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

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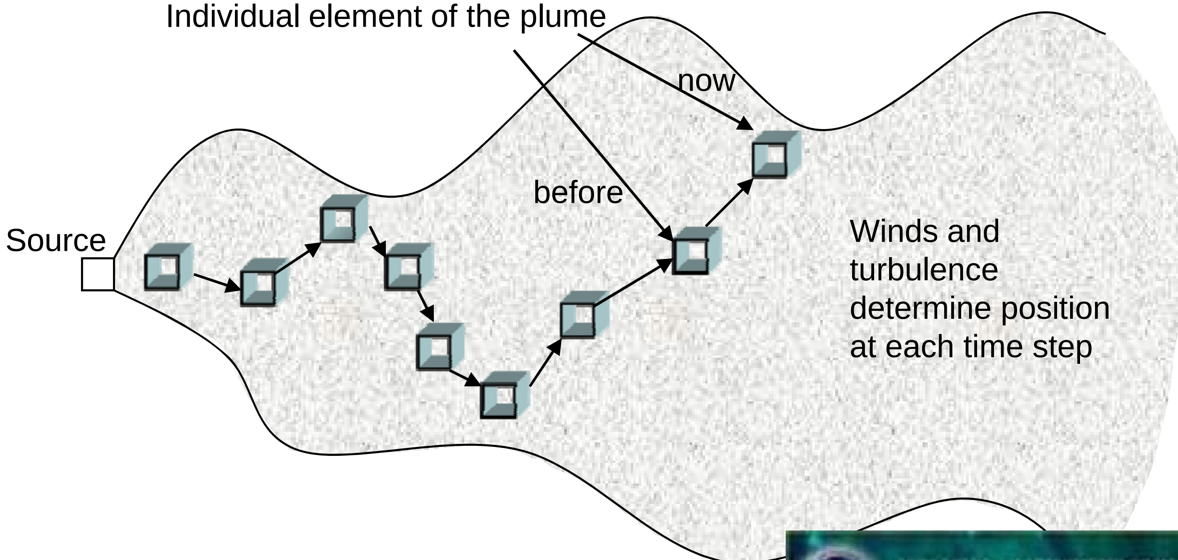
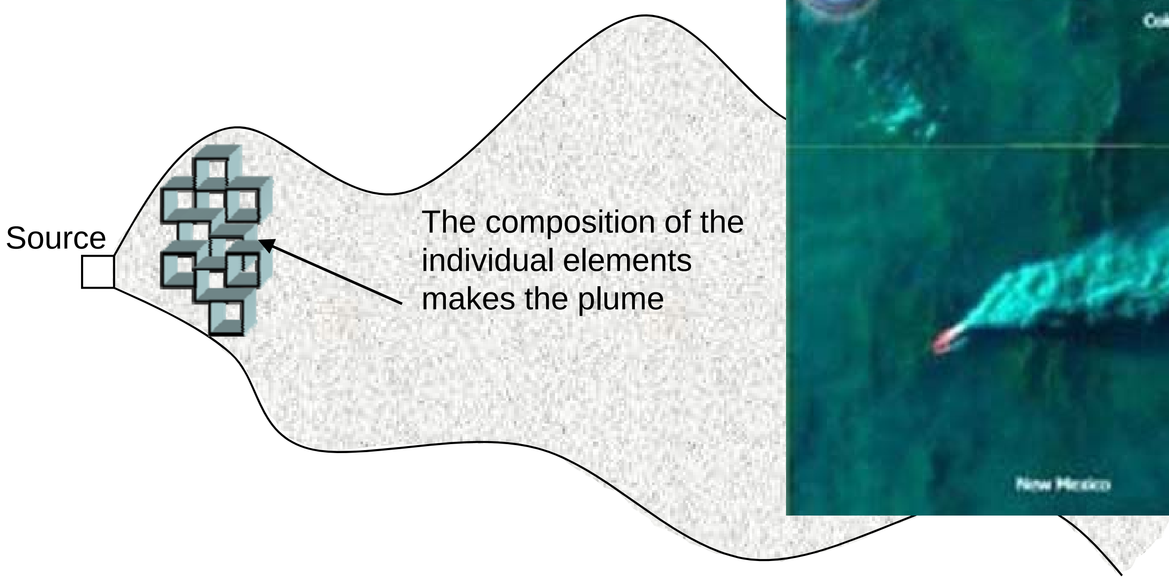
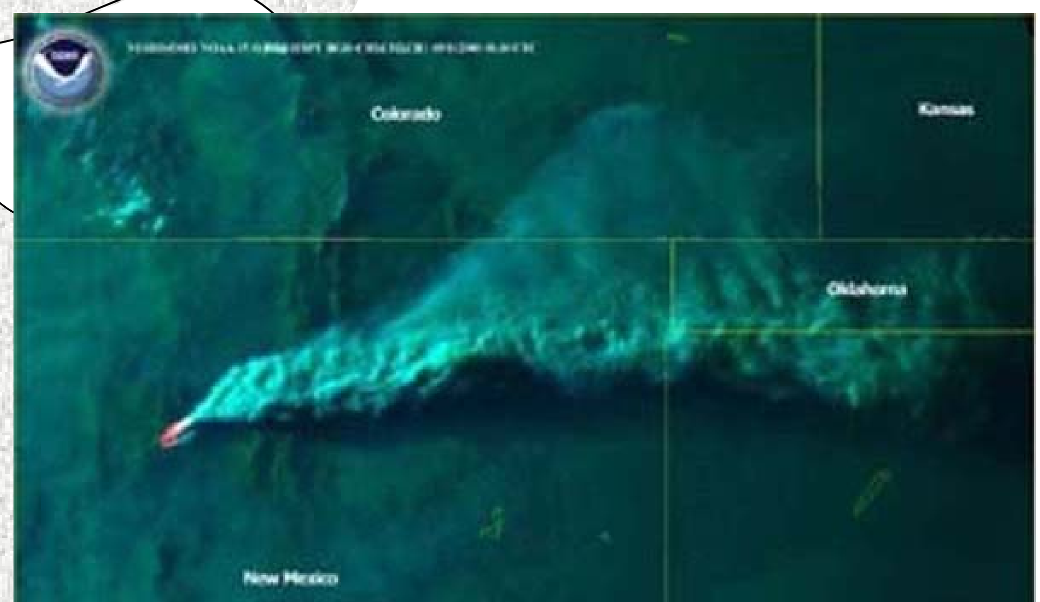
Lagrangian Random Particle Dispersion Modeling



•No fixed dimensions of the plume
•Applicable to any terrain
•Applicable to any surface type
•Applicable to any meteorological conditions



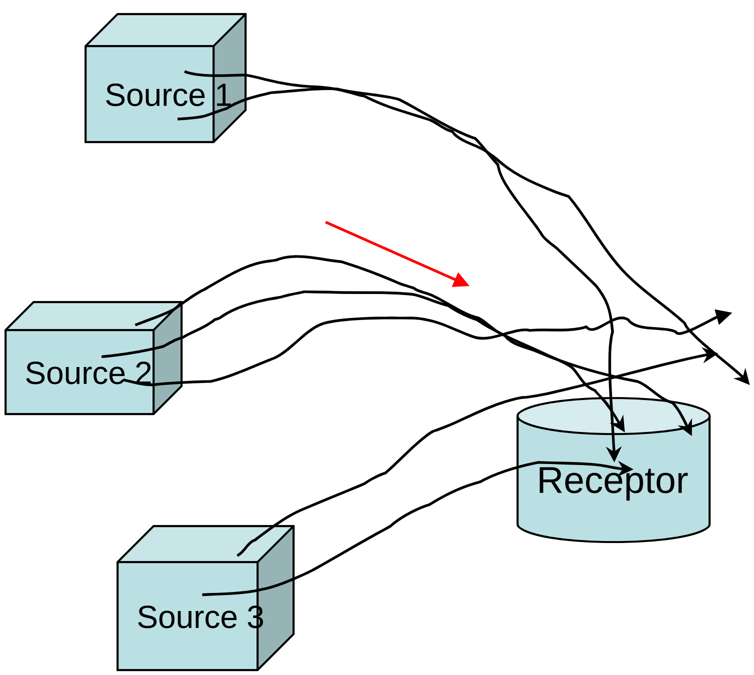


Lagrangian random particle dispersion model - Main principles

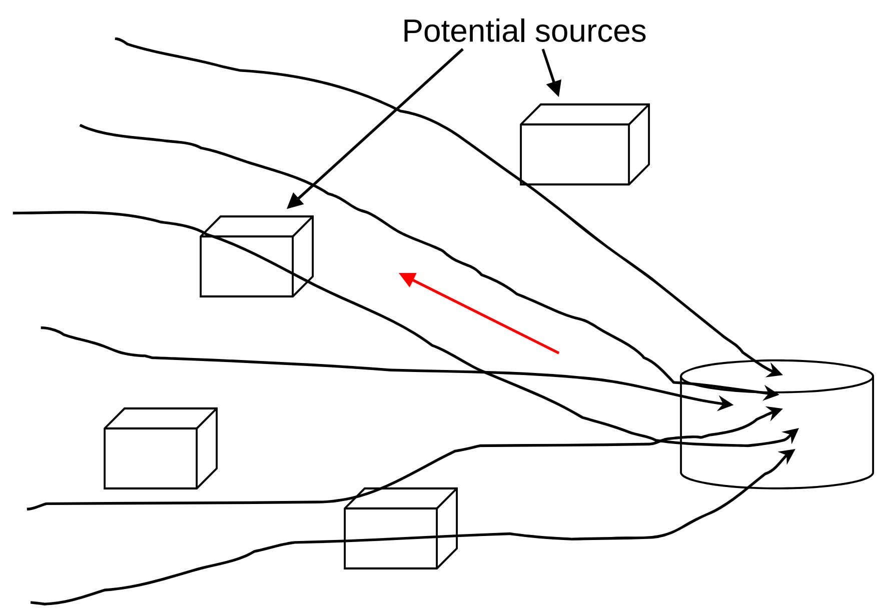
- Numerical model which uses a large number of hypothetical particles to simulate the transport and dispersion of atmospheric pollutants
- Particles are subjected to 3D atmospheric fields
- Dispersion of the simulated plume is directly linked to the turbulence structure *without* the Gaussian assumption
- Typically, 500 particles per minute are emitted from each source
- The particles are continuously traced in time and space and their population represents the plume structure

Forward and backward models using the same particle modeling tool

Forward model: particles released from sources are traced



For receptor-oriented modeling, the sign of the time step is reversed and trajectories are run backward.



Computation of concentrations

Pollutant concentration

Mass emission source

$$C(x,t) = \int_{-\infty}^{t} \int_{-\infty}^{\infty} S(x_0, t_0) \underbrace{P^f(x, t \mid x_0, t_0) dx_0 dt_0}$$

probability that a fluid element initially at *(x0,t0)* is found at time *t* in the volume *dx* centered on *x*.

Flesch, Wilson, Yee, 1995, JAM

Particle residence time

Receptor volume

$$T^{f}(x, V_{rec} \mid x_0) = \int_{V_{rec}} \int_{t=0}^{\infty} P^{f}(x', t \mid x_{0,0})\,dx'\,dt$$

Simple discrete form:

particles

$$C^{v}(x) = S \frac{V_{src}}{V_{rec}} \frac{1}{N} \sum_{n=1}^{N} T_n^{f}(x, V_{rec} \mid V_{src})$$

Lagrangian modeling – Theoretical basis (II)

- 1908 Langevin

$$\frac{du}{dt} = -a_1 u + b\, f(t)$$

u – particle velocity; t – time

a_1 – damping coefficient due to viscous drag

b – coefficient

$f(t)$ – rapidly varying acceleration component from a irregular and asymmetrical molecular bombardment of the particle.

Lagrangian modeling – Theoretical basis (III)

- The Langevin equation is a Lagrangian stochastic differential equation.
- *Lagrangian framework – system of coordinates based on the position (x,y,z) of a particle at time t relative to its position (a,b,c) at a reference time* t_0.
- Lagrangian coordinates are more natural for describing fluid motion, but are more difficult to use compared to Eulerian coordinates.

Lagrangian random particle (LAP) model – Main algorithms (II)

- The subgrid-scale velocity components are iteratively determined as:

$$u_r(t) = u_r(t-\Delta t)R_u(\Delta t) + u_s(t-\Delta t)$$
$$v_r(t) = v_r(t-\Delta t)R_v(\Delta t) + v_s(t-\Delta t)$$
$$w_r(t) = w_r(t-\Delta t)R_w(\Delta t) + w_s(t-\Delta t)$$

- R_u, R_v, and R_w are the Lagrangian autocorrelation functions for each velocity component, and u_s, v_s, and w_s are the random fluctuations of the velocity components.

