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## Air Pollution, Modeling and GIS based Decision Support Systems for Air Quality Risk Assessment

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### 1. Introduction

Air Pollution is a state of the atmosphere with predominant presence of hazardous substances that are harmful to humans and animals. The air-borne pollutants degrade the air quality and constant exposure to polluted air may lead to several health problems such as cardiopulmonary disease, bronchitis, asthma, wheezing and coughing etc. Average composition of the atmosphere below 25 km indicates that nitrogen, oxygen, water vapor, carbon dioxide, methane, nitrous oxide, and ozone are the major constituents and their balance is important to the maintenance of the Earth's biosphere. An imbalance of these constituents for a considerable long time may lead to serious implications of air quality and weather and climate. The pollutants are categorized as primary and secondary, primary pollutants are directly emitted from a source and secondary pollutants result from reaction of primary pollutants in the atmosphere. The primary pollutants are the ash from volcanoes, carbon monoxide and sulfur dioxide emissions from vehicles and factories and combustion of fossil fuels etc whereas secondary pollutants are tropospheric ozone resulting from photolysis of nitrogen oxides and hydrocarbons in the presence of sunlight and smog from a mixture of smoke and sulfur dioxide. The sources of air pollution are classified as natural and anthropogenic. Volcanoes, forest fires and biological decay providing sulfur dioxide and nitrogen oxides, large barren lands providing dust, vegetation producing volatile organic compounds come under natural sources whereas anthropogenic sources are categorized as mobile and stationary sources. Different forms of transportation such as automobiles, trucks, and airplanes come under mobile sources whereas power plants and industrial facilities are the stationary sources. Stationary sources are further classified as point and area sources, wherein a point source refers to a fixed source such as a smokestack or storage tank that emits the pollutant and an area source refers to several small sources affecting the air quality in a region such as dry cleaners, gas stations, auto body paint shops and a community of homes using woodstoves for heating. Air pollutants are also categorized as 'criteria' and 'hazardous', where the criteria pollutants refer to the commonly

and frequently observed six chemicals which are carbon monoxide, lead, nitrogen dioxide, ozone, particulate matter, and sulfur dioxide and hazardous pollutants are toxic pollutants which cause cancer and other serious health problems or lead to adverse environmental effects.

Anthropogenic primary pollutants such as carbon monoxide, particulate matter, nitrogen oxides and lead are detrimental to health as well as environment. Sulfur dioxide and nitrogen oxides get transformed as sulfuric acid and nitric acid in the atmosphere due to chemical reactions and may fall as acid rain. Some details of these pollutants are briefly described as follows:

Carbon monoxide is a colorless, odorless, poisonous gas produced from burning of fuels with carbon and so the major source is road transport vehicles. Due to oxidation process, CO will be transformed as carbon dioxide. The background levels of carbon monoxide are in the range of 10-200 parts per billion (ppb) and urban concentrations generally vary between 10 to 500 parts per million (ppm). Continuous exposure to higher levels (>500 ppm) for longer time periods (> 30 minutes) may lead to headache, dizziness and nausea and also death.

Nitric oxide (NO) is a colorless, odorless gas produced during burning of fuel at high temperatures in cars and other road vehicles, heaters and cookers. Mostly, nitrogen dioxide in the atmosphere is formed from the oxidation of nitric oxide (NO). Nitrogen dioxide reacts to form nitric acid and organic nitrates and plays an important role in the production of surface ozone. Mean concentrations in urban areas are in the range of 10-45 ppb reaching as high as 200 ppb. Continuous exposure to NO<sub>2</sub> leads to respiratory problems and lung damage.

Particulate matter comprises of both organic and inorganic substances, mainly from dust, fly ash, soot, smoke, aerosols, fumes, mists and condensing vapors and is regarded as coarse particulates with a diameter greater than 2.5 micrometers (μm) and fine particles less than 2.5 micrometers. The acid component of particulate matter (PM) generally occurs as fine particles. Primary sources of the particulate matter are from road transport (25%), non-combustion processes (24%), industrial combustion plants and processes (17%), commercial and residential combustion (16%) and public power generation (15%). In urban areas, secondary particulate matter occurs as sulfates and nitrates with mean values in the range 10-40 μg/m<sup>3</sup> and may rise up to higher than 100 μg/m<sup>3</sup>. Primary PM sources are derived from both human and natural activities which include agricultural operations, industrial processes, fossil fuel burning etc and secondary pollutants such as SO<sub>2</sub>, NO<sub>x</sub>, and VOCs are considered as precursors as they help form PM. Measures to reduce these precursor emissions will have a controlling impact on PM concentrations. Fine PM will cause asthma, lung cancer, cardiovascular issues, and premature death and estimated to cause 20,000 - 50,000 deaths per year in US.

Sulfur dioxide (SO<sub>2</sub>) is a colorless, nonflammable gas with an odor that irritates the eyes and air passages. The most common sources of sulfur dioxide are fossil fuel combustion, smelting, manufacture of sulfuric acid, conversion of wood pulp to paper, incineration of refuse and production of elemental sulfur. Coal burning is the single largest man-made source of sulfur dioxide accounting for about 50% of annual global emissions, with oil burning accounting for a further 25-30%. The most common natural source of sulfur dioxide is volcanoes. The mean concentrations are in the range of 5-15 ppb but hourly peak values may reach to 750 ppb. The health effects include asthma, respiratory illness and cardiovascular disease. Sulfur dioxide pollution can be more harmful when particulate and other pollution concentrations are high which is known as the "cocktail effect".

Secondary pollutants, resulting from the conversion of primary pollutants through complex chemical reactions, are potentially more harmful than their precursors. Since much of the pollutant chemistry is driven by the presence of sunlight, these are commonly referred to as photochemical pollutants. A well-known secondary photochemical pollutant is ozone ( $O_3$ ) formed due to oxidation of benzene and other volatile organic compounds in the presence of nitrogen oxides. In urban areas with high  $NO_x$  concentrations, ozone concentrations tend to be lower due to scavenging effect ( $NO_x$  react with ozone to form  $NO_2$  and  $O_2$ ), but tend to be higher due to downwind transport of  $NO_x$  and its reaction with VOCs under sunlight. Ozone is a colorless, pungent, highly reactive gas and is the principal component of smog, which is caused primarily by automobile emissions, predominantly in urban areas. Ozone concentrations in urban areas rise in the morning, peak in the afternoon, and decrease at night. Higher frequencies of higher concentrations are dependