# SIMULATION OF TRANSPORT AND DISPERSION OF POLLUTANTS FROM ELEVATED POINT SOURCES IN MISSISSIPPI GULF COAST USING A MESOSCALE ATMOSPHERIC DISPERSION MODELING SYSTEM

Venkata Srinivas Challa, Jayakumar Indracanti, Loren D. White, Chuck Patrick, John Young, Robert Hughes and Yerramilli Anjaneyulu\* Trent Lott Geospatial and Visualization Research Centre @Mississippi e-Centre, Jackson State

University, MS USA

# 1. INTRODUCTION

Increasing urbanization, industrial growth and consequent population rise in coastal areas needs the study of air pollution dispersion at various scales that cause impact scenarios in local and long ranges. Dispersion in the coastal regions is influenced by the meso-scale circulations of land and sea breeze which develop due to the differential land-sea temperatures. These complex thermal circulations and the surface temperature contrast between ocean and land initiates a thermal internal boundary layer (TIBL), which has a critical effect on dispersion (Pielke et al 1991). These local effects need to be accounted in the coastal dispersion simulation for realistic estimations of pollutant concentrations. Simple gaussian plume models do not account these effects over distances of a few tens of kilometers. Numerical models have proved to be useful in simulating atmospheric mesoscale phenomena including air-pollution transport (eg., Pielke et al 1991; Boybeyi and Sethu Raman, 1995, Draxler and Hess, 1998). The present study explores application of а meso-scale atmospheric dispersion modeling system to estimate the ground level concentrations of air pollutants (SO<sub>2</sub>, CO and PM10) from the major elevated point sources in the Mississippi Gulf Coast.

# 2. NUMERICAL SIMULATIONS

The numerical modeling systems consists of the Weather Research and Forecast Model (WRF ARW) (Skamarock et al., 2005) to provide the input data, especially the wind and turbulence fields and a three-dimensional Hybrid Integrated Trajectory Particle Dispersion Model (Hysplit) (Draxler and Hess, G.D, 1998). Summer synoptic conditions are considered in the study as they represent weak synoptic forcing with significant land-sea temperature contrast conducive to the development and sustenance of local meso-scale circulations in Mississippi. Three nested grids with 54x40 grid points (36 km grid spacing), 109x76 grid points (12 km grid spacing) and 187x118 grid points (4 km grid spacing) and with 34 vertical layers are used in the model (Fig 1). The area of interest is the inner fine grid (4km) covering the MS Gulf coast. Initial and lateral boundary conditions are taken from NCEP FNL data and model is integrated for 48 hours during 01-03. June 2006. The physics used in the model consists a 5-layer soil model for ground temperature prediction, Yonsei University (YSU) PBL scheme for boundary layer turbulence, Kain-Fritisch scheme for convective parameterization on the outer grids, WSM3 class simple ice scheme for explicit moisture, Dudhia scheme for short wave radiation and RRTM model for long wave radiation processes (Table.1).



Figure 1. Modeling domains used in WRF-ARW

Dispersion simulation is done over a range of 100 km around the sources. A horizontal grid of  $1.5^{\circ} \times 1.5^{\circ}$  with resolution of  $0.005^{\circ} \times 0.005^{\circ}$  (roughly 500m x 500m) and with seven vertical levels (50 m, 100 m, 200 m, 500 m, 1000 m, 2000 m and 5000 m above ground level) is considered in Hysplit dispersion model. Four major elevated sources of emission located along the Mississippi gulf coast are considered (Table 2).

Pollutant concentrations are sampled and averaged every 2 hours. The turbulence mixing is computed using a diffusivity approach based upon vertical stability estimates and the horizontal wind field deformation. The puff dispersion is treated as linear with time. Ground level concentrations are

<sup>\*</sup>*Corresponding author:* Yerramilli Anjaneyulu, Director, Trent Lott Geospatial and Visualization Research Centre,e-mail: yerramilli.anjaneyulu@jsums.edu

computed as averages for the lowest 50 m within each horizontal grid cell.