Lagrangian random particle (LAP) model – Main algorithms (VII)

- The bounds for the random components are determined from the statistical properties of the turbulence transfer and the autocorrelation function :

$$\sigma_u = \sqrt{(\overline{u'u'}) \cdot \{1 - R_u^2(\Delta t)\}}$$

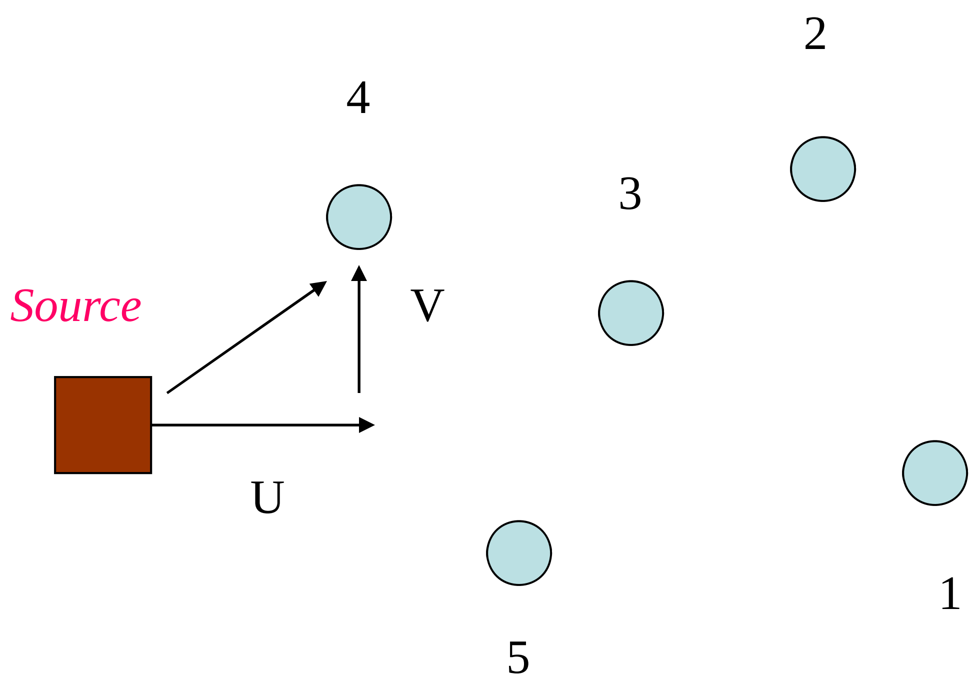
$$\sigma_v = \sqrt{(\overline{v'v'}) \cdot \{1 - R_v^2(\Delta t)\}}$$

$$\sigma_w = \sqrt{(\overline{w'w'}) \cdot \{1 - R_w^2(\Delta t)\}}$$

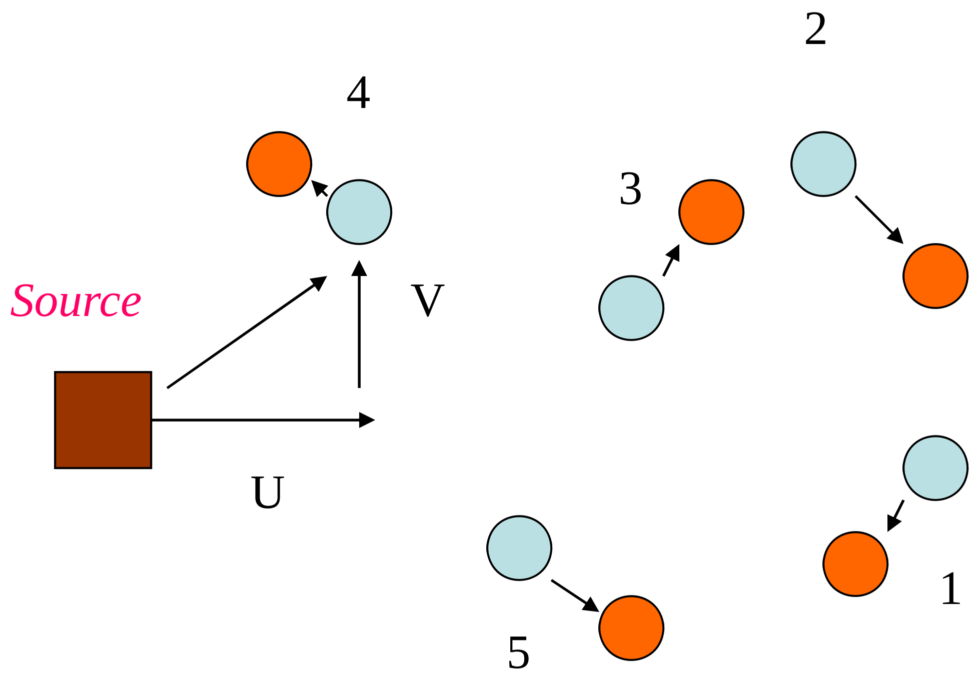
$\sigma_u, \sigma_v, and\ \sigma_w$ - standard deviations around zero mean for the range of random components u_s, v_s, and w_s .

$\overline{(u'u')}$, $\overline{(v'v')}$, $\overline{(w'w')}$ - variances at the particle location

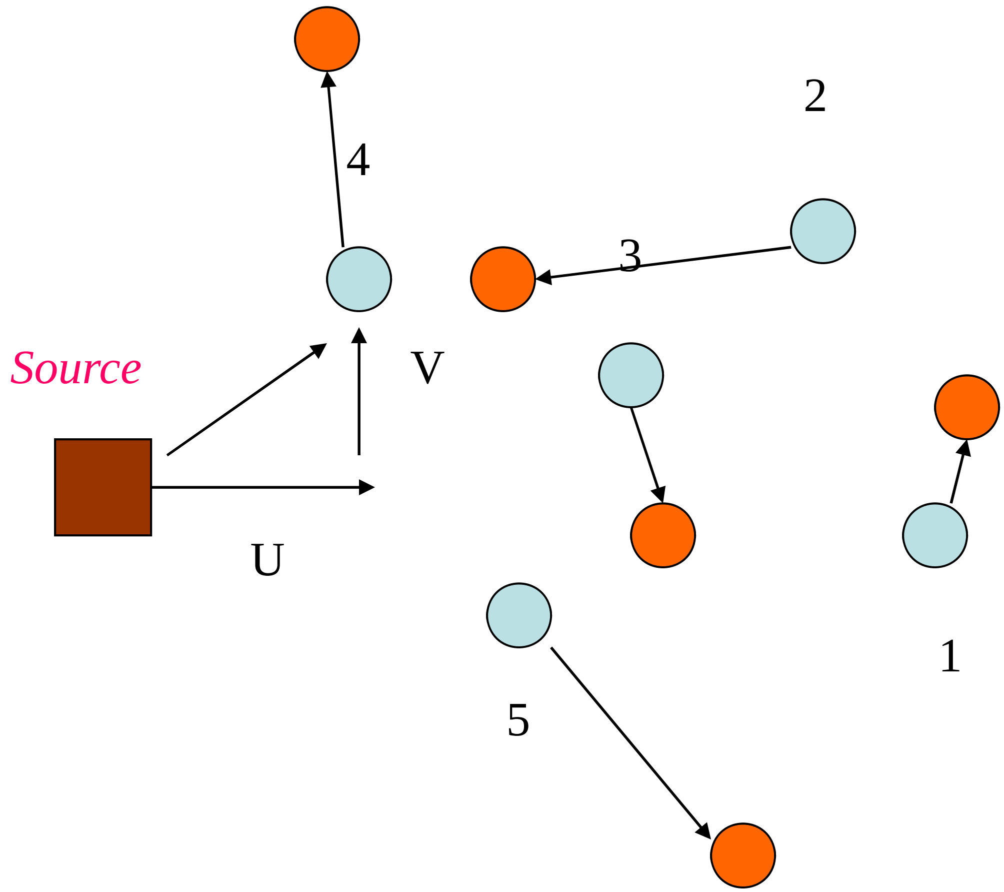
Initial distribution of particles – only wind, no turbulence, no dispersion



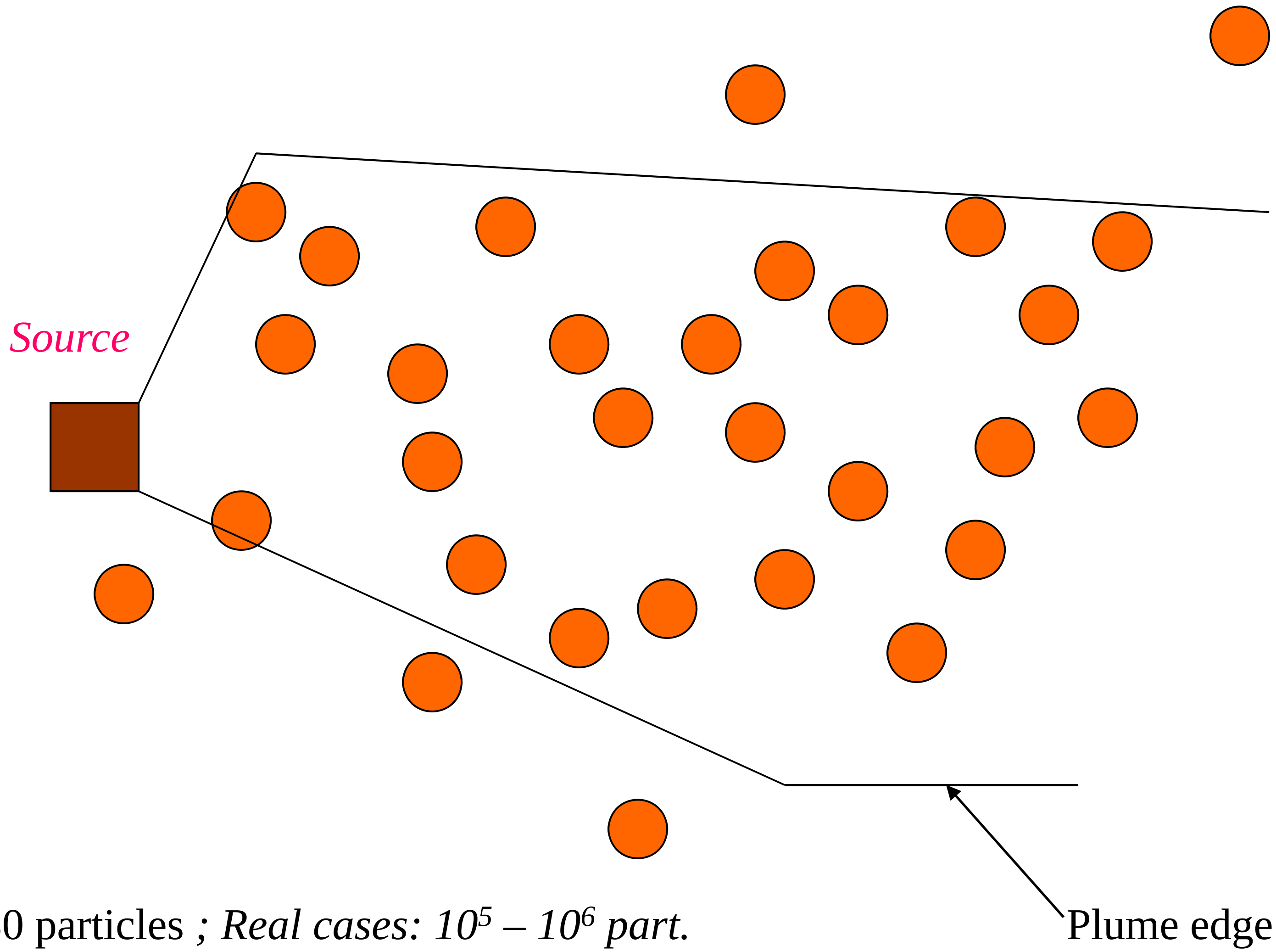
Distribution of particles – STABLE conditions: wind + low turbulence = *weak dispersion*



Distribution of particles – UNSTABLE conditions: wind + high turbulence = *strong dispersion*

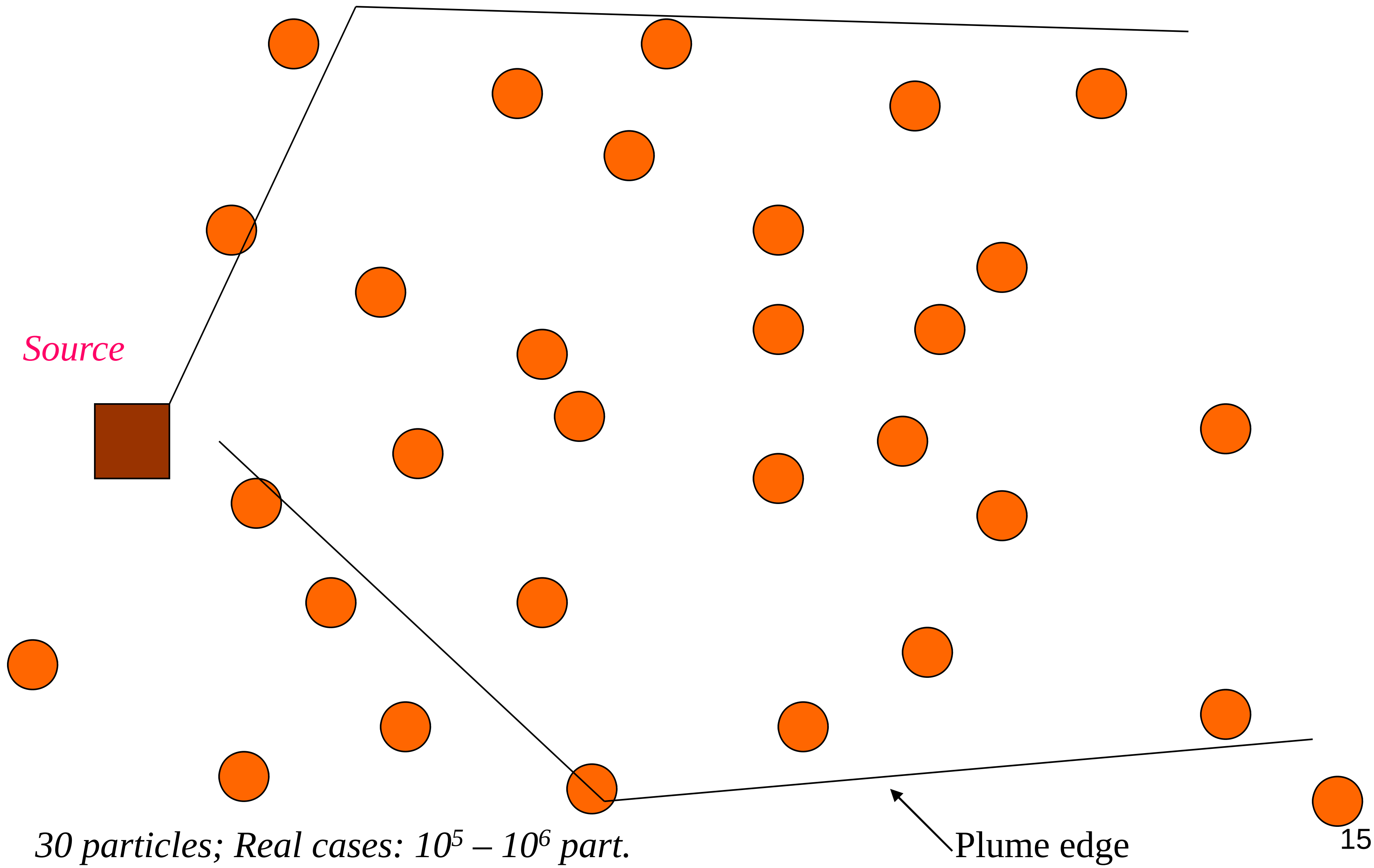


Population of particles – STABLE conditions: wind + low turbulence = *weak dispersion*



