J3.4 EVALUATION OF $PM_{2.5}$ SOURCE REGIONS OVER THE MISSISSIPPI GULF COAST USING WRF/HYSPLIT MODELNG APPROACH

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ABSTRACT

Fine particulate matter ($PM_{2.5}$) is formed by precursors such as sulfur dioxide, nitrogen oxides, volatile organic compounds, and trace metals, which are emitted largely from intense industrial operations and transportation activities. $PM_{2.5}$ is known to cause serious respiratory problems. Evaluation of source regions and assessment of the contribution of various sources in the Mississippi Gulf Coast region will be useful for implementation of regulatory and mitigation measures.

In the present study, output from the HYbrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) Model driven by the Weather Research and Forecasting (WRF) Model is used as a tool to assess source location, transportation trends, and the extent of contribution to $PM_{2.5}$. Meteorological and air pollution ($PM_{2.5}$ sulfate) observations were collected during a joint atmospheric dispersion field experiment in summer 2009 at two locations in southern Mississippi.

The WRF model was used to simulate meteorological parameters at a resolution of 4 km and was designed to have three two-way interactive nested domains with horizontal resolutions of 36, 12 and 4 km, and the inner-most domain covered the region of interest. The vertical resolution included 43 levels, with 33 levels confined to below 500 hPa to simulate boundary layer flow characteristics. The model was integrated for 72 hours starting from 00UTC on 16, 17 and 18 June 2009. The initial and boundary conditions were adopted from National Centers for Environmental Prediction Final Analyses (NCEP FNL) data available at one degree horizontal resolution. The model derived meteorological fields were validated with in-situ observations collected at the two locations.

The HYSPLIT model was integrated with WRF model-derived meteorological fields to identify the source location using backward trajectory analysis. The backward trajectories were plotted for every one hour with different heights in the mixed layer. Trajectories were plotted for a 24-hr period starting from two observations, and a cluster analysis method was used to estimate the probable contribution from each source. As a second step, forward trajectories were plotted with different identified source locations using data from observations at elevated point sources. Concentration levels were calculated and compared with in-situ observations to examine and assess possible relative contributions from different sources.

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1. INTRODUCTION

Contamination of the environment due to pollution from anthropogenic sources is a serious concern due to its potential impact on human and ecosystem health. Observed patterns of pollutant deposition indicate their transport and dispersion at local, regional and global spatial scales. The atmosphere may be considered as a "shared resource" to carry pollutants that have the potential to affect many ecosystems. Sulfur and nitrogen oxides, emitted into the atmosphere primarily from fossil fuel combustion, react in the atmosphere to form compounds that can be transported long distances and subsequently deposited as particulate matter (i.e., sulfates, nitrates) (Myles et al. 2009). Fine particulate matter ($PM_{2.5}$) is a mixture of solid and liquid atmospheric particles of less than 2.5 µm diameter which are formed from gaseous precursors like SO_2 and NO_x that mainly originate from anthropogenic sources such as thermal power plants, automobile emissions, and industrial processes. $PM_{2.5}$ in the ambient atmosphere can degrade air quality, reduce visibility, and contribute to respiratory illnesses.

Study of atmospheric dispersion is essential for air quality management and environmental impact assessment. Atmospheric dispersion models are used to compute the spatio-temporal air concentrations and depositions of given contaminants based on meteorological fields and source characteristics. Conventional methods use simple Gaussian plume models for air quality assessments, which do not account for the spatial and temporal variations in wind field and eddy diffusivity (Hanna et al. 1982). Recent advanced models based on Lagrangian methods consider the variability in wind field as well as the eddy diffusivity in downwind regions by coupling with meteorological models and using surface layer turbulence parameterizations. This approach is preferred when the region of interest extends up to hundreds of kilometers from the emission source where air pollutants are influenced by mesoscale flow fields. Coastal regions are particularly complex as topographic variations and land-sea interactions govern local flow. Dispersion in coastal zones is influenced by development of mesoscale circulations as a result of differential heating of land and water surfaces (Pielke et al. 1991; Lu and Turco 1995).

