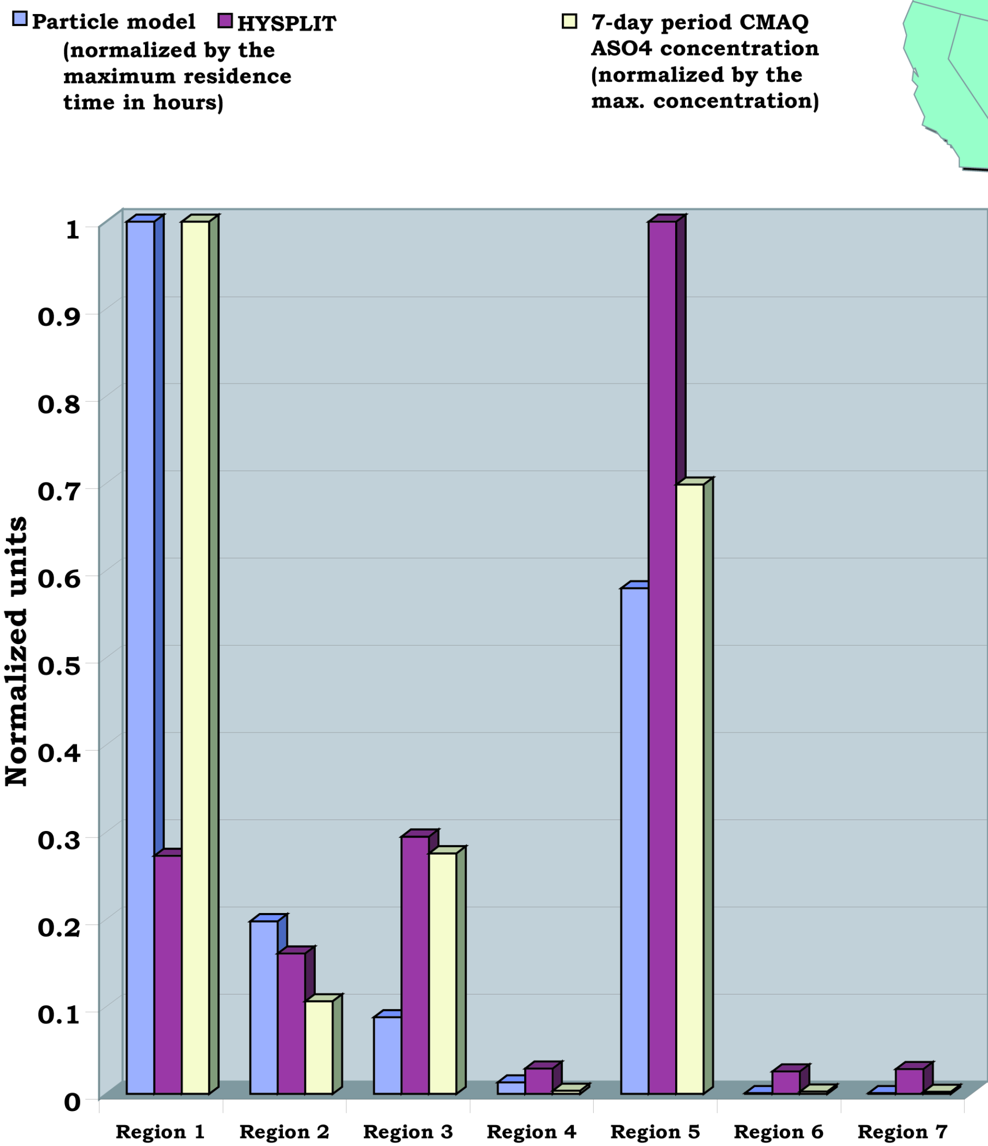
- Create a "model data base"
- EPRI/Sonoma Technology provided "synthetic" IMPROVE data sets using the SMOKE/ CMAQ/MM5 modeling system for the eastern U.S.
- Synthetic IMPROVE data are computed at the Brigantine National Wildlife Refuge (BRIG), NJ, and Great Smoky Mountains National Park (GRSM), TN, for summer (July-September) and winter (January-March), 2002.
- HYSPLIT trajectory computations
- Lagrangian stochastic dispersion model (Koracin et al. 2007, AtmEnv; Luria et al. 2005, AtmEnv; Erez et al. 2008, AtmEnv)