Table. 2 Emission parameters of different sources used for the model simulations (Hs – Physical stack height, Ds – Stack exit diameter, Qs – source strength)

Plant	Stack Height (m)	Stack Diameter (m)	Source strength
Mississippi Power Plant Jack Wa	115.12	3.85	24869.5
Chevron Refinery	54.1	1.35	1742.8
Mississippi Power Plant Victor	105.0	10.23	12522.2
Dupont Delisle Facility	45.0	3.0	1270.5

# 3. RESULTS

Simulated meteorological fields by WRF model show the presence of synoptic flow, landbreeze in the morning hours and significant seabreeze circulation in the day time through the late evening. The flow in the Mississippi Gulf coast region is altered at the lower levels by the mesoscale land and sea-breeze circulations in the course of the day (Figure 2).



Figure 2. Horizontal wind vectors at 10 m level for Domain 3 on June 1 A) 6:00 B) 16:00

Simulated surface flow in Mississippi is northwesterly off-shore during morning time and gradually becomes strong southerly by the onset of sea breeze, horizontal extent of the onshore flow increased towards the late evening time. Circulation up to 500 m above ground level (AGL) followed this pattern which is modified by synoptic flow upwards. Examination of vertical crosssection of simulated horizontal winds, potential temperature, divergence/ convergence and vertical winds in north-south vertical section across the Mississippi coast indicate development of a shallow unstable layer near the coast after the onset of sea breeze (Fig 3). Simulated internal boundary layer height is about 300 - 500 m AGL across the coast.



Figure 3. Vertical section of potential temperature (K) and circulation vectors ( $ms^{-1}$ ) across the Mississippi Coast at 16:00 LST on June 1, 2006

Development of sea breeze front is noticeable at 1600 LST with ascending winds at the leading edge, return flow aloft and subsidence behind the front (Fig 3). The lowest 600 m layer is dominated by southerly sea breeze flow which gradually advances further north (inland) in late evening hours. Sea breeze is seen to extend up to 80 km inland in the simulation.

A qualitative agreement is found between the simulated and observed surface parameters (winds, temperature) at the Pascagoula coastal meso-net station (Fig 4). Forward trajectories computed using Hysplit model from WRF wind fields, showed recirculation of air parcels at the coast indicating the influence of sea breeze and land breeze (Fig 5) flow on pollutant plume.



Figure 4. Simulated and observed wind speed (a), wind direction (b) and air temperature (c) at Pascagoula location in the MS Gulf coast.



Figure 5. Forward trajectories from the sources computed using WRF meteorological fields.

Simulated ground level  $SO_2$  concentration distribution averaged every 2 hours for the lowest 50 m layer is presented in Fig.6. The plume evolution followed the simulated diurnal wind flow pattern. Temporal variation in the plume spread is noticed according to changes in stability, strength of wind and the spatial variations in the wind field. The plume lies in the east-northeast direction along the coast during night (0400 - 0600 UTC), it shifts gradually southward in the morning (1200 -1400 UTC) under land breeze influence. Plume turns gradually to land in the day time on sea breeze development and completely stays on land with full sea breeze establishment. Similar diurnal transition is found in the plume in the next 24 hours. Concentration pattern shows the plume is narrow during the stable morning conditions and dispersed over a wider area at the incidence of sea breeze in the afternoon time (Fig 6C). The plume is narrow in the region of sea breeze influence and is wide spread further away due to spatial variations in the wind field across the sea breeze zone. This is because the wind field is governed by synoptic flow at distances of 100 km from the coast and the sea-land breeze near the coast. During the transition times i.e., during the onset of LB or SB distinctly different patterns of dispersion can be noticed, one near the source region in the direction of local circulation and the second due to earlier spread releases in the direction of the large scale flow.