Mesoscale atmospheric models are widely used for complex terrain to capture the complex flow and meteorological parameters essential in dispersion estimations (e.g. Physick and Abbs 1991; Kotroni et al. 1999; Wang et al. 2004). Sulfur dioxide (SO_2) concentrations from major elevated sources in Southern Florida were studied with a coupled dispersion model by Segal et al. (1998) which showed that local sea-breeze circulations led to complex dispersion patterns and higher concentrations on the eastern coast of the USA. Moran and Pielke (1996) used a coupled mesoscale atmospheric and dispersion modeling system for tracer dispersion over complex topographic regions. Jin and Raman (1996) studied dispersion from elevated releases under the sea-land breeze flow using a mesoscale dispersion model which included the effects of local topography, variability in wind, and stability.

The Mississippi Gulf Coast is a typical coastal urban terrain that is experiencing multiple pollution problems due to changes in air and water quality and widespread disruption of hydrology as a consequence of human activities such as oil and gas development, thermal power plants, and transportation. High concentrations of precursor pollutants are found generally in the winter season under prevailing high pressure conditions and mesoscale circulations. Atmospheric dispersion over the Mississippi Gulf Coast region using an integrated mesoscale weather prediction and atmospheric dispersion models was studied by Anjaneyulu et al. (2008, 2009) and Challa et al. (2008, 2009). In this work, a numerical modeling approach has been adopted to examine environmental SO_2 and NO_2 concentrations from some significant elevated sources near the Mississippi Gulf Coast. The HYbrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model was used to simulate dispersion in the coastal environment. Meteorological fields for the study period were predicted by using the Weather Research and Forecasting (WRF) mesoscale model (Skamarock et al. 2008). We used applications of HYSPLIT driven by WRF to assess the source location, transportation trends, and extent of contribution to $PM_{2.5}$ using meteorological and air pollution ($PM_{2.5}$ sulfate) observations that were collected during the Mississippi Coastal Atmospheric Dispersion Study (MCADS), a joint Jackson State University Trent Lott Geospatial Visualization Research Centre and NOAA Air Resources Laboratory summer 2009 field experiment.

2. MODELS, DATA, AND METHODOLOGY

2.1 Description of Atmospheric Model

The Advanced Research version of WRF (ARW) was used to produce atmospheric fields at a high resolution over the study region. This model system has versatility to choose the domain region of interest, horizontal resolution, and interactive nested domains with various options to choose parameterization schemes for convection, planetary boundary layer (PBL), explicit moisture, radiation, and soil processes (Skamarock et al. 2008). The Advanced Research version of WRF is suitable for use in a broad range of applications, across scales ranging from meters to thousands of kilometers.

2.2 Description of Air Quality Model

HYSPLIT (rev. 4.9) was used to compute simple air parcel trajectories for complex dispersion and deposition simulations. HYSPLIT computes the advection of a single pollutant particle, or simply its trajectory. The dispersion of a pollutant is calculated by assuming either puff or particle dispersion. In the puff model, puffs expand until they exceed the size of the meteorological grid cell (either horizontally or vertically) and then split into several new puffs, each with its share of the pollutant mass. In the particle model, a fixed number of initial particles are advected about the model domain by the mean wind field and a turbulent component. The default configuration assumes a puff distribution in the horizontal direction and particle dispersion in the vertical direction. Greater accuracy of the vertical dispersion parameterization of the particle model is combined with the advantage of having an ever-expanding number of particles represent the pollutant distribution.

