Correlating an Upwind Source-Footprint with Urban Emissions Data Using the MM5/MCIP/CALPUFF Modeling System

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ABSTRACT

A modeling system has been developed relying on plume diffusion theory to yield the upwind source area and emissions responsible for a measured downwind concentration. Three steps comprise this modeling strategy. Application of the MM5 meteorological model to yield a regional wind field, processing of the wind field through the Models-3/CMAQ meteorological processor (MCIP), inversion of the resulting wind field, and finally application of the CALPUFF puff dispersion model to the inverted wind field. In this manner, plume dispersion theory is applied to map the upwind pollutant source area (source-footprint) for a measured downwind concentration. This method has been applied to the Boston, MA area for a period in May of 1999 when the Urban Respiration and Trace Gas Metabolism project was conducting field studies in the south Boston area. An emission inventory was obtained from the Massachusetts Department of Environmental Quality and correlated with the inverted CALPUFF plume to yield the fractional source contribution of the downwind sources to a receptor in urban Boston, MA. The data indicate that 92% of the impacting emissions come from within a radius of 30 km and that over a 5 hour period emissions from Connecticut and Rhode Island also influenced the Boston area.

INTRODUCTION

Cities and their associated industrial areas are dynamic entities that consume and metabolize atmospheric trace gases in daily and seasonal cycles. Evaluating the metabolites of urban areas both quantitatively and qualitatively for emission inventory purposes is therefore a complex task. The Urban Metabolism and Trace Gas Respiration project funded by the National Aeronautical and Space Administration (NASA) is studying urban and industrialized areas as entities that consume, metabolize and respire a wide range of trace gases. As part of this project, an urban source-footprint modeling system is being developed to predict upwind pollutant source areas from downwind concentration measurements. These upwind source areas are then correlated with emission inventories and/or real-time emission and tracer data to yield insights into emission sources contributing to a downwind receptor concentration. Thus, this is a methodology for directly evaluating the impacts of emissions on downwind receptors for a given meteorological situation.

Plume diffusion modeling along a forward trajectory maps out the distribution of pollutant concentrations due to an upwind source. Application of plume diffusion theory along a back-trajectory yields the upwind source distribution (source-footprint) affecting a receptor at the trajectory initial point. Thus, our approach is to use available modeling systems to derive a detailed wind field, and then apply the CALPUFF model in reverse along back trajectories. The results yield the upwind source distribution of sources affecting a downwind receptor.

Three components comprise this source-footprint modeling strategy: 1) Mesoscale modeling of the regional wind field, 2) Application of MCIP, the Models-3/CMAQ meteorological processor, then inversion of the resulting wind field, 3) Application of the CALPUFF plume dispersion model to the inverted wind field. The MM5 prognostic meteorological model (Dudhia et al., 1994) provides detailed hourly wind fields to the MCIP (Byun et al., 1999) model utilized here primarily to reformat the MM5 output for input into CALPUFF (Scire et al., 1999). Finally, the winds are inverted and the CALPUFF model is applied. By applying CALPUFF to the inverted wind field, the resulting plume trajectory and puff dispersion indicates the upwind pollutant source area affecting a downwind receptor. Correlation of this source-footprint with existing emissions data yields the fractional contribution of the applicable upwind emissions to a downwind receptor. The source-footprint is correlated with emissions data collected from a field study conducted May 1999 in Boston, Massachusetts and with a gridded 1988 emission inventory obtained from the Massachusetts Department of Environmental Quality.

DOMAIN AND METEOROLOGY

The MM5 meteorological model was applied to simulate the wind field for the Northern New England coast for May 24-26, 1999; the period during which extensive measurements of NO, NO2, O3, CO2, and CO was carried out throughout the South Boston area. A four-nested domain was utilized where grid resolutions were 27km, 9km, 3km, and 1km. The 3km domain encompassing Massachusetts, Connecticut, Rhode Island, and parts of New Hampshire and Maine was chosen as the study area. Figure 1 depicts the overall domain, and figure 2 depicts the 3km domain.

A sodar was operating at the Massachusetts Institute of Technology (MIT) near downtown Boston yielding a vertical profile of wind speed, wind direction, and other meteorological statistics with a vertical resolution of 7 m and maximum height of 280 m. Figure 3 compares the MM5 predicted wind field with the sodar data at the MIT location for May 25, 1999 at 5pm EST. The MM5 data tend to be smooth compared to the sodar but both profiles exhibit the surface southwest winds that were reported for the day by Logan International Airport. The sodar was situated in an urban area with a tall building directly to the southwest, which thus influenced the wind field by decreasing the wind speed and skewing the wind direction at approximately the 80 m height.

The MM5 wind field was also compared with radiosonde (raobs) data archived by the National Climatic Data Center (NCDC) and the Forecast Systems Laboratory (FSL). Figure 4 depicts vertical profiles of wind direction and wind speed for MM5 and the raobs data at Chatham, MA at 7pm EST May 25, 1999. Wind speeds are similar up to a height of approximately 400 m, then the raob data exhibit increasing winds vertically in a logarithmic profile while the MM5 winds remain approximately constant with height. Wind direction data are very similar between the two sounding indicating that winds were from the southwest.
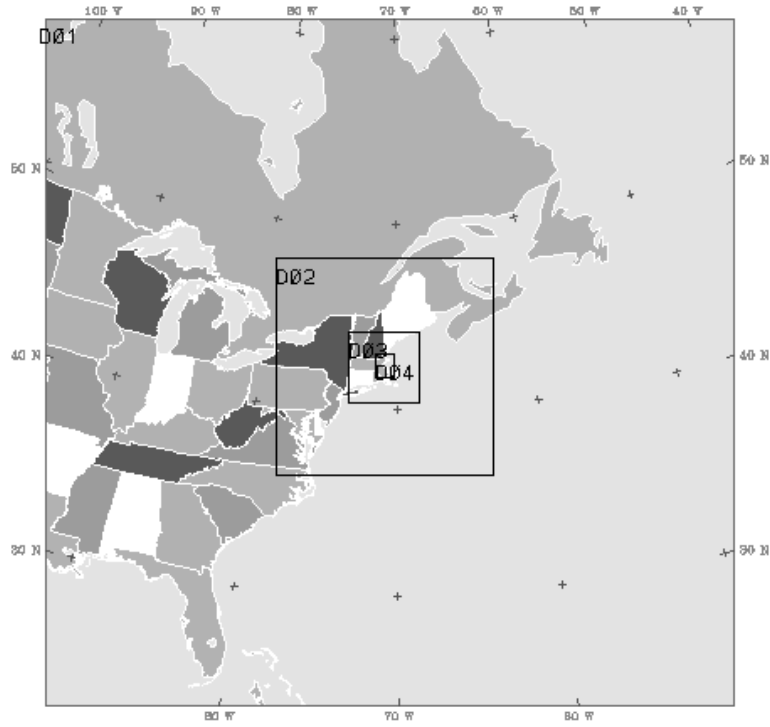
Figure 1. 27 km MM5 Model Domain for Northern New England.

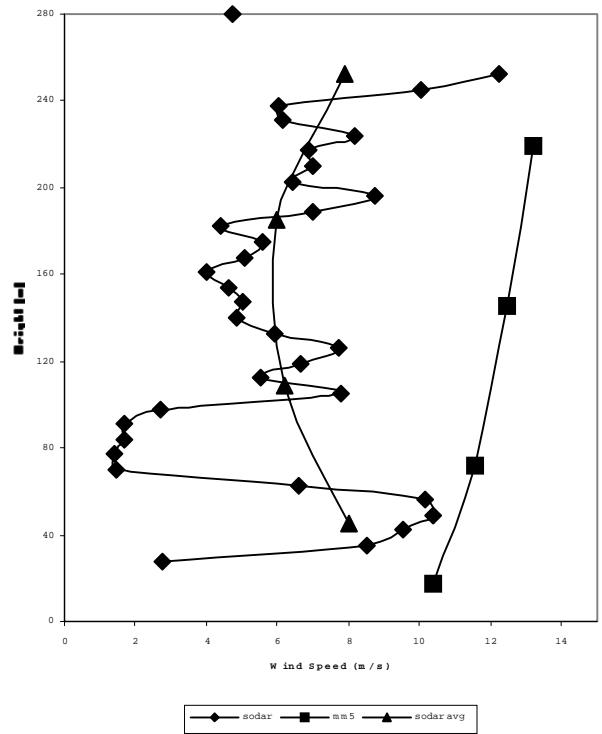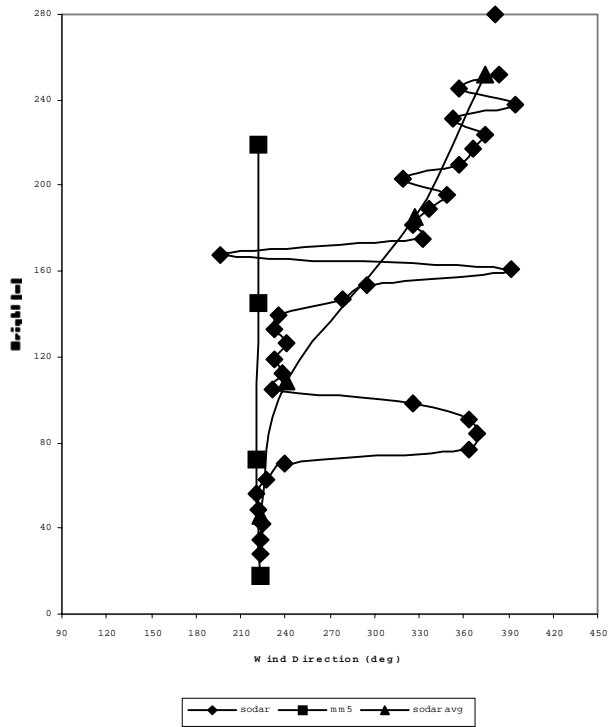Figure 2. 3 km MM5 Model Domain for Northern New England.

Figure 3. Comparison of Sodar and MM5 (a) wind direction and (b) wind speed at MIT on May 25, 1999 at 5pm EST.
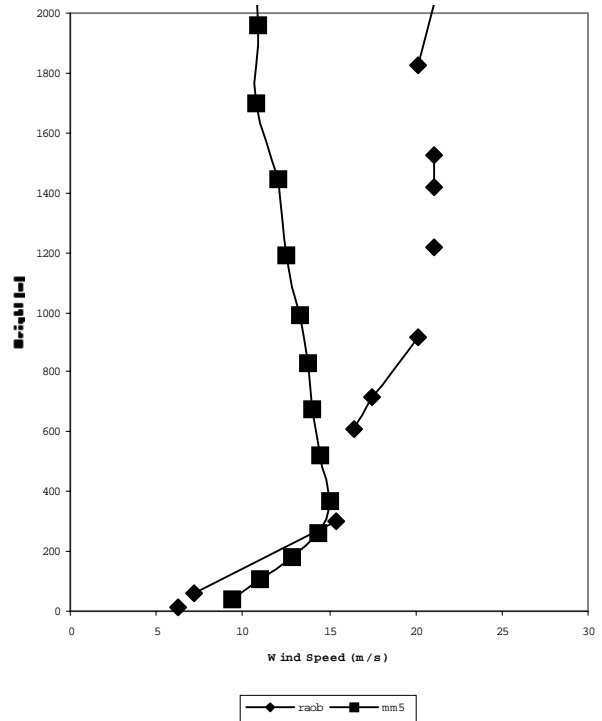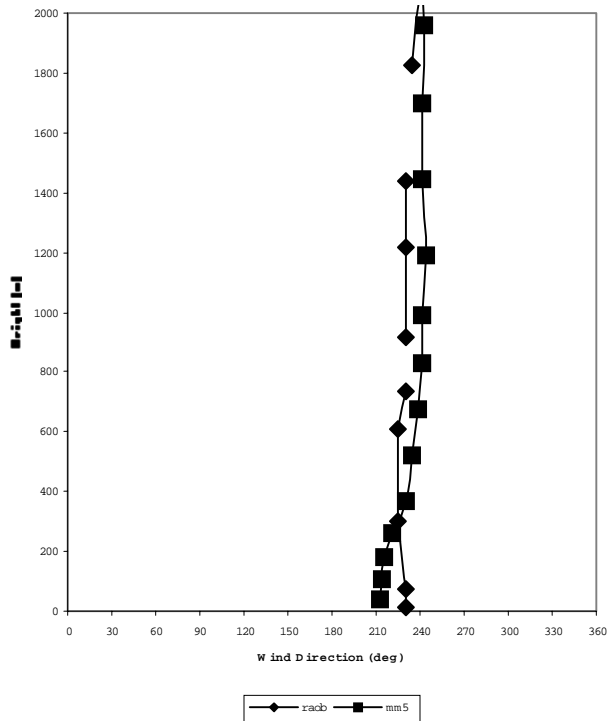

Figure 4. Comparison of MM5 and NCDC/FSL Radiosonde archived (a) wind direction and (b) wind speed at Chatham, MA on May 25, 1999 at 7pm EST.

EMISSIONS DATA

1) Gridded Emission Inventory Data

The Massachusetts Department of Environmental Quality provided a 1988 5 km gridded emission inventory suitable for the carbon-bond IV chemical mechanism. Since we are not yet at the point where we can validate pollutant source strength, these data are used as an indicator of the spatial distribution of emissions within Boston and its surrounding areas. The emission inventory data are normalized by the total emission rate and the assumption made that pollutant source locations and relative strengths have not changed appreciably in the previous 11 years. Data for June 21, 1988 (Tuesday) in particular were extracted from the emission inventory to coincide as closely as possible with the May 25, 1999 (Tuesday) field data. Processing was required to merge the area and point source emission data, and to re-grid the 5km data to the 3 km MM5 grid. NOx (NO + NO2) was chosen as the pollutant of interest. Figure 5 illustrates the normalized distribution of pollutants across the domain from the gridded emission inventory for point and area sources used to represent May 25, 1999 at 5 PM EST.
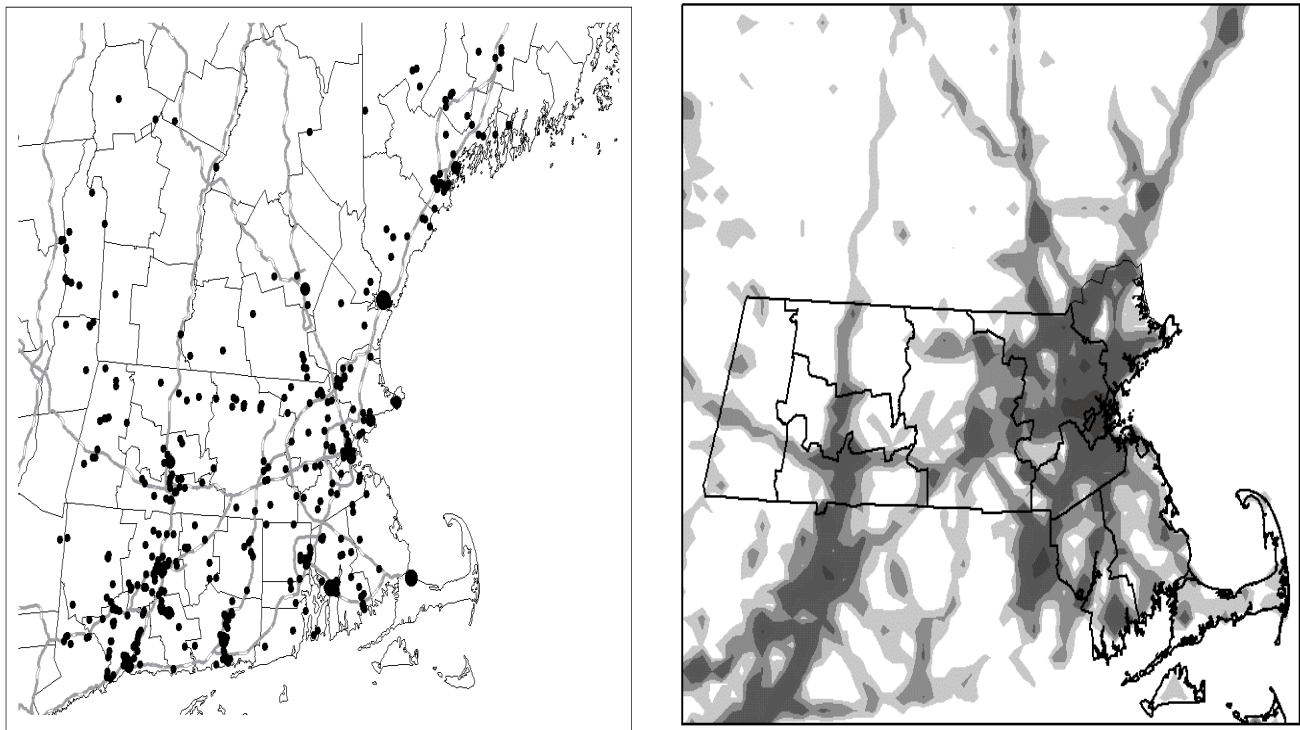

Figure 5. NOx (a) Point and (b) Area emission inventory data for New England applied to May 25, 1999 at 12 PM.

2) Field Measurements

A 10 day field study was conducted in May of 1999 in the Boston, Massachusetts areas of Dorchester and Roxbury. The measurement region covered an area 4 km by 6 km; approximately the area of one to two standard grid modeling cell. An instrumented mobile laboratory was deployed containing a tunable diode laser (TDL) system measuring NO and NO2 at 1 Hz, a Licor NDIR CO2 instrument, a TSI condensation nuclei instrument for particulates detection, a uv adsorption ozone instrument, and an Eppley total ultraviolet radiometer. See Lamb et al. (1995), and Zahniser et al. (1995) for further details regarding the real-time TDL system.

"Mapping" of the study area was accomplished by driving the city streets and highways with the mobile laboratory continually taking data. The day of May 25, 1999 (Tuesday) was chosen as a particular day of interest because a tracer test was conducted that day, extensive data were obtained both in rush-hour traffic and off-hour traffic, and data were obtained both in crowded city streets and park settings. The data contains many sharp peaks that correlated with CO_2 indicating that the peaks were due to discrete nearby sources such as individual automobiles or trucks directly affecting the sensor. Thus, filtering was applied to the data to extract the slowly varying background concentrations and averaging done to yield approximately one hour averages of NOx. These one hour averages were used to represent receptor concentrations for the CALPUFF model.

INVERSE MODELING APPROACH

CALPUFF was applied to simulate the upwind source probability distribution for a receptor by application of plume dispersion theory along a back trajectory. South Boston was chosen as the receptor of interest because of the extensive mapping data available from the field study. Figure 6 depicts a backward plume originating from South Boston May25, 1996 at 5 PM EST. This backward plume depicts the probability source distribution for Boston for pollutants undergoing advective and dispersive processes during the previous 5 hours. The winds were steady from the southwest thus causing a narrow plume and indicating that pollutants could have traveled from Connecticut and Rhode Island during the previous 5 hour period.
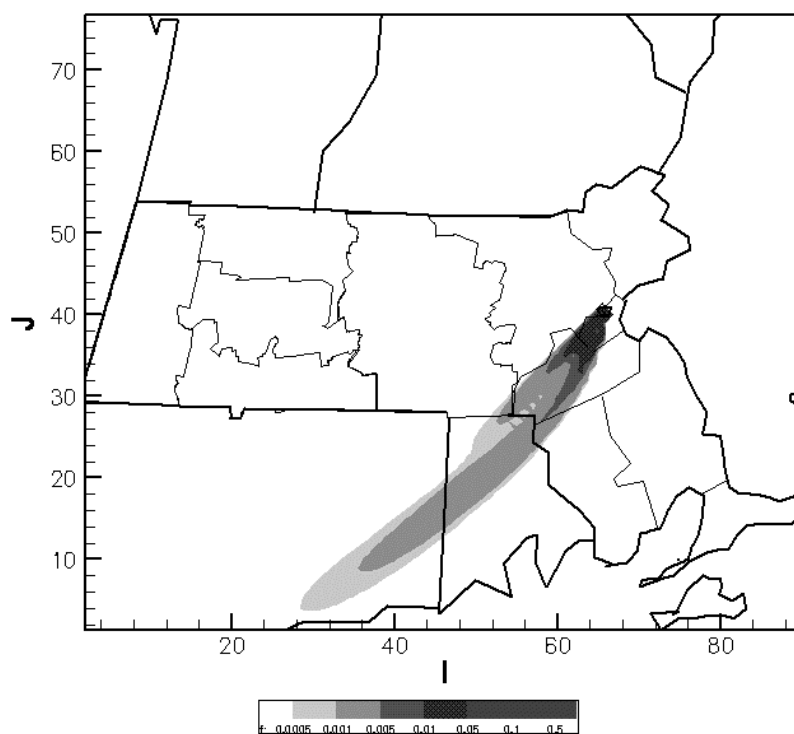

Figure 6. Upwind source area influencing Boston, MA at 5pm EST May 25, 1999.

To correlate the source-footprint with an emission inventory, knowledge of travel time is necessary because concentrations at a receptor at a particular time t are due to emissions upwind at an earlier time (t-travel time). Furthermore, each grid in the domain can be impacted by more than one puff; thus CALPUFF was modified to include a procedure to compute the average travel time (t_{avg}) for a puff, weighted by its concentration contribution, to travel from grid i,j to the receptor for each grid of the domain, for every time t:

$$t_{avg}(i, j, t) = \frac{\sum_{k=1}^{N} T(i, j, t, k) * C(i, j, t, k)}{C_T(i, j, t)} \qquad (1)$$

Where,

N = Number of puffs emitted from the receptor from the beginning of the simulation to time t.
$T(i,j,t,k)$ = Travel time of puff k from the receptor to the grid location i,j, at time t.
$C(i,j,t,k)$ = Concentration that puff k contributes to grid location i,j, at time t.
$C_T(i,j,t)$ = Total concentration from all puffs at grid location i,j, at time t.

Figure 7 depicts the gridded hourly average pollutant source travel times for 5 PM EST, May 25, 1999 for Boston, MA.
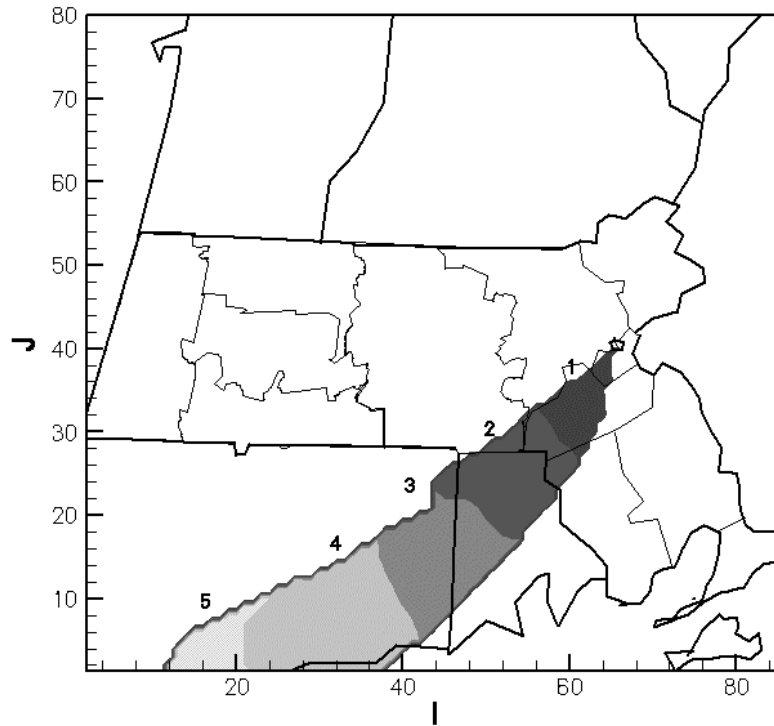

Figure 7. Average pollutant source travel times in relation to Boston, MA at 5 PM EST, May 25, 1999.

Once the average travel time from emission point i,j to the receptor is known (i.e. t_{avg}), then the emission rate at grid i,j that contributed to the receptor concentration is simply the emission rate at t-t_{avg}. In this way time varying emission inventories can be investigated with this method. The final result is a two-dimensional footprint of the hourly emission inventory for the species of interest in which each grid point contributed to some extent to the concentration at the receptor. The fractional contribution of a particular grid point emission to the concentration recorded at the receptor can then be calculated by:

$$f(i, j, t) = \frac{Emis(i, j, t - t_{avg}(i, j, t)) * Conc(i, j, t)}{\sum_{i=1}^{R} \sum_{j=1}^{C} Emis(i, j, t - t_{avg}(i, j, t)) * Conc(i, j, t)} \qquad (2)$$

Where,

　　C, *R* = Number of columns and rows in the domain.

　　Emis(i,j,t-t$_{avg}$(i,j,t)) = Emission rate from the emission inventory contributing to the receptor concentration at time t.

　　Conc(i,j,t) = Concentration (as an indicator of probability) from the backward CALPUFF plume.

　　Figure 8 depicts the fractional source contribution of NOx on the receptor concentrations at Boston, MA at 5 PM EST May 25, 1999.
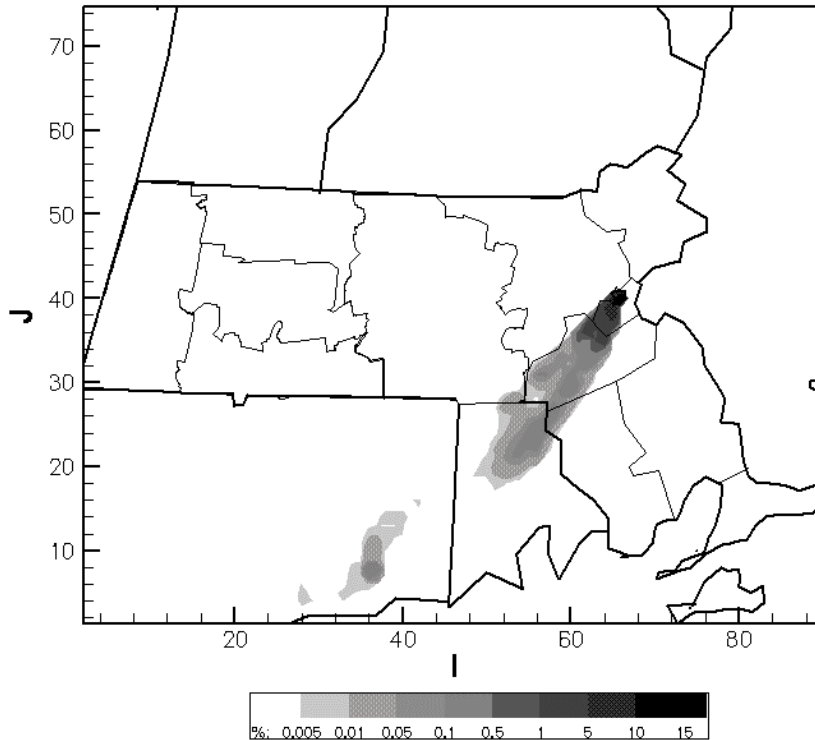

　　Figure 8. Fractional source contributions of NOx on the receptor concentrations at Boston, MA at 5 PM EST May 25, 1999.