Annual Emissions by Region

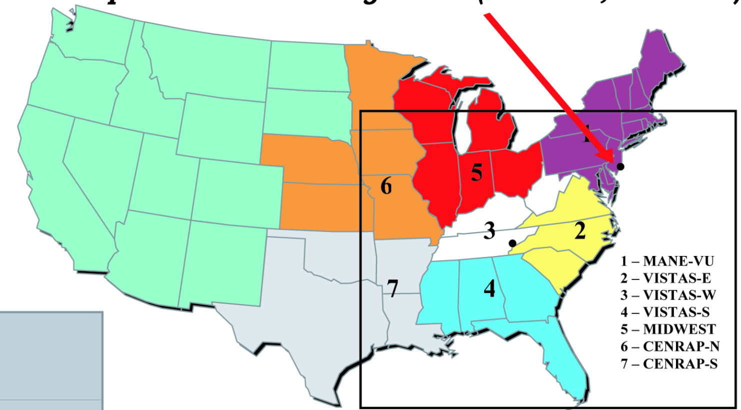




Particle model inverse mode simulations initialized on 20 July 2002 at 00 UTC



Receptor location = Brigantine (74.45 W; 39.46 N)



24-hour average sulfate concentration (Site: Brigantine; units in ng/m**3) (source: CMAQ)

	12 Jul 2002	13 Jul 2002	14 Jul 2002	15 Jul 2002	16 Jul 2002	17 Jul 2002	18 Jul 2002	19 Jul 2002	Total
1	1294.7	436.2	554	4350.2	2443.2	2050.5	4206.8	3794.7	**19130.4**
2	1.09	0.43	217.98	600.49	146.99	18.38	236.49	809.54	2031.39
3	0	0	27.72	170.74	187.6	0.04	1636.48	3253.91	**5276.49**
4	0	0	19.88	29.9	2.25	0	0.67	17.18	69.88
5	0	0	27.5	79.1	377.5	0.7	4208.9	8672.9	**13366.6**
6	0	0	7.55	14.75	1.29	0	0.32	30.47	54.38
7	0	0.04	1.53	3.07	0.59	0	0	41.12	46.35

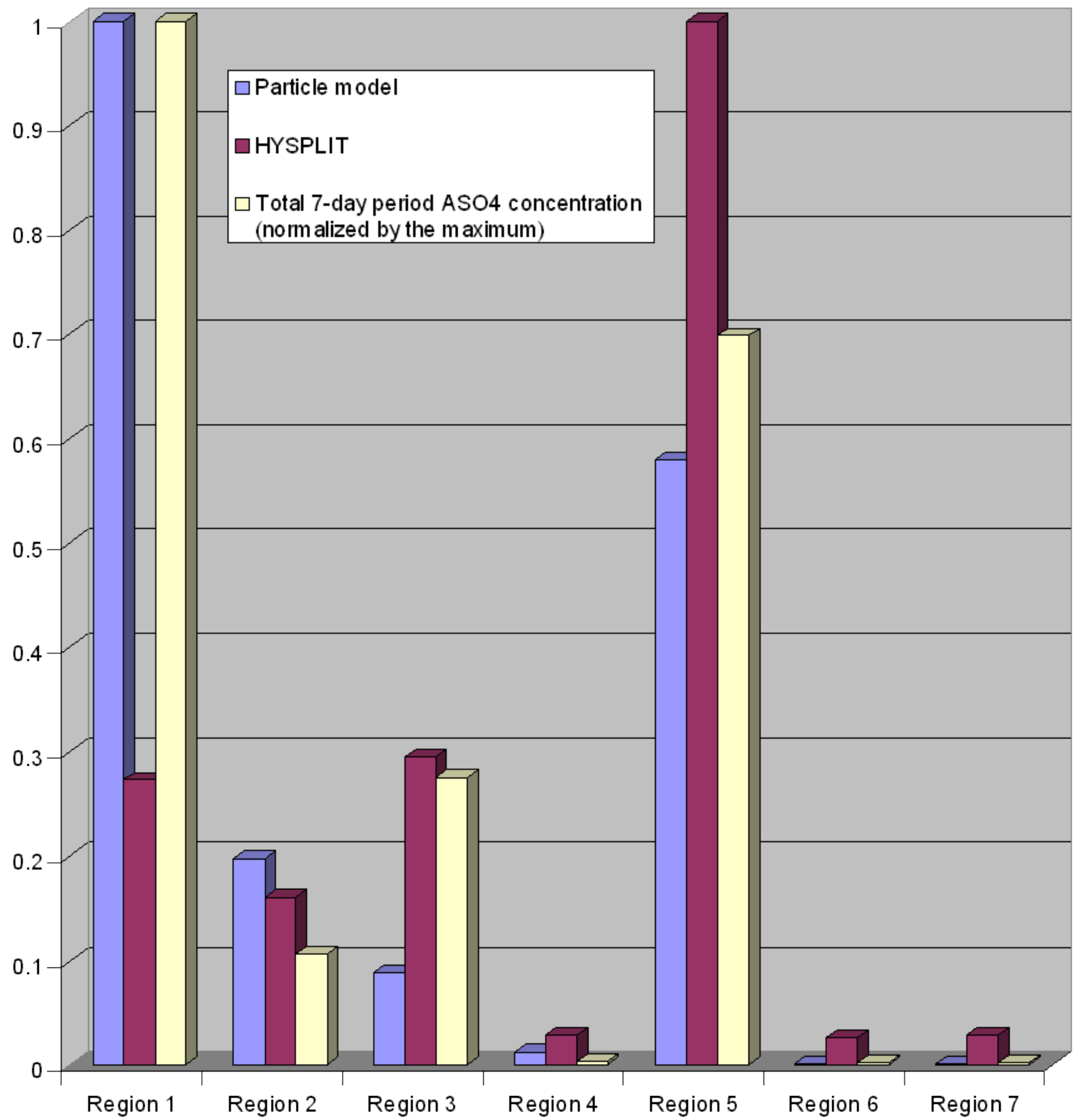
Total residence time of particle and HYSPLIT backtrajectories over 7-day period given in hours (no. of regionalwise hits in the backward simulations given in brackets)