2.3 Methodology

WRF and HYSPLIT were integrated to identify emission sources using backward trajectories and then computing the dispersion of pollutants from the source location. Integrated measurements of $PM_{2.5}$ sulfate were made every six hours from 17-19 June 2009 at two locations in southern Mississippi: Harrison Central High School (30.5N, 89.1W) and Wiggins/Stone County Airport (30.8N, 89.13W). These measurements were used to compute accumulated daily values as representative at 00 UTC of each day of the three-day sampling period. Locations of the Harrison and Wiggins monitoring sites along the Gulf Coast with emission sources around the study region are shown in Fig. 1. As the second step, WRF was designed with three nested domains; the innermost domain at 4 km resolution covered the Mississippi Gulf Coast region (Fig. 2). WRF was integrated for 48 hours starting at 00 UTC on 16, 17 and 18 June 2009 to produce atmospheric flow fields over the domain regions. HYSPLIT was run, driven by the simulated atmospheric fields, to produce back trajectories of parcels originating from a monitoring location. These back trajectories provided the Lagrangian path of the air parcels that could have contributed to the observed $PM_{2.5}$ sulfate concentrations at the monitoring sites. Possible sources were identified from back trajectories and were matched with Mississippi Department of Environmental Quality (MDEQ) observation sources of the region for the corresponding time period. Once the sources were identified, HYSPLIT was run with hypothetical emission data from the MDEQ observation locations to produce spatial dispersion of $PM_{2.5}$ for a 24-hr period. For the present study, three emission sources of $PM_{2.5}$ [(a) Hood Industries, Inc. in Waynesboro, MS (b) Hood Industries, Inc. in Wiggins, MS and (c) Mississippi Power Co. Victor J. Daniel Plant in Escatawpa, MS] fell in the mean path of backward trajectories and were analyzed.

2.4 Data

The initial and boundary conditions required for WRF model integrations and FNL data at one degree interval as available from NCEP were used. Boundary conditions were updated at 6-hr intervals (00, 06, 12 and 18 UTC) during the period of model integration. Measurements of $PM_{2.5}$ sulfate collected at Harrison and Wiggins were used for back trajectory analysis.

3. RESULTS

The 24-hr accumulated PM_2 (sulfate) concentrations, which are representative of $PM_{2.5}$ at Harrison and Wiggins, are given in Table 1. These data indicate that the magnitudes of 24-hr accumulated values are in the range of 20-30 μg/m^3 for sulfate. High resolution atmospheric fields were provided as input to HYSPLIT for computing back trajectories, source identification, and spatial atmospheric dispersion characteristics. The model-derived wind flow at 10 m height corresponding to 09 and 21 UTC on 18 June are presented in Fig. 3. The wind flow shows clockwise circulation indicating the presence of a high pressure system near the surface during this period. Temperatures were high, mostly above 90 F and heat wave conditions were indicated. At 0900 UTC on 18 June, winds were from the north and northeast over eastern parts of the domain, and predominantly from the east over western parts of the domain. The wind direction had a more northerly component over the land and easterly component over the ocean in parts of the eastern domain. Conversely, the wind had a slightly northern component over land and southern component over the ocean in parts of western domain. At 2100 UTC, wind flow was predominantly from the northeast over eastern parts of the domain and from the east over western parts of the domain. Wind speed was higher (10-15 m/s) over southwest parts of the domain in the western ocean region as compared to 5-10 m/s over eastern parts of the ocean and most parts of the land region. Wind flow was less than 5 m/s over northeast parts of the domain. Differences in wind flow regime between 09 and 21 UTC, which correspond to early morning and evening hours, indicate diurnal changes over this Gulf Coast region under the influence of a large-scale high pressure system. The establishment of sea breeze, as expected during the summer period along the coastal regions, is not distinctly indicated due to the dominant high pressure system, which induced a clockwise wind circulation leading to northerly flow over the eastern parts and easterly flow over western parts.