Figure 6. Simulated diurnal plume concentration distribution pattern.

During the morning time releases occur with in a stable boundary layer, the ground level concentration near the release locations (< 5 km) is 0.1  $\mu$ g m<sup>-3</sup> which falls to 0.01  $\mu$ g m<sup>-3</sup> at distance rage of 20 to 50 km and 0.001  $\mu$ g m<sup>-3</sup> in 50-100 km in the northeast direction (Fig 6 A). After the incidence of sea breeze there is a reduction in the concentration (0.01- 0.001  $\mu$ g m<sup>-3</sup>) due to

advection by strong sea breeze winds (Figs .6 C ). Once sea breeze is fully established, the plume is well alienated over land in northeast direction and maximum concentration (0.1  $\mu$ g m<sup>-3</sup>) occurs at distance ranges of 25 km to 40 km (Fig.6 D). Contours corresponding to the value of 0.10-0.01  $\mu$ g m<sup>-3</sup> are extending to large downwind distances in the late evening time. This coincides with the formation of internal boundary layer at the coast during sea breeze time, that causes fumigation and reflection of plume. It is noticeable that the concentrations are higher during the morning hours than during the day time, due to low wind speeds and stable conditions. Thus the highest 2h average SO<sub>2</sub> concentrations simulated by the WRF-Hysplit modeling system in a distance range of 50 km around the release locations are 0.1 ug m<sup>-3</sup>. This occurs during two conditions, one in the stable morning time upto 20 km in the eastward direction and the second during the fumigation time in the day time associated with sea breeze and confined to about 40 km in the northeast. The second highest concentration 0.01  $\mu$ g m<sup>-3</sup> occurs during most of the day.

#### 3.1 Comparison with observations

Modeled concentration is compared with ambient air quality data for SO<sub>2</sub> at Pascagoula to assess the diurnal trends in the simulation. Concentration in the initial 6 hr is below observations due to WRF model spin up time and Hysplit model grid instauration. Model values are closer to observations up to 32 hours of simulation (Fig 7a) and show increased bias thereafter probably because of deterioration in simulated meteorological fields.



Figure 7. a) Modeled and observed concentration at Pascagoula site , b) model plume centerline concentration at 16:00 LST

Maximum concentrations are noticed at distances of 10 to 40 km in the afternoon (Fig 7b) probably due to the sea breeze development and shallow mixing near coast as simulated by WRF.

# 3.2 Surface concentrations using Gaussian Model

Although the Gaussian Plume Model (GPM) has limitations in accounting the significant temporal and spatial variations of the meteorological fields in the coastal region, it provides conservative estimates for different wind, stability and mixing height categories. Uniform winds speeds, mixing heights at different hours along with a neutrally stable condition are assumed in the GPM calculation (Table 3). It can be noticed that the concentration falls by 2 orders at distances of 100 km, which is also simulated by the mesoscale dispersion system in the present case. However, the concentrations predicted by Hsyplit model are about an order less than the GPM estimations. The hysplit model takes into account the spatial and temporal variations in wind speed, mixing depth and the stability condition of the atmosphere and hence gives more realistic estimates. Estimations from GPM however are qualitative indications of the performance of Hysplit model

# 4. CONCLUSION

The present simulation study clearly shows the typical atmospheric dispersion in the Mississippi gulf coast region. WRF model simulations show the occurrence of meso-scale land -sea breeze circulation and formation of shallow mixing layer in the Mississippi Gulf coast and are validated with meso-net observations. Simulations using Hysplit dispersion model show the effects of the above phenomena on the concentration pattern up to 50 kilometers inside the coast. Concentrations are generally more during the stable morning time. During sea breeze time maximum concentrations are noticed at ranges of 20-40 km and associated with internal boundary layer formation in the coastal area. Calculated concentrations follow the observed trends and those calculated using a standard Gaussian Plume model.

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