Residence time in hours	R1	R2	R3	R4	R5	R6	R7
Particle model	19.33 (19114553)	2.92 (3786418)	1.09 (1684377)	0.24 (251552)	11.02 (11080649)	0.03 (16917)	0.02 (18781)
HYSPLIT	19.45 (934)	10.12 (486)	23.02 (1105)	1.58 (76)	73.89 (3547)	2.12 (102)	2.37 (114)

Particle model simulations:
Area sources (0.5 x 0.5 deg centered at Brigantine)
50 particle emitted per time step
(emission rate = 1.11 g/sec)

PM and HYSPLIT trajectory positions = hourly
48 HYSPLIT trajectories
and 1014000 PM trajectories for this case study

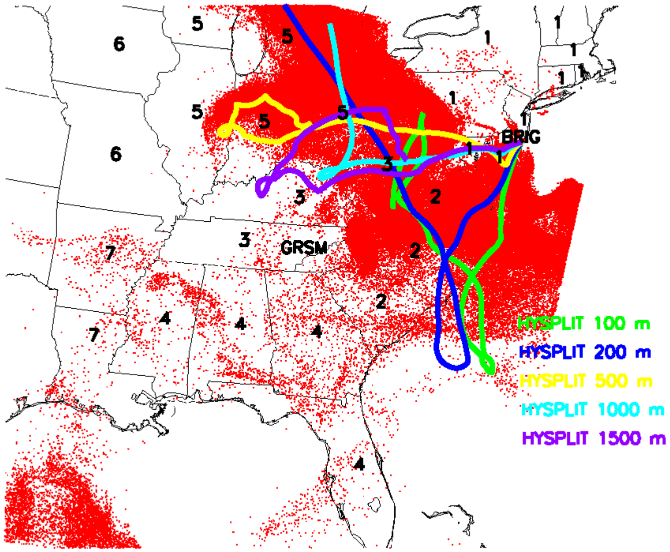
Results: Apportioned normalized contribution of sulfate by regions at Brigantine Hybrid model (blue) and HYSPLIT (red) vs. "true contribution" (yellow)