30 particles ; *Real cases:* $10^5 - 10^6$ *part.*

Population of particles – UNSTABLE conditions: wind + high turbulence = *strong dispersion*



30 particles; Real cases: $10^5 – 10^6$ part.

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) and WRF (Skamarock et al. 2005)
- Lagrangian stochastic dispersion model (Koracin et al. 2007, AtmEnv, 2010, JAWMA; Luria et al. 2005, AtmEnv; Erez et al. 2008, AtmEnv; Lowenthal et al. 2010, JAWMA)
- Eulerian chemical model with RACM (Stockwell et al. 1997, JGR)

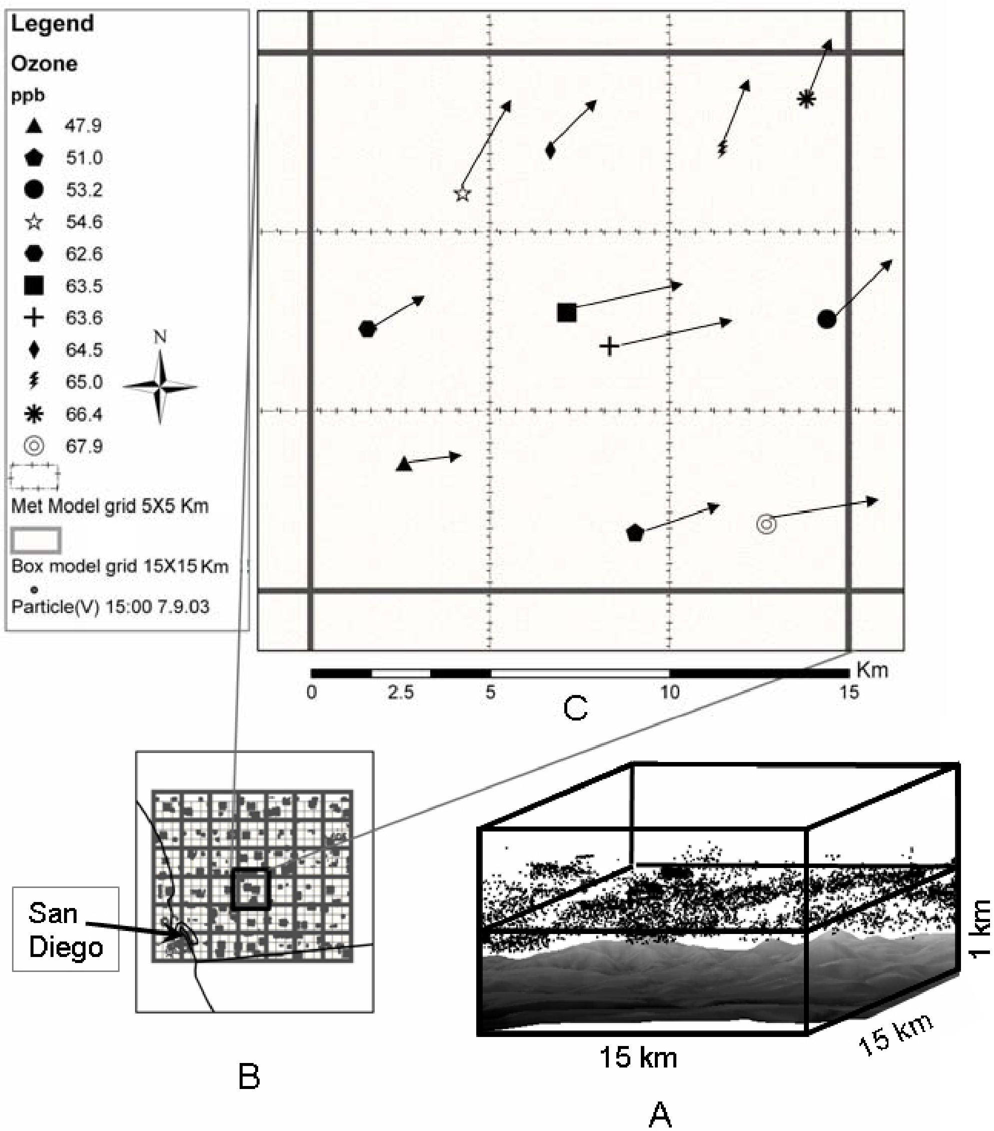
Lagrangian stochastic dispersion modeling within complex modeling systems

- 2. Inverse LS modeling: Evaluation of receptor modeling & assessment of regional emission sources (eastern U.S.)

- EPA generated Meteorological model MM5 (Grell et al. 1994, NCAR) fields for the summer 2002
- CMAQ baseline simulations (synthetic data set)
- HYSPLIT and EDAS trajectory computations
- Lagrangian stochastic dispersion model (Koracin et al. 2007, Atm. Environ.)

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 troposphere



Model domains

Grid resolution

- MM5: 5x5 km2
- Box chemistry model: 15x15 km2

Each particle is apportioned by the emissions and carries "chemical dimensions"

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

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

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*

$P_{Tot(n)}$ – total mass of chemical *n* from all particles in the grid cell is converted into concentration of 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)

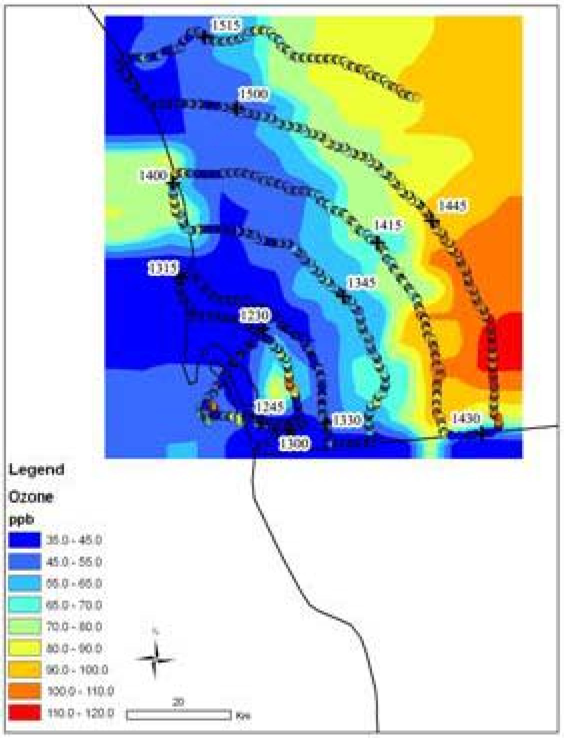
$Particle_k(x,y,z,T,RH,p,chm_i....chm_j,ID,t)$

Distribution of newly formed species is based on a factor *f* intermixing efficiency as a function of diffusion, time scale, mixing height, and turbulence intensity
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 the time steps t and $t+\Delta t$ for particles that had the new chemical species

Aircraft measurements



Comparison: Hybrid & CAMx models vs. aircraft data

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

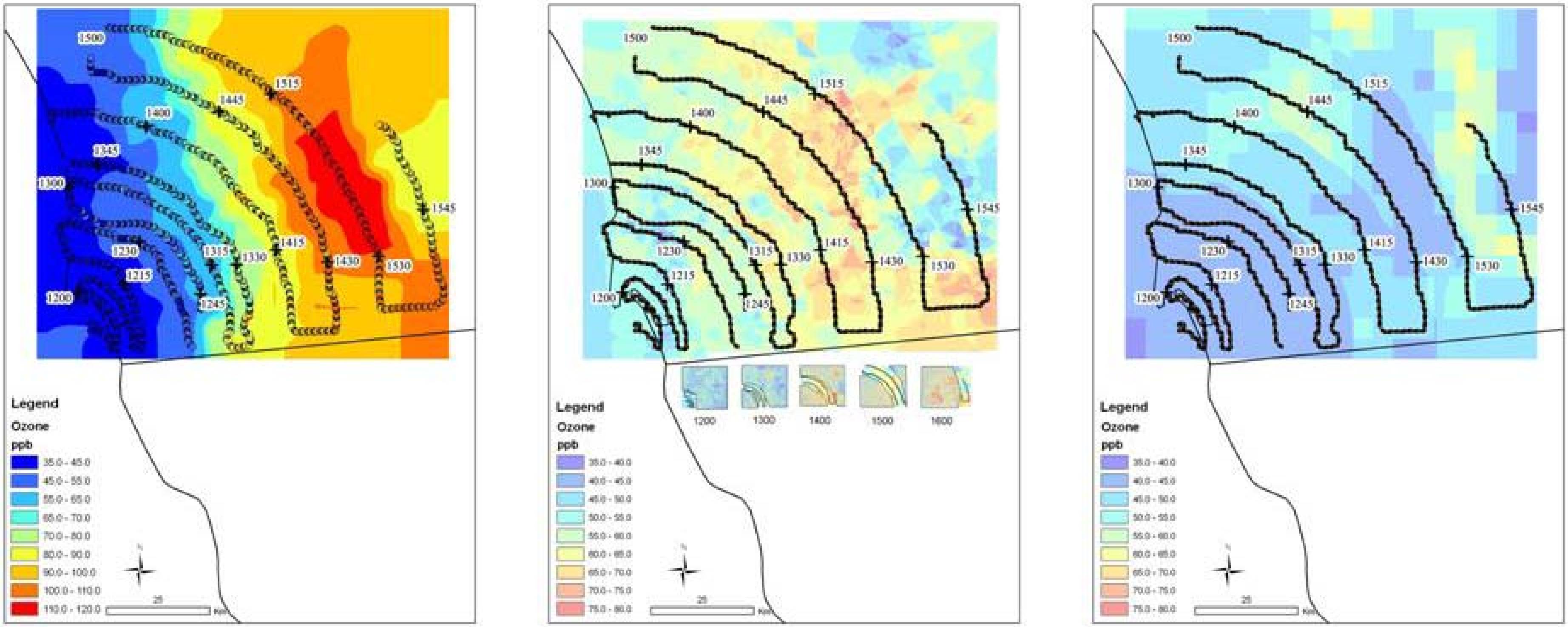
A mapped hourly predictions of ozone by the Hybrid and CAMx models were cut in hourly sections corresponding to the aircraft flight time and locations.