　　Further deductions regarding the area source contribution can be obtained by tracking radial upwind areas contributing to the overall fractional contribution. In this manner, fractional source contribution from 0-15 km, 15-30 km, 30-75 km, and 75-150 km can be determined. Table 1 lists the percent contribution of emissions to the receptor concentration at Boston for May 25, 1999 at 5 PM EST for each of the radial distance ranges. Within a five hour upwind period, 93% of the emissions contributing to the receptor concentration are within 30 km of Boston. Figure 9 shows the fractional source contribution of emissions within approximately 75 km of the receptor at Boston, MA.

Table 1. Percent Contribution of Emissions to the Boston Receptor at Incremented Radial Distances.

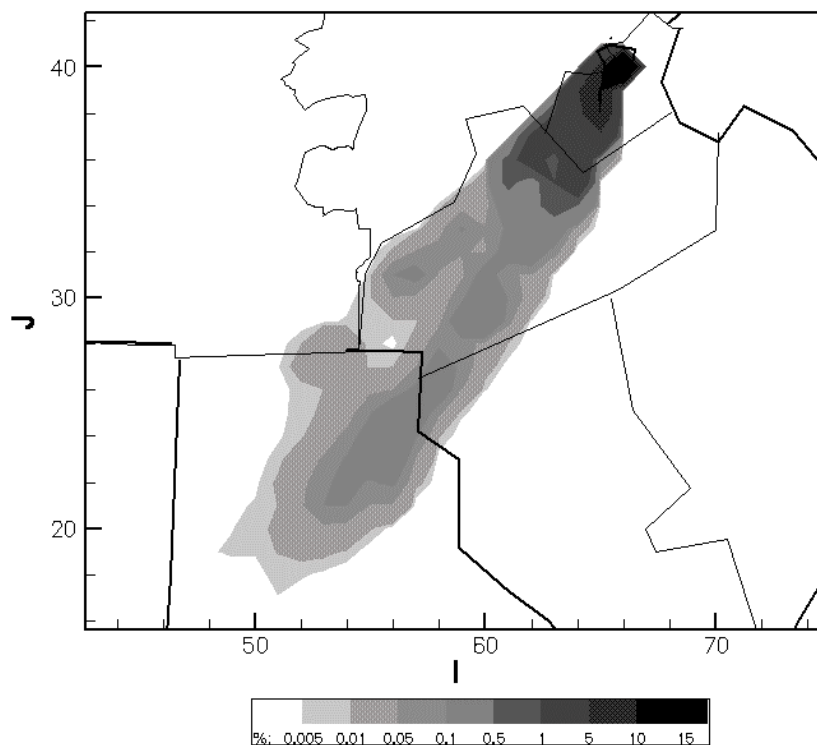| Radial Number of Grids	0 - 5	5 - 10	10 - 25	25 – 50
Radial Distance (km)	0 - 15	15 - 30	30 - 75	75 – 150
Contribution (%)	83.1	9.4	6.0	1.5

Figure 9. Fractional source contributions of NOx within approximately 75 km of the receptor, Boston, MA at 5 PM EST May 25, 1999.

SUMMARY

The source-footprint modeling system is a simple means to identify upwind source areas responsible for downwind pollutant concentrations. By linking puff dispersion with emission inventories, the picture of the resulting upwind source area takes into account distance and source strength and thus yields a fine scale structure where specific source influences become more obvious. In this application the system identified the upwind area extending from Boston southwest to eastern Connecticut as the area responsible for regional pollutants impacting Boston, MA when winds prevail from the southwest. Further investigation of this methodology is necessary to determine the scale of its applicability. Comparison with other footprint type methodologies such as inverse modeling and/or stochastic Lagrangian backward trajectory methods is also underway.

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