With this wind flow regime, HYSPLIT was used to produce back trajectories at one-hour intervals starting from 00 UTC on 19 June 2009 with duration of back trajectories as 24 hr. Back trajectories were produced from both Harrison and Wiggins (Fig. 4). Computed back trajectories show that the air parcels had paths distributed in the octant between northeast and east. The paths were mostly confined to heights below 1.5 km, within the planetary boundary layer. The back trajectories distinctly indicated source locations to be towards the northeast. A number of known industrial sources of $PM_{2.5}$ in Mississippi and neighboring states are present in this sector (Fig. 1). Three probable sources, as identified from MDEQ data, were located in the path of the back trajectories within their time duration. These sources were Hood-Waynesboro (31.39N, 88.37W), Hood-Wiggins (30.49N, 89.07W), and Victor J. Daniel Plant (30.32N, 88.33W). Since the emission strength of $PM_{2.5}$ at these sources is not known for the period of study, hypothetical emission strengths were assumed, based on the annual emission values of $PM_{2.5}$ sulfate for the prior years. A total magnitude of 100 μg/m^3/day sulfate was assumed. With this input to HYSPLIT, forward dispersions were computed originating from these sources. HYSPLIT produced ground based atmospheric dispersion maps that are presented in Fig. 5. It is noted that the dispersion of $PM_{2.5}$ from the three sources is mostly towards the west and covers the Gulf Coast region where Harrison and Wiggins are located. Hood-Waynesboro contributes significantly with dispersion confined to a narrow cone region towards the west and with maximum intensity extending over a large distance. Victor J. Daniel Plant shows dispersion towards the west but with a slightly lower value than from the Waynesboro source. Hood-Wiggins shows dispersion towards the west but with strength less than the other two sources. It should be noted that these simulations indicate that all three sources are likely to contribute significantly to $PM_{2.5}$ concentrations in the western Gulf Coast region as influenced by the prevailing wind flow field. The forward dispersion characteristics from these three different sources also confirm that the pollutant sources located towards the east of Harrison and Wiggins may also have significant contributions to the observed $PM_{2.5}$ sulfate measured in this study. Limitations with the availability of data restricted this study to hypothetical emission strengths and to the three sources analyzed.

4. CONCLUSIONS

The present study demonstrates the application of the integrated HYSPLIT atmospheric dispersion model driven by the WRF (ARW) mesoscale atmospheric model to assess source location, transportation trends, and the extent of contribution to $PM_{2.5}$. Meteorological and air pollution ($PM_{2.5}$ sulfate) measurements were collected during MCADS in summer 2009 along the Mississippi Gulf Coast. The back trajectory capability of HYSPLIT is useful for identification of possible source locations/regions. Back trajectory and dispersion features from HYSPLIT are dependent on atmospheric flow fields; the need for precise prediction of these fields at the desired high resolution is emphasized. Similarly, the applicability of HYSPLIT in producing the forward atmospheric dispersion characteristics of the pollutants is also demonstrated. It may be noted that this methodology could be adopted for source location for other atmospheric pollutants.

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TABLE 1. Measurements of $PM_{2.5}$ sulfate at Harrison and Wiggins during MCADS.

Date/ Start Time (CDT)	Date/ End Time (CDT)	Harrison SO_4 (ug/m^3)	Wiggins SO_4 (ug/m^3)
6/17/2009 14:00	6/17/2009 20:00	8.38	5.94
6/17/2009 20:00	6/18/2009 2:00	7.14	8.89
6/18/2009 2:00	6/18/2009 8:00	6.91	8.2
6/18/2009 8:00	6/18/2009 14:00	6.57	7.18
6/18/2009 14:00	6/18/2009 20:00	6.48	6.16
6/18/2009 20:00	6/19/2009 2:00	6.74	3.4
6/19/2009 2:00	6/19/2009 8:00	6.9	5.2
6/19/2009 8:00	6/19/2009 14:00	7.1	6.37
6/19/2009 14:00	6/19/2009 20:00	6.08	6.87
6/19/2009 20:00	6/20/2009 2:00	10.1	8.21
6/20/2009 2:00	6/20/2009 8:00	6.68	5.33
6/20/2009 8:00	6/20/2009 14:00	6.7	---