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

a. Aircraft

b. Hybrid model

c. CAMx model

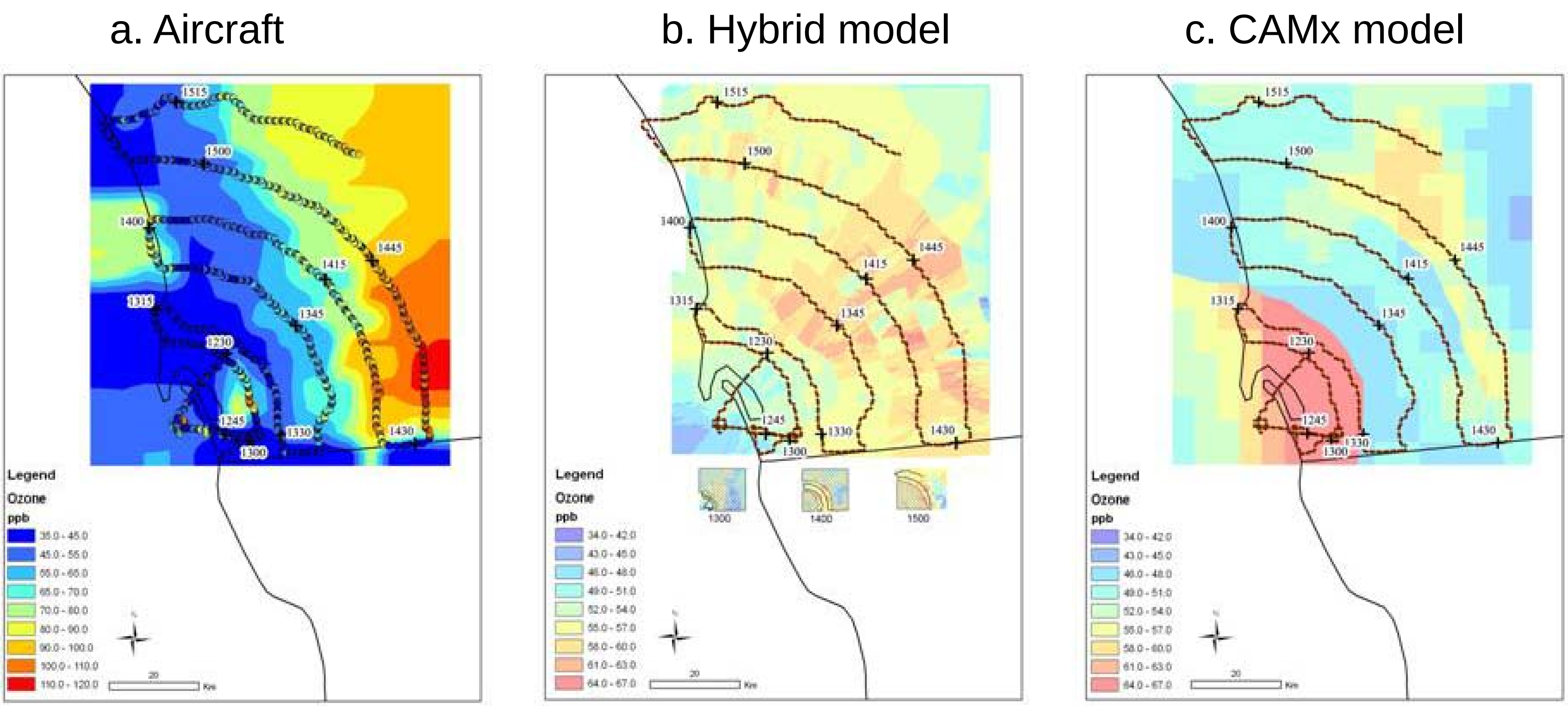


7 July 2003

a. Ozone concentration (ppbv) at 300 m AGL from kriged 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 LAPIB 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



9 July 2003

a. Ozone concentration (ppbv) at 300 m AGL from kriged 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 LAPIB 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

- 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)

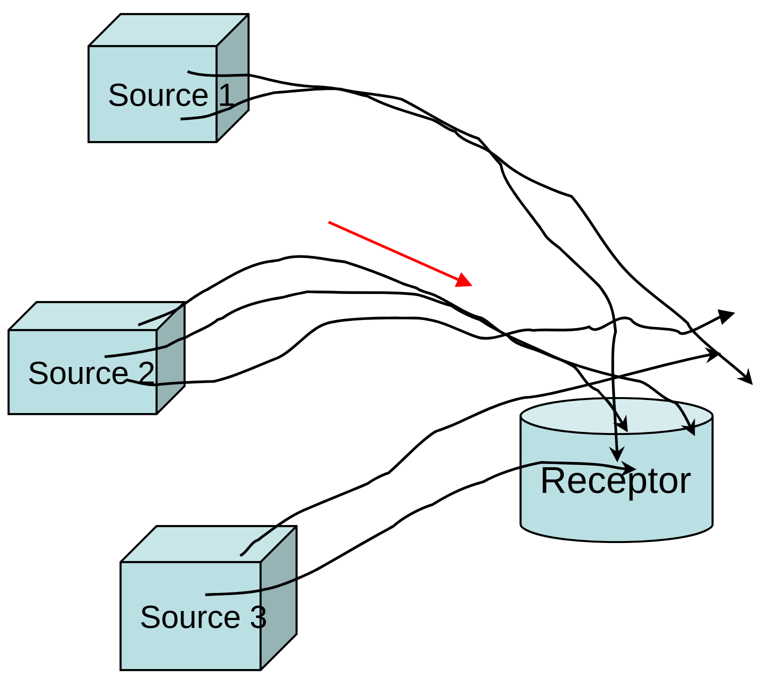
Lagrangian stochastic dispersion Inverse modeling

- 2. 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 Brigantine National Wildlife Refuge (BRIG), NJ, and Great Smoky Mountains National Park (GRSM), TN, for summer (July-September) and winter (January-March), 2002.
- HYSPLIT and EDAS trajectory computations
- Lagrangian stochastic dispersion model (Koracin et al. 2007, 2010, AtmEnv; Luria et al. 2005, AtmEnv; Erez et al. 2008, AtmEnv, Lowenthal et al. 2010, JAWMA)

Forward and backward models using the same particle modeling tool

Forward model: particles released from sources are traced



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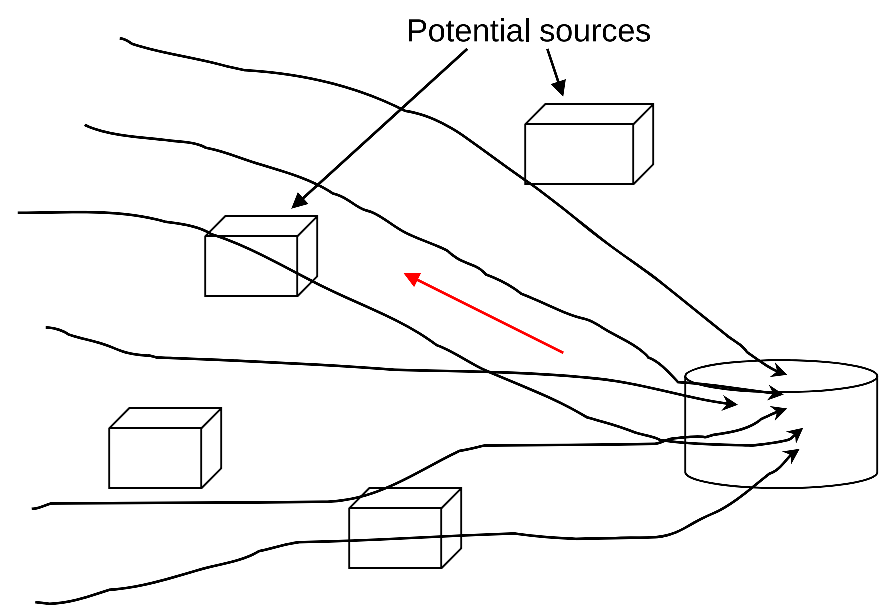


Backward Lagrangian stochastic dispersion modeling

- Particles released at *(x,t)* and collected at *(x_0,t_0)* with the backward-time conditional probability density P^b *(x_0,t_0/x,t)*

$$C^v(x) = \frac{S}{V_{sens}} \int_{sens} T^b(x_0, V_{src} / x)\, dx$$

$$C^v(x) - Concentrations$$

$$S - Emission\ rate$$

$$T^b - Backward\ residence\ time$$

$$In\ a\ discrete\ form:$$

$$C^v(x) = \frac{S}{N} \sum_{n=1}^{N} T_n^b(x_0, V_{src} / x)$$

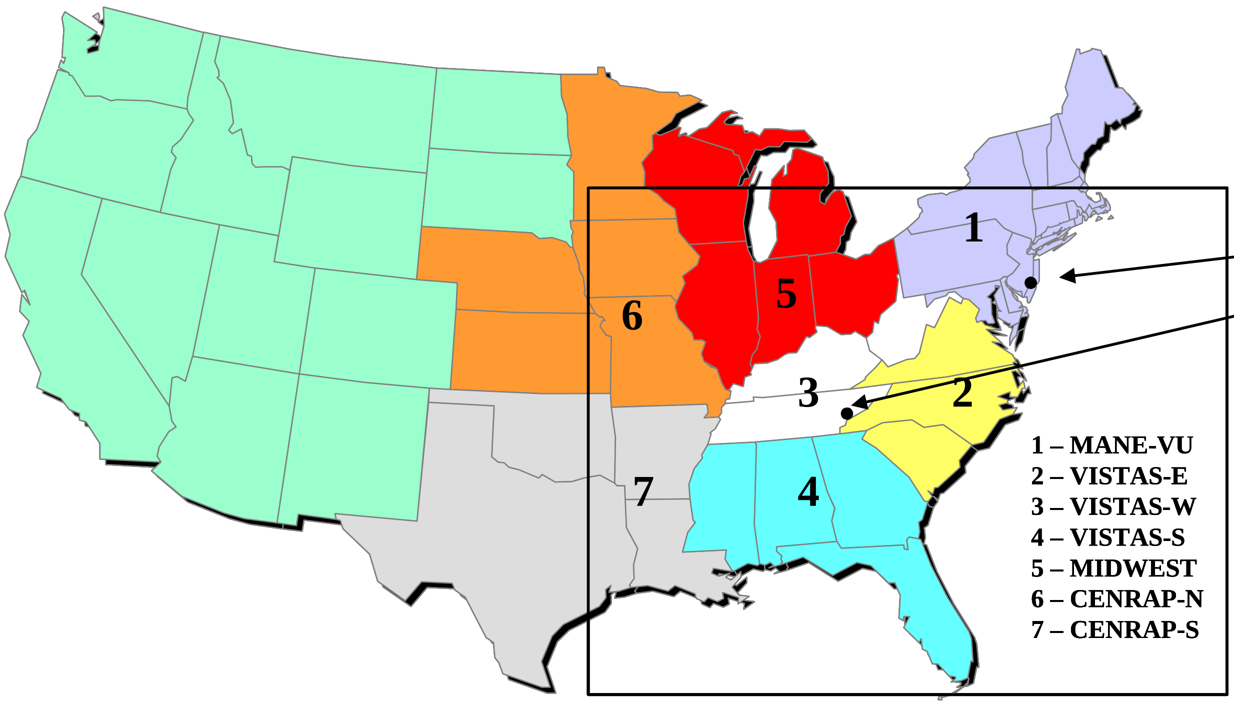
$$N\ particles\ are\ released\ from\ V_{sens}$$

$$T_n^b - Individual\ particle\ residence\ times$$

Flesch, Wilson, Yee, 1995, JAM

Lagrangian stochastic dispersion modeling within complex modeling systems

- 2. Inverse LS modeling: Assessment of regional sources (eastern U.S.)



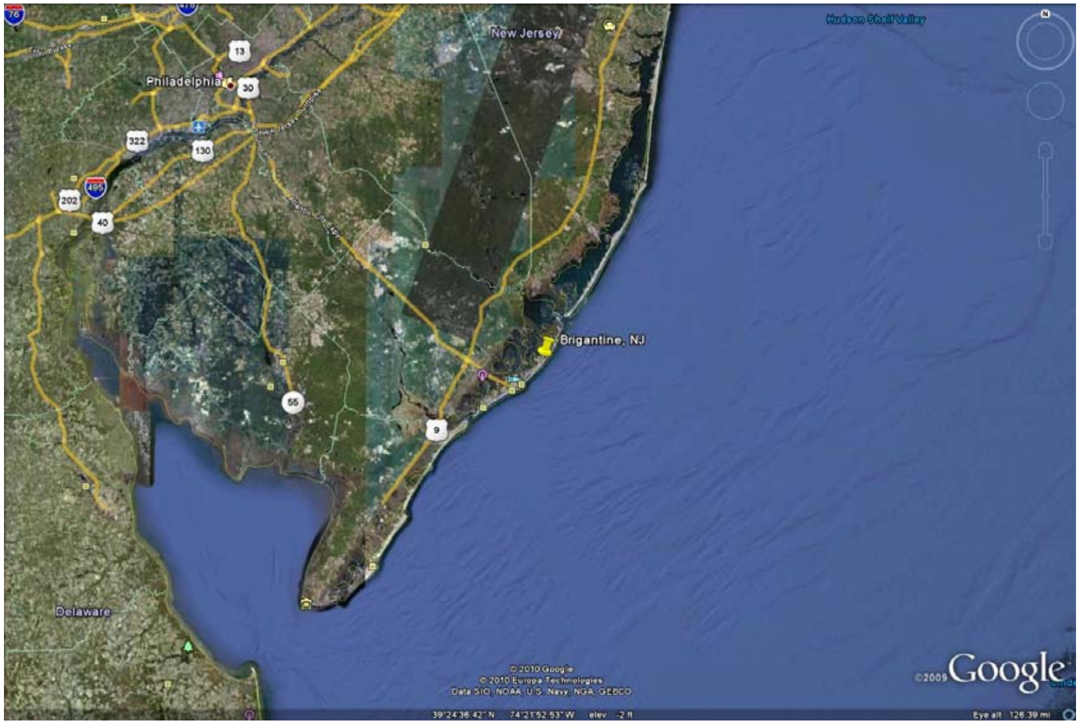
7 regions

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

Specifics of the “synthetic” model results

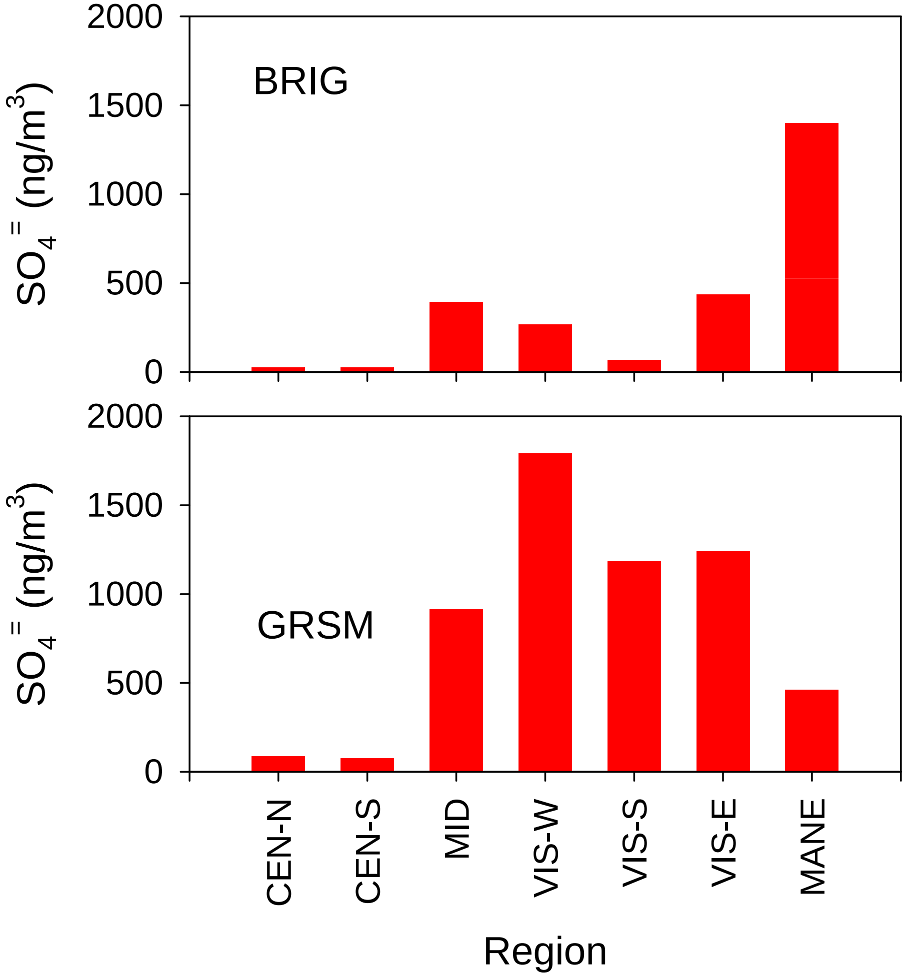
- Primary PM2.5 source profiles for 43 source categories were taken from the EPA’s Speciate and DRI’s PM source profile libraries. The profiles were used in the CMAQ model to produce hourly multi-species IMPROVE-style concentration data (EPRI/STI).
- The meteorological input to CMAQ was 12 km resolution data generated with the NCAR Mesoscale Meteorological Model (MM5) (EPA).
- 43 additional variables were added to each source profile, with unique values equal to the primary PM2.5 emitted by that source. This allows us to follow each source’s primary PM2.5 contribution to each receptor site.
- Contributions from each of the seven regions were estimated by sequentially running the model with 30% of a given region’s anthropogenic emissions removed.
- For summer, the “true” regional contributions were provided to DRI as a guide in the receptor modeling analysis.
- Hourly average PM2.5 concentrations at BRIG and GRSM were given to DRI for a “blind” analysis, which means that the “true” contributions were retained by EPRI and were not provided to DRI.

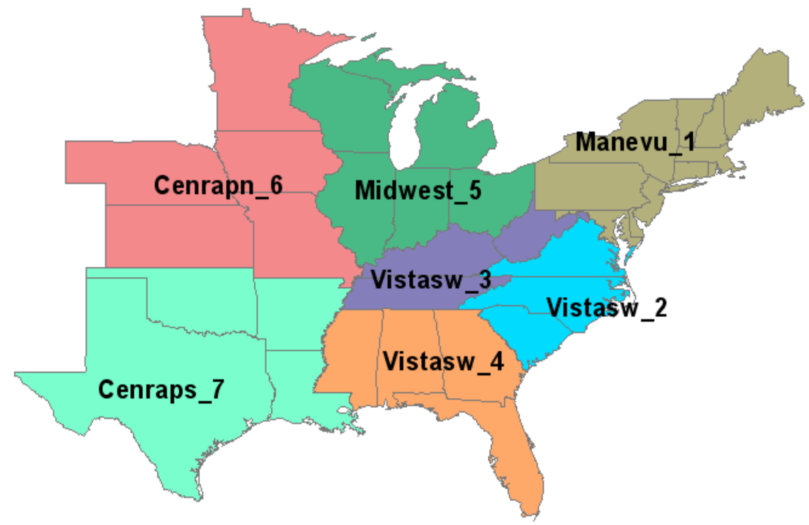
Great Smoky, TN



Brigantine, NJ

Average "True" Regional Contributions to Sulfate at Brigantine and Great Smoky





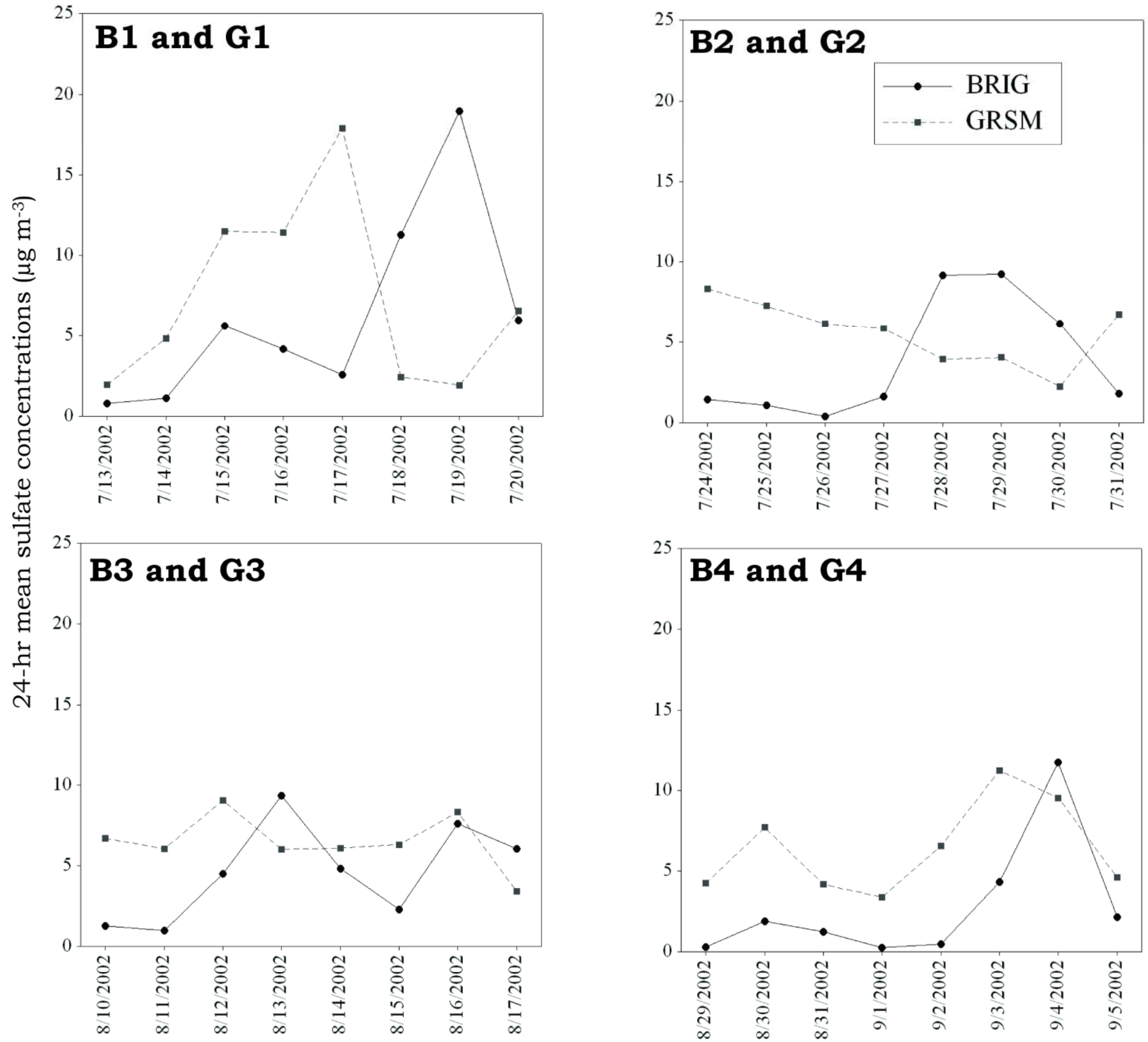
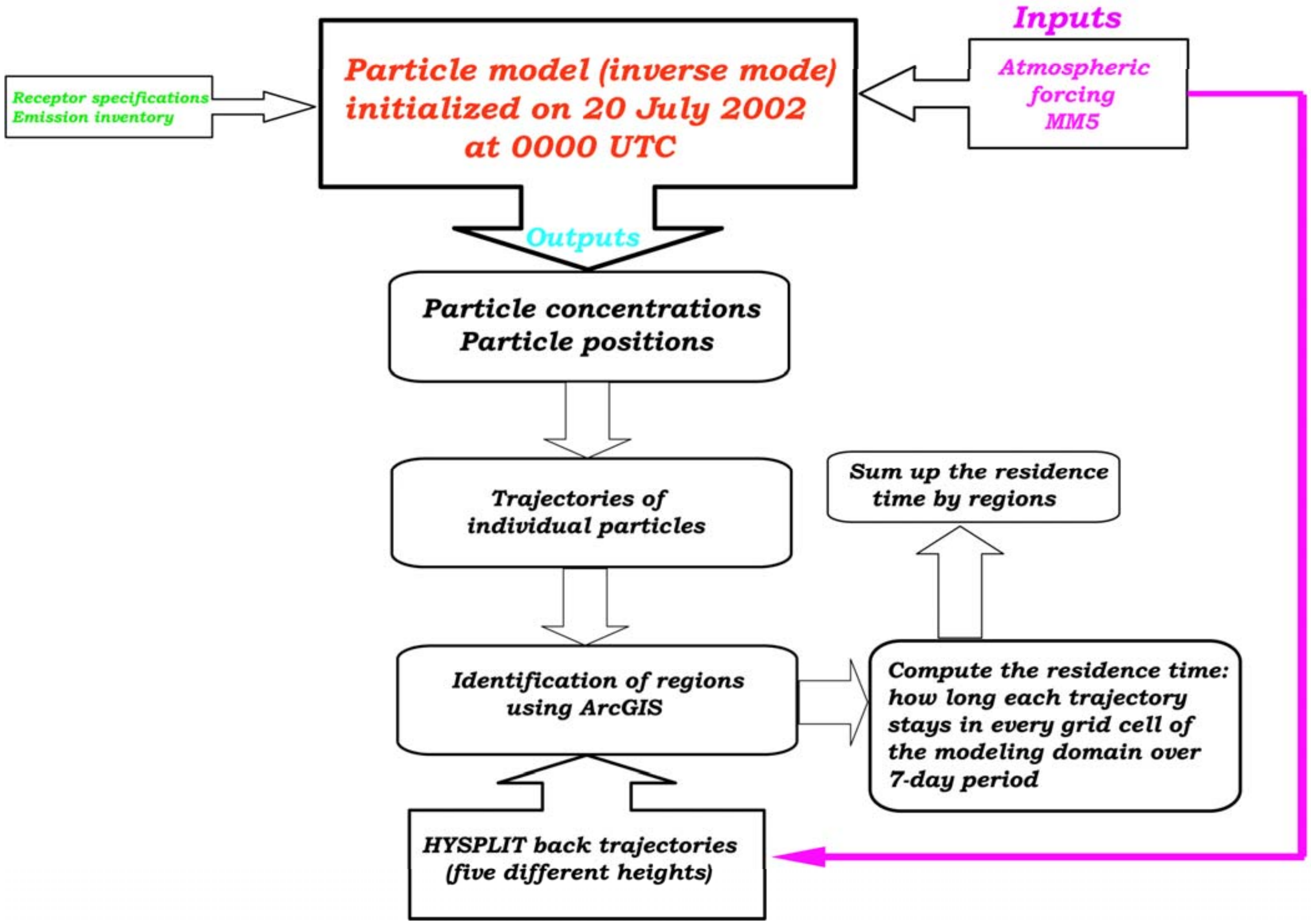


Figure 2. CMAQ-simulated 24-hr average SO_4^{2-}concentrations (µg m^{-3}) at BRIG (dashed) and GRSM (solid) from all regions R1-R7 shown in Fig. 1 for the four case periods.

Flowchart


Inputs
Receptor specifications
Emission inventory
Particle model (inverse mode) initialized on 20 July 2002 at 0000 UTC
Atmospheric forcing MM5
Outputs
Particle concentrations
Particle positions
Trajectories of individual particles
Sum up the residence time by regions
Identification of regions using ArcGIS
Compute the residence time: how long each trajectory stays in every grid cell of the modeling domain over 7-day period
HYSPLIT back trajectories (five different heights)

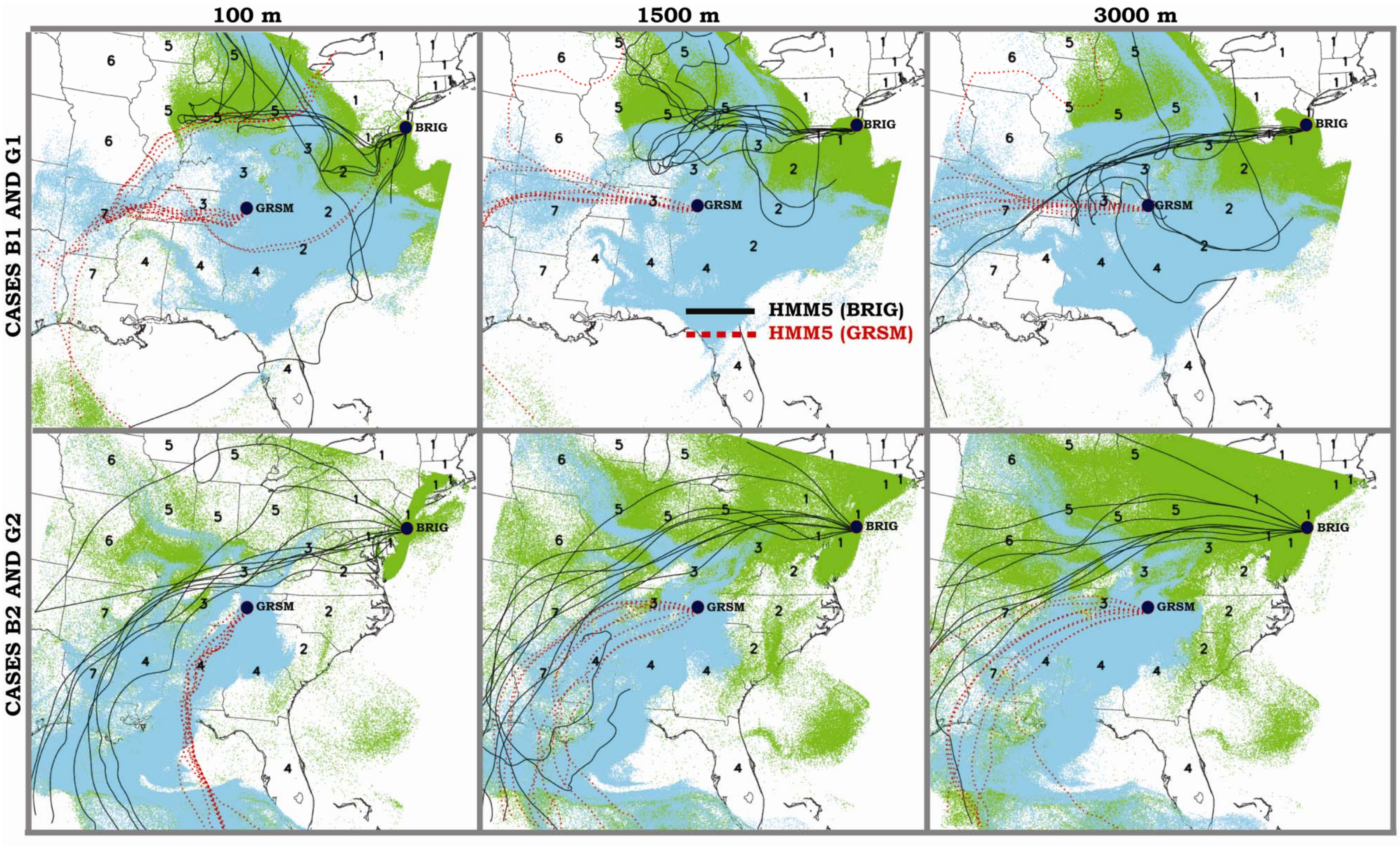
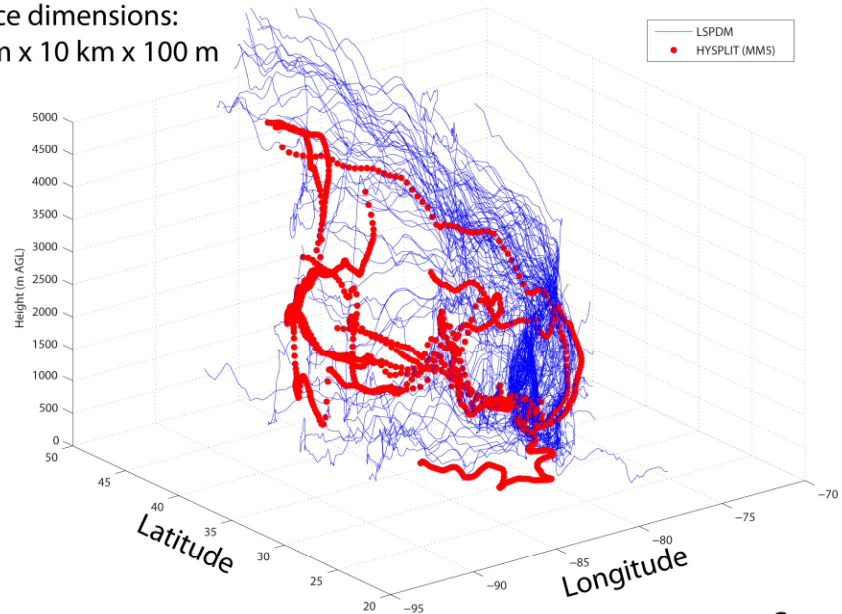
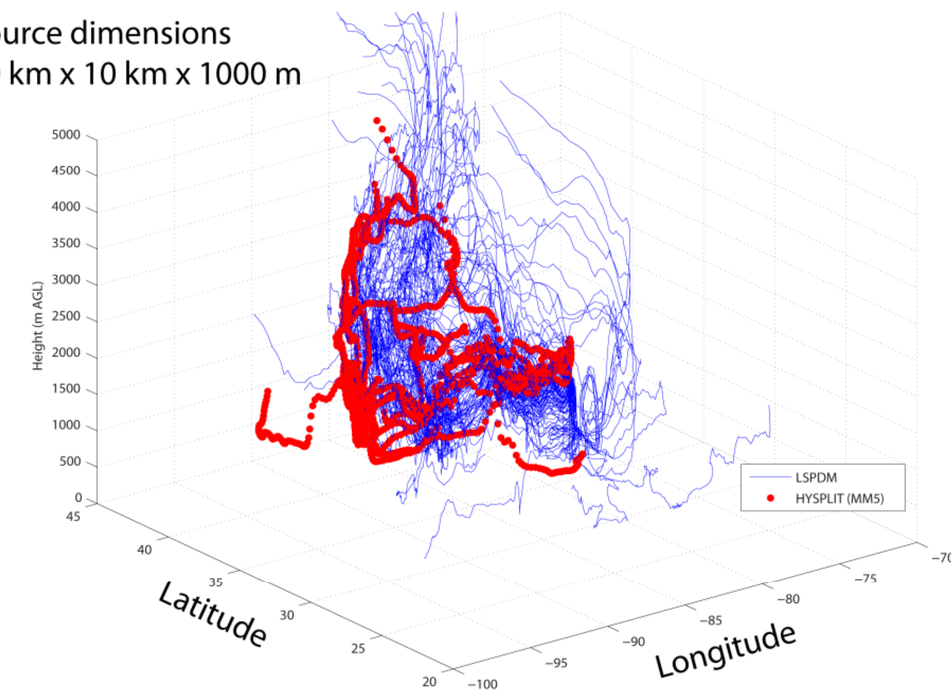


Figure 3. The spatial distribution of LSPDM particles from the baseline simulations (green from BRIG receptor and light blue from GRSM) at -168 hrs for cases B1 and G1 (top panel), and B2 and G2 (bottom panel). MM5-HYSPLIT (HMM5 = H^M used in the text) back trajectories from BRIG (solid black) and GRSM (dashed red) for 100 m, 1500 m, and 3000 m heights above ground are superimposed. Emission source region numbers and the receptor sites BRIG and GRSM are also shown in the figure. Note that LSPDM particles simulated using receptor depth 1500 m or less are shown in the figure under the 1500 column.

Source dimensions:
10 km x 10 km x 100 m



Source dimensions
10 km x 10 km x 1000 m



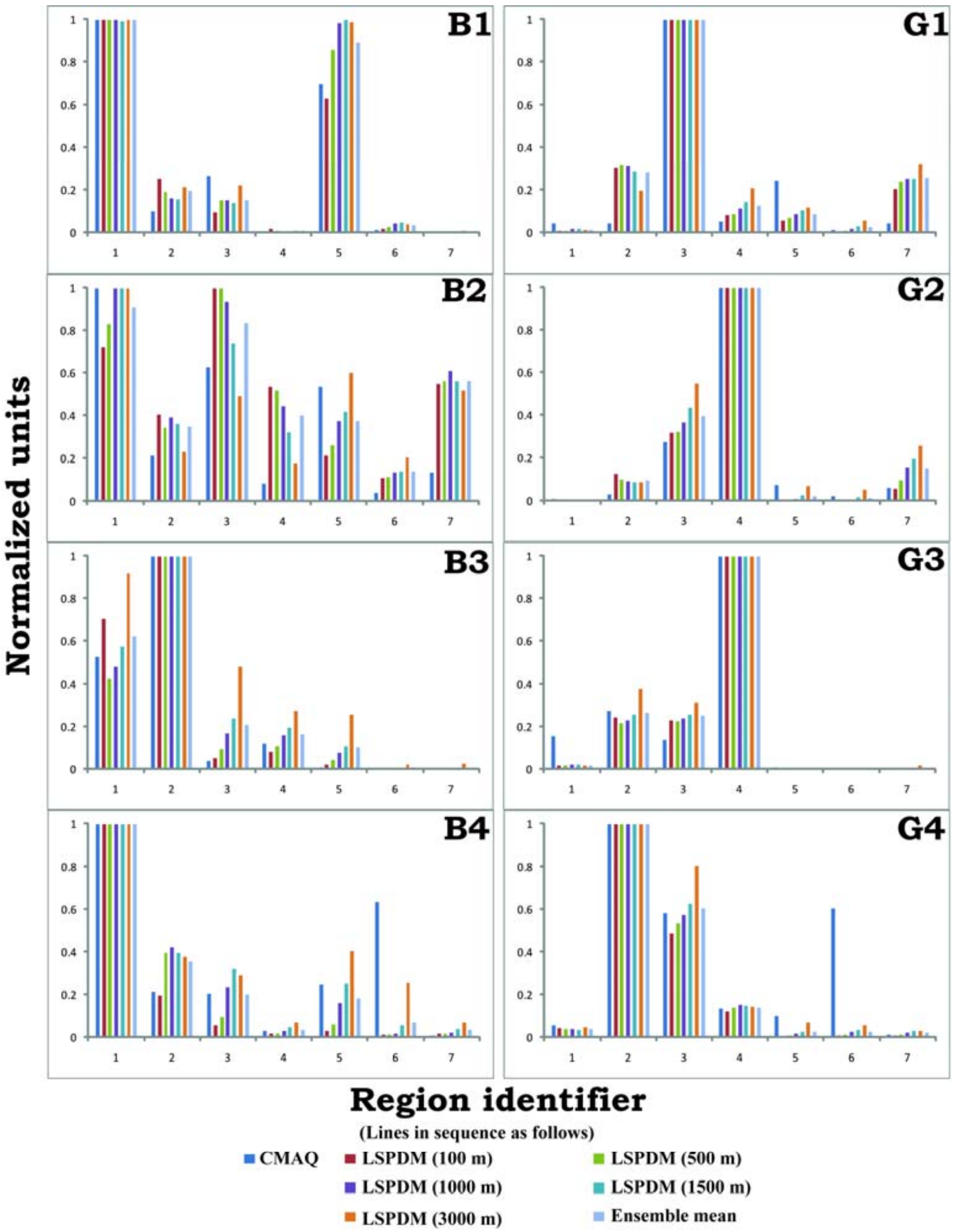


Figure 5. Histograms of normalized average residence times (y-axis) for each region obtained from the baseline 168 hr simulated LSPDM particle back trajectories for the BRIG (B1-B4; a,b,c,d) and GRSM (G1-G4; e,f,g,h) cases. CMAQ simulated 168 hr totals of 24-hr averaged SO_4^{2-} concentrations in the regions R1-R7 is normalized by their regional maximum. Lines in the figure indicate as follows: CMAQ, LSPDM (100 m), LSPDM (500 m), LSPDM (1000 m), LSPDM (1500 m), LSPDM (3000 m) and the total or ensemble mean (from the normalized pairs that are used in the computation of Overall[c] in Tables 2-5).

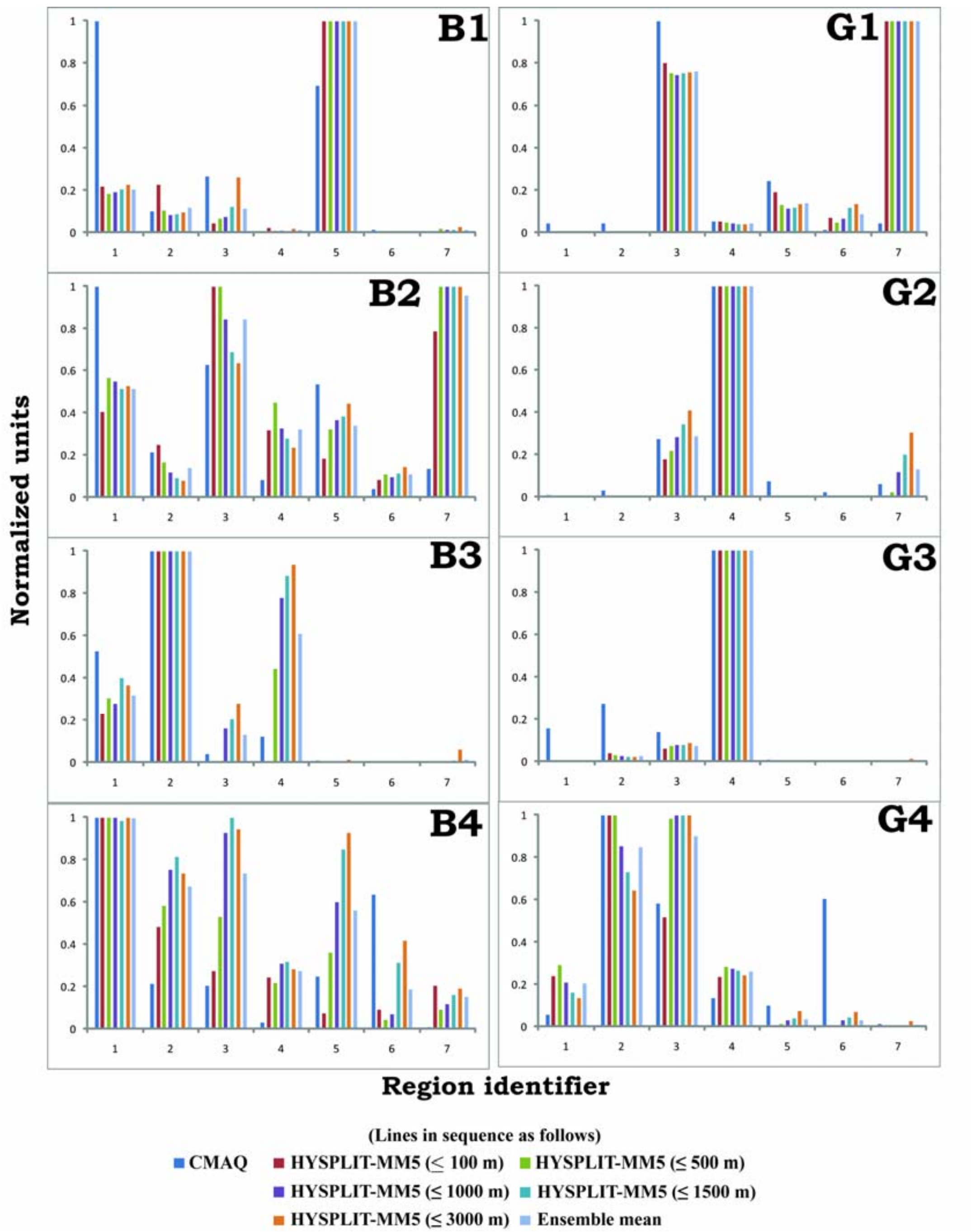
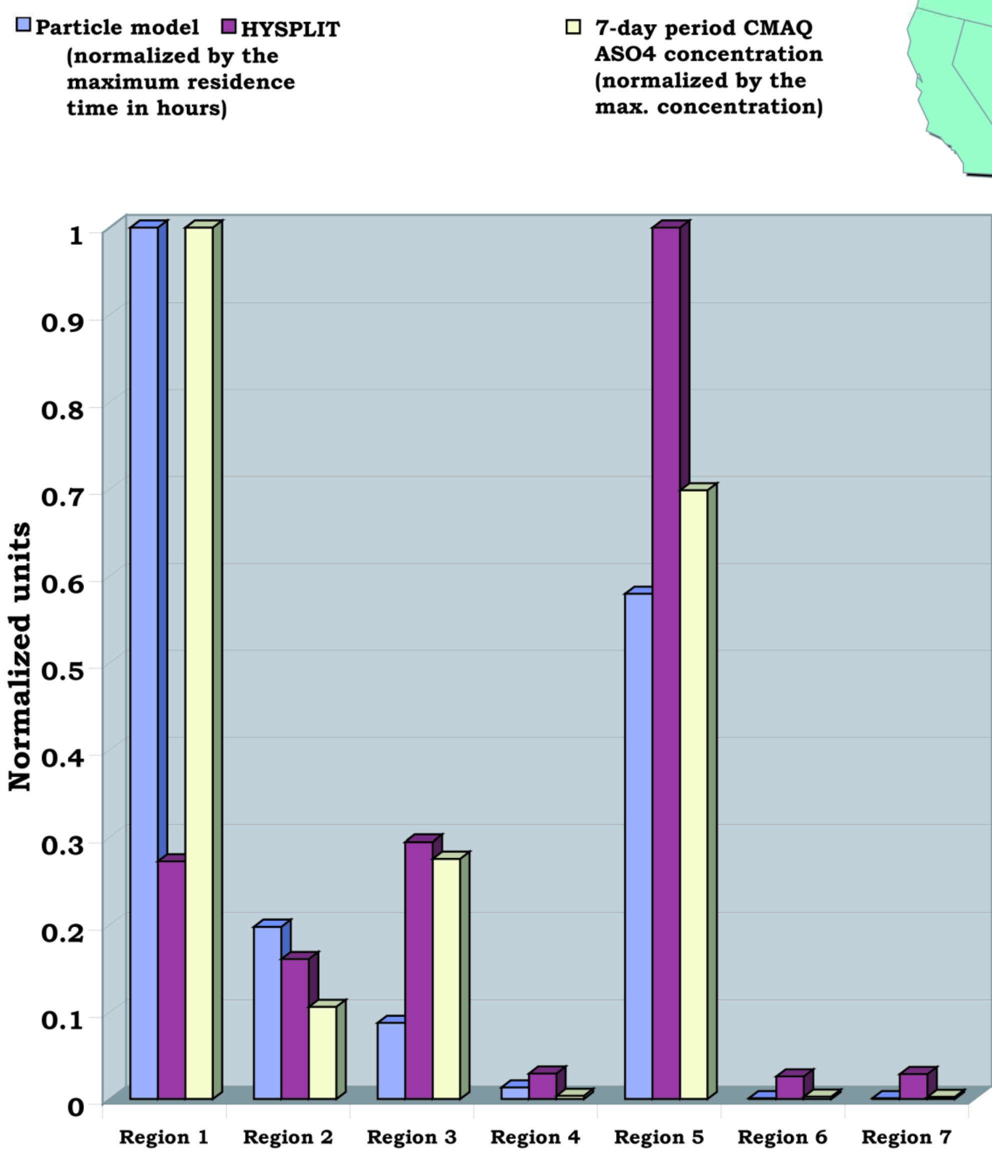
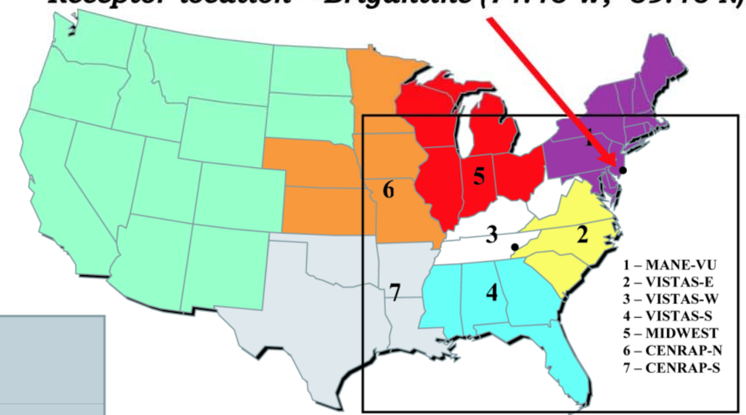


Figure 6. Histograms of normalized average residence times (y-axis) for each region obtained from the baseline 168 hr simulated HYSPLIT particle back trajectories (using MM5 inputs) for the BRIG (B1-B4; a,b,c,d) and GRSM (G1-G4; e,f,g,h) cases. CMAQ simulated 168 hr totals of 24-hr averaged SO_4^{2-} concentrations in the regions R1-R7 is normalized by their regional maximum. Lines in the figure indicate as follows: CMAQ, HYSPLIT (100 m), HYSPLIT (500 m), HYSPLIT (1000 m), HYSPLIT (1500 m), HYSPLIT (3000 m) and the total or ensemble mean (from the normalized pairs that are used in the computation of Overall[c] in Tables 2-5).

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

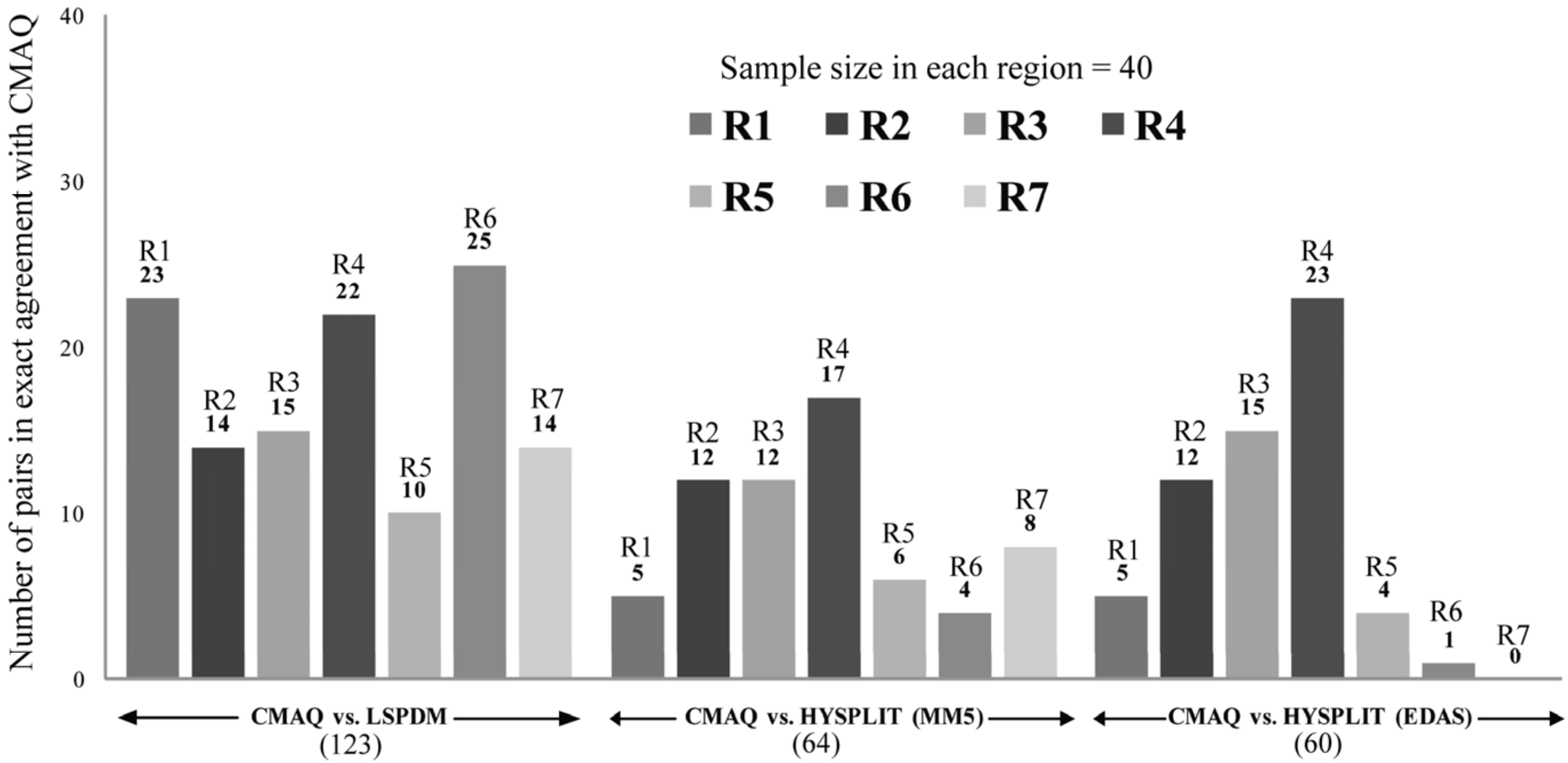
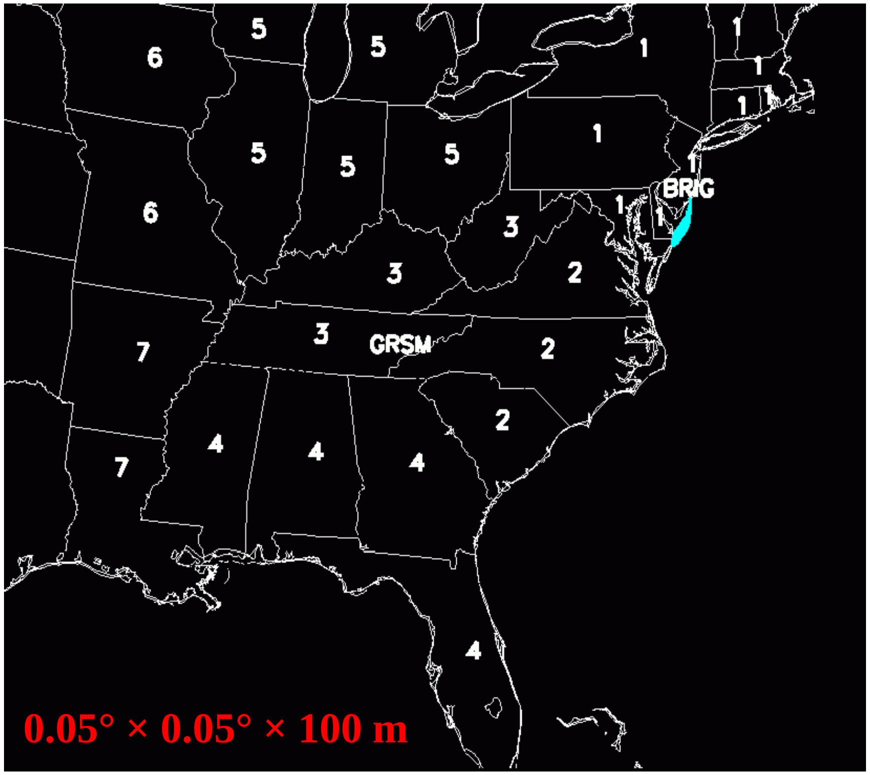
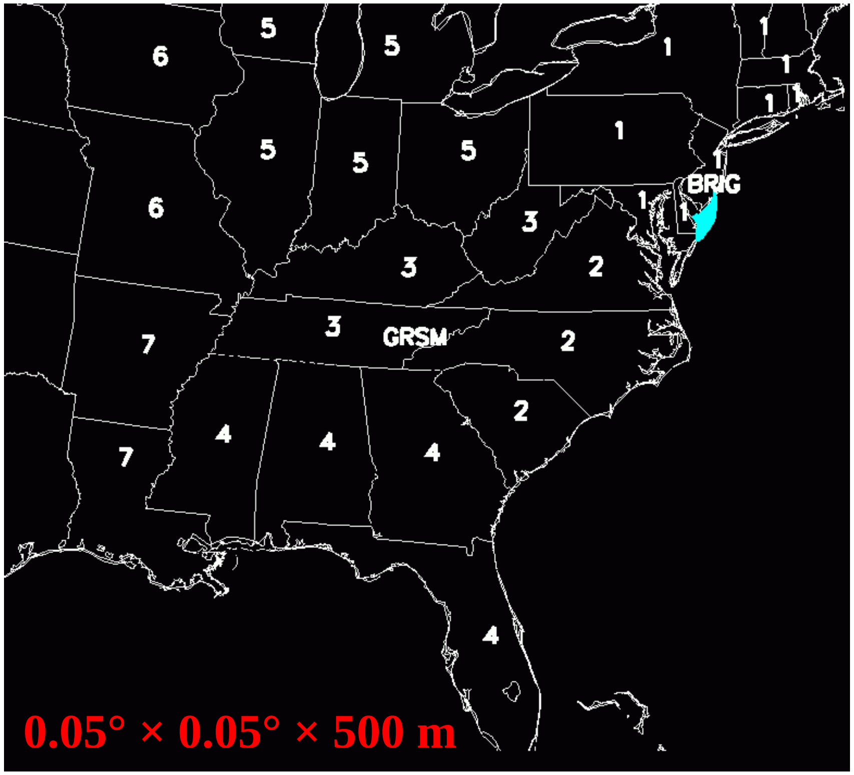