Comments: HYSPLIT back trajectories

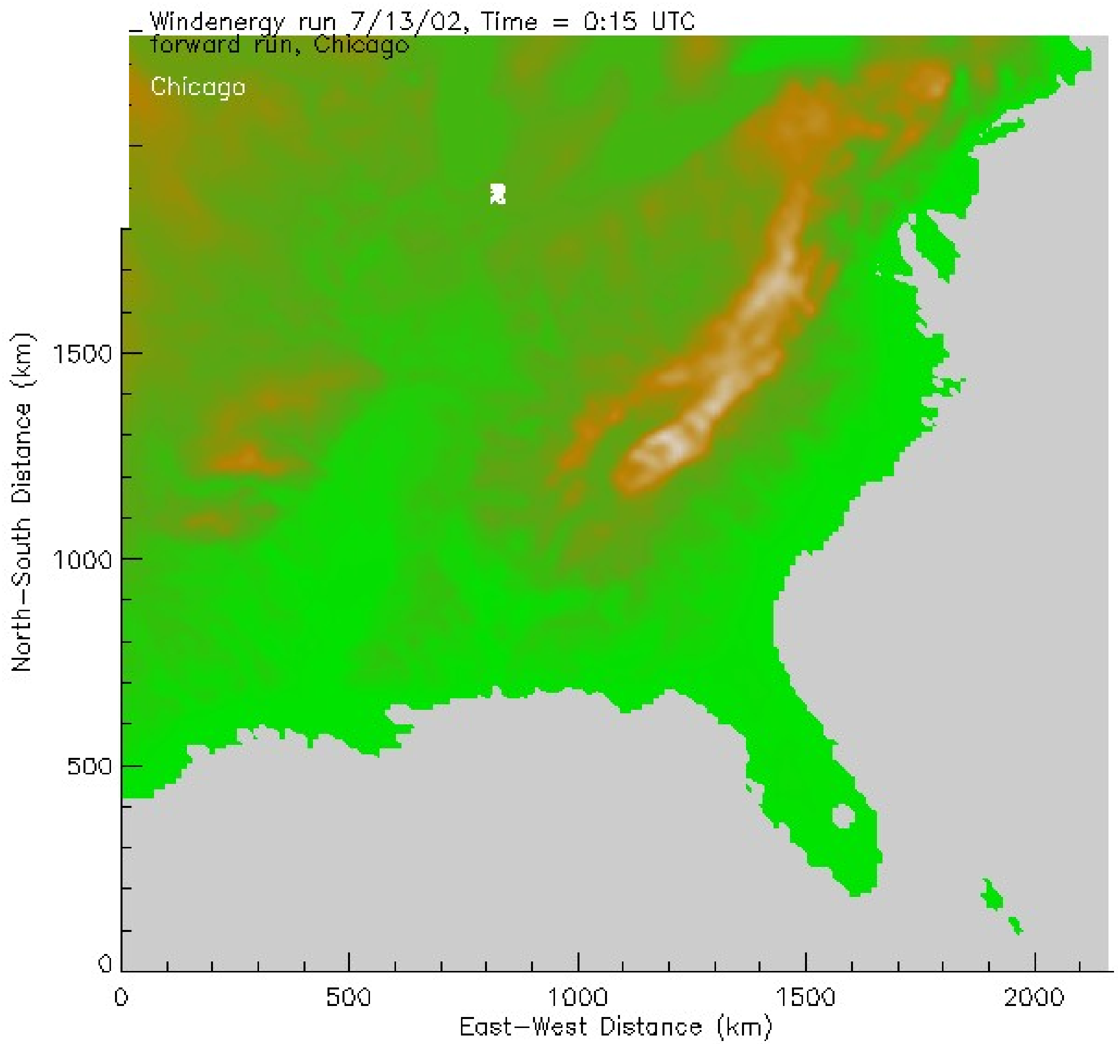
- underestimate near by contributions (Region 1) and

- overestimate distant sources (Region 5)



End of the inverse run indicates possible emission sources in Region 5

Forward run from Region 5



Summary

- Lagrangian stochastic dispersion models show significant capabilities in complex atmospheric and environmental conditions on variety of scales – they should be more tested and utilized in regulatory applications.
- Hybrid modeling offers possibilities of linking chemical modules of various complexities.
- Lagrangian dispersion – no numerical diffusion – applicable to high resolution, complex topography.
- Currently, Lagrangian dispersion with Eulerian chemistry is a feasible tool.
- Inverse modeling offers enhancement of standard back trajectory and receptor modeling approach.
- Another advantage in using Lagrangian stochastic approach is possibility of either forward or inverse modeling. Or, in a dual mode (inverse and forward) when investigation has to start from receptors in the area of complex sources. This dual method can be valuable for estimation of clean-air corridors and other environmental planning.
- New observational and modeling methods should be developed for efficient model evaluation.