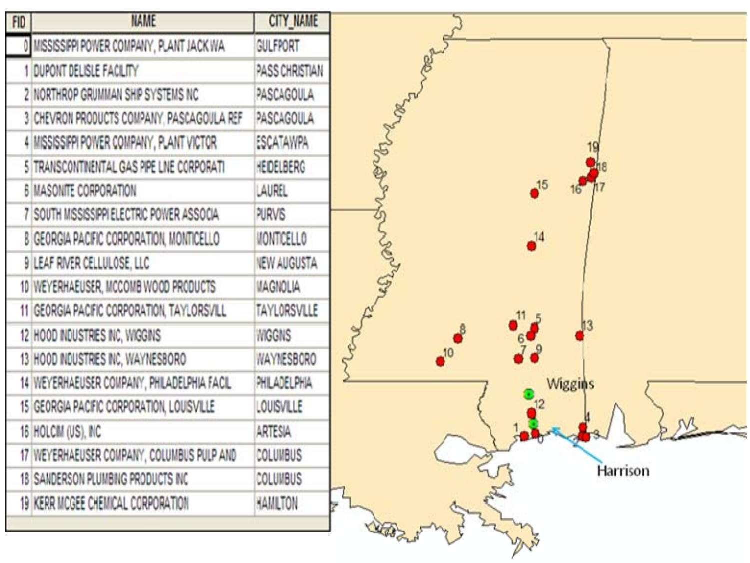

FIG. 1. A map of Mississippi showing $PM_{2.5}$ emission source locations, identified from MDEQ data (red circles). Green circles denote locations of monitoring sites at Harrison Central High School and Wiggins/Stone County Airport.

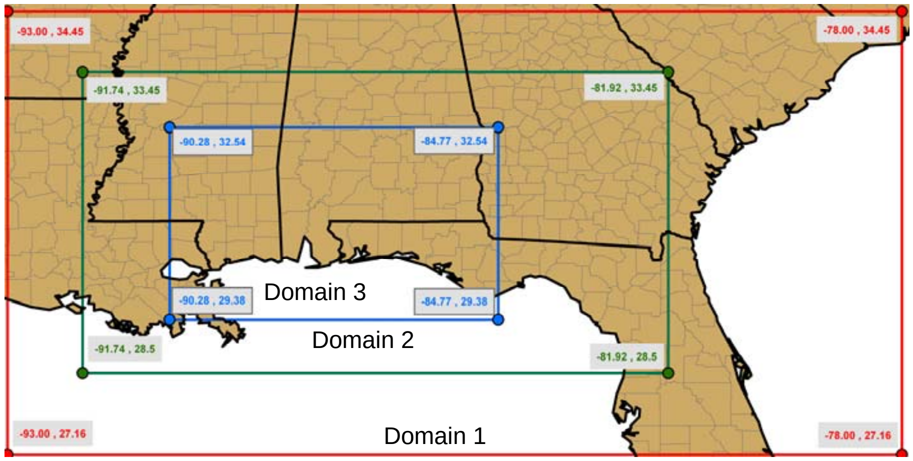

FIG. 2. WRF model domains for the Mississippi Gulf Coast Region.