Figure 8. of the pairs of exact agreement for each emission source region R1-R7 between CMAQ and baseline-LSPDM (left), CMAQ and H^M(center), and CMAQ and H^E(right panel). A sample size of 40 (=4 cases × 2 receptors × 5 vertical depths) is used.

Animation of 12 hour particle positions obtained from the
Particle model backward (Inverse mode) simulations
and backtrajectories obtained from
HYSPLIT (**HY**brid **S**ingle-**P**article **L**agrangian **I**ntegrated **T**rajectory) model
7 days (168 h) backward
from 07/20/02 at 00 UTC – 8 PM EST on 07/19/02
to 07/13/02 00 UTC – 8 PM EST on 07/12/02





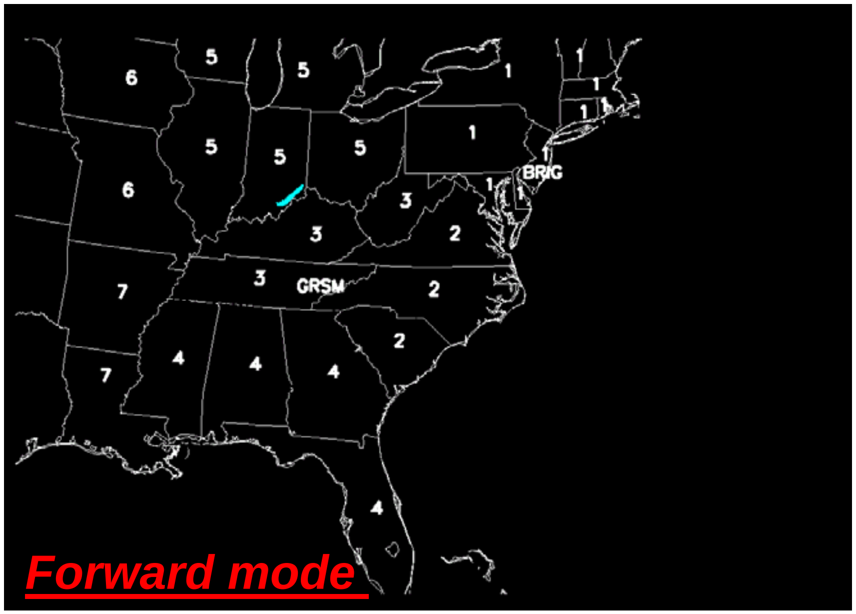
Area source (0.05º)

Receptor location :
BRIG: Brigantine (74.45º W, 39.46º N)
Particulate emission rate =
50 particles/30 sec (time step)

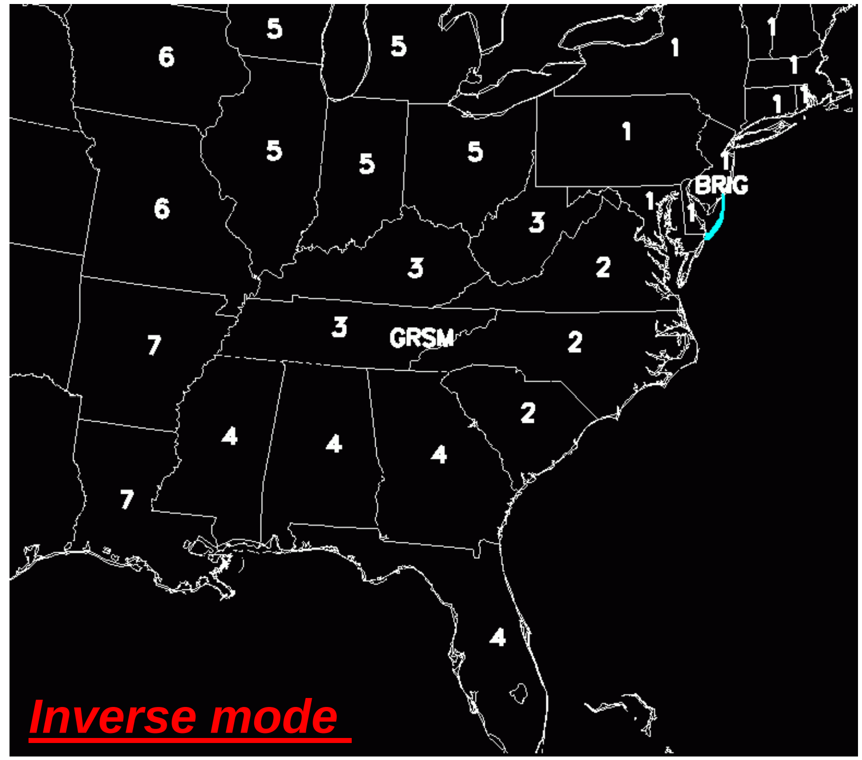
Atmospheric forcing: MM5 outputs (12-km grid resolution)

Forward and Inverse simulations

0.05° × 0.05° × 10 m
Source: Indianapolis

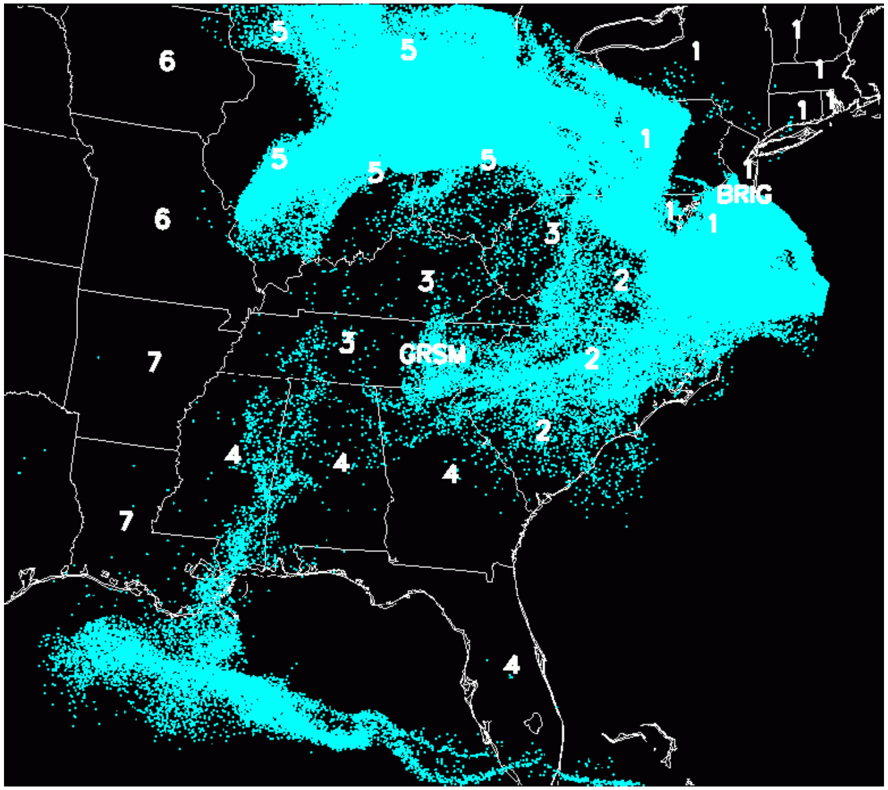


single source (a priori) and many receptors. Source in region 5 (state of Indiana) and BRIG and GRSM are the receptors.



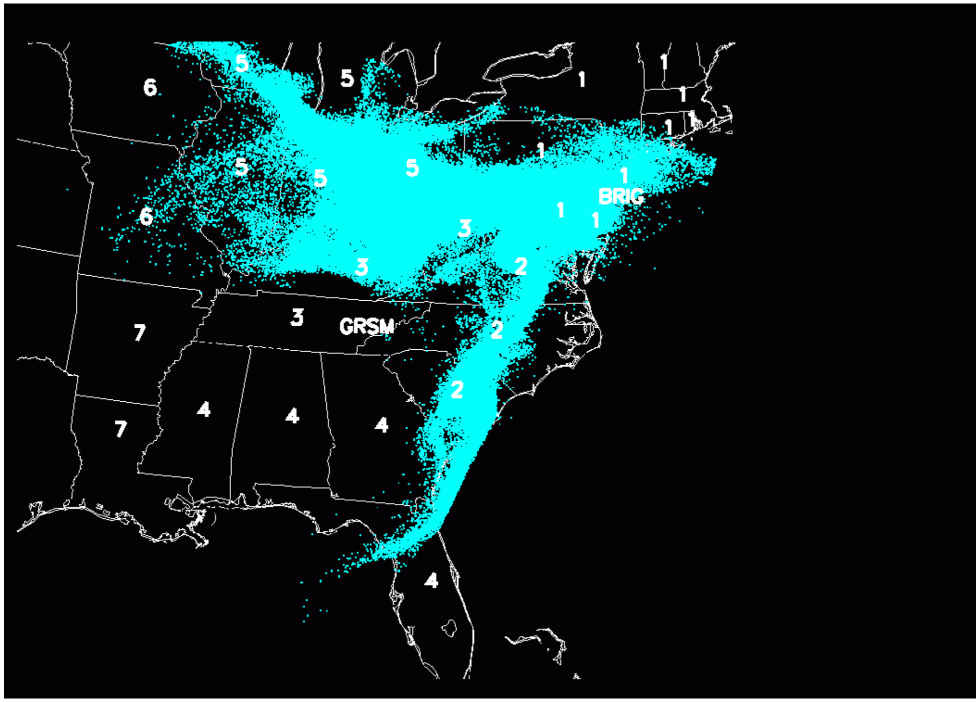
single receptor (BRIG) and many source elements (from the regions 1-7).

Developed inversion modeling tools confirm the particle dispersion in the forward mode (where the particles go to) with the regional identification of sources that contributes the receptor at BRIG using inversion approach (where the particles originate from).



Backward (inverse) simulations
20 July 2002 at 00 UTC - 144 hrs

Forward simulations
13 July 2002 at 00 UTC + 144 hrs



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.
- Currently, Lagrangian dispersion – Eulerian chemistry is a feasible tool.
- Next research and applications: linking Lagrangian dispersion with Lagrangian chemistry.
- Another advantage in using Lagrangian stochastic approach is possibility of either forward or inverse modeling.
- Inverse modeling offers enhancement of standard back trajectory and receptor modeling approach.