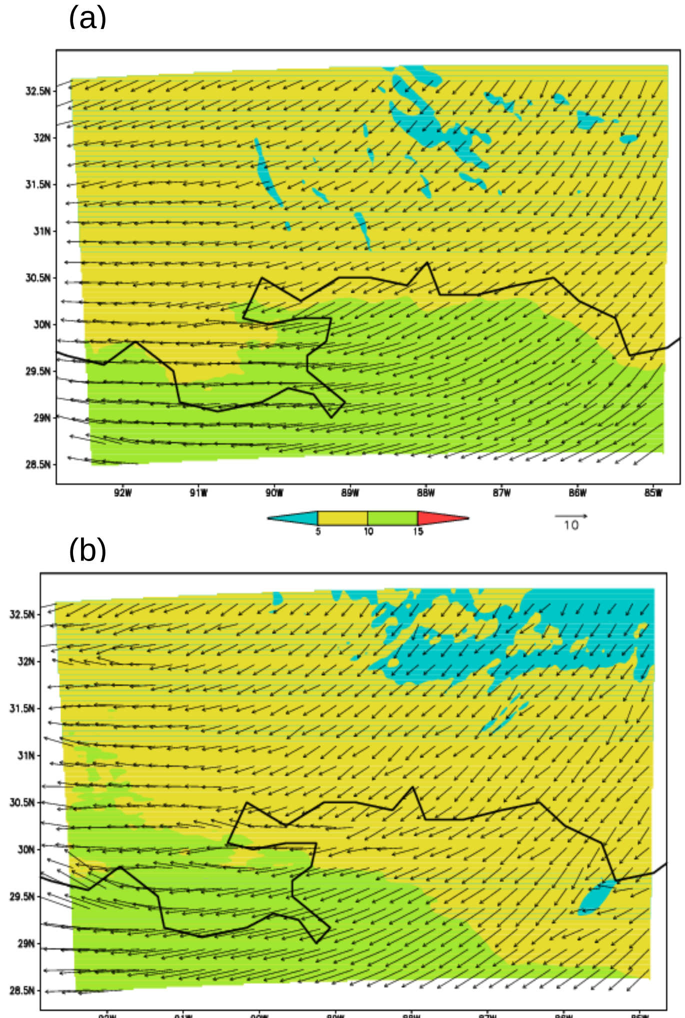

FIG. 3. Model-simulated wind flow at 10 m over the study region at (a) 0900 UTC and (b) 2100 UTC on 18 June 2009.

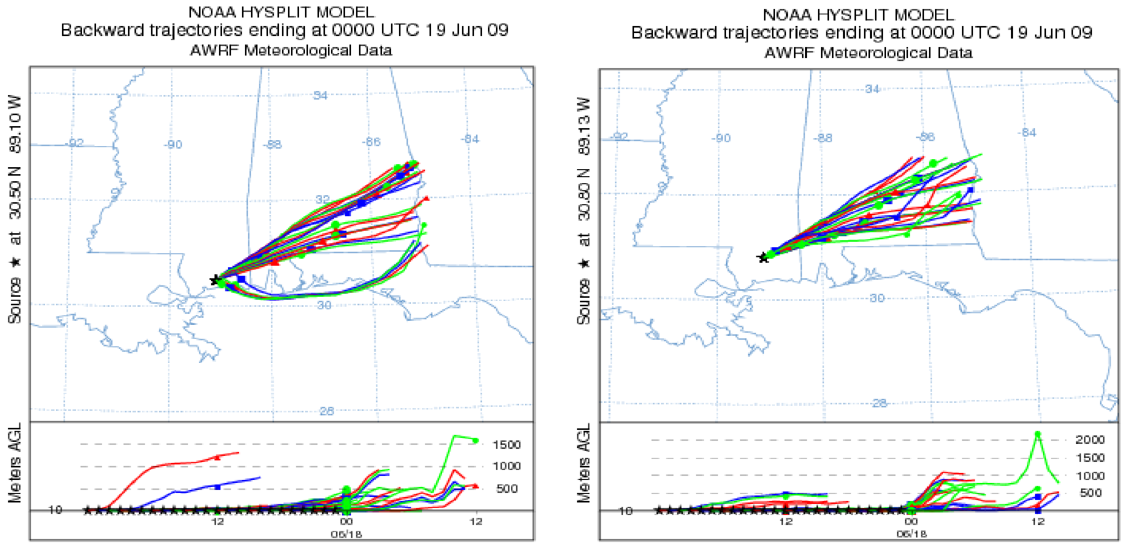

FIG. 4. Computed back trajectories at 1-hr intervals for the 24 hour period ending 00 UTC on 19 June 2009. Upper portions of the figure show the horizontal path, and lower potions show the vertical path of the trajectories.

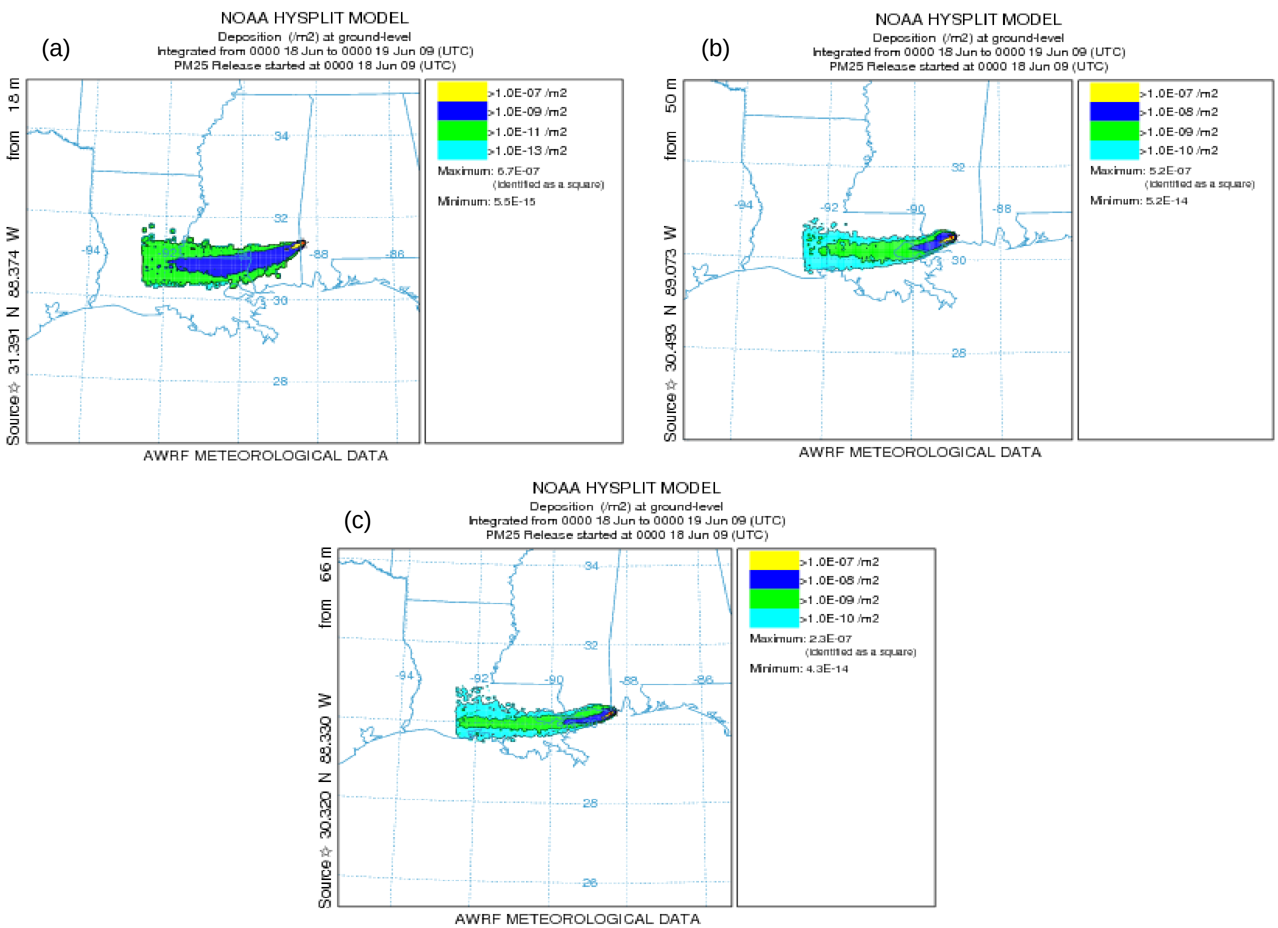

FIG. 5. Atmospheric dispersion characteristics of $PM_{2.5}$ originating from three sources – (a) Hood Industries, Inc. in Waynesboro, MS; (b) Hood Industries, Inc. in Wiggins, MS; and (c) Mississippi Power Co. Victor J. Daniel Plant in Escatawpa, MS during the 24-hr period starting from 00 UTC on 18 June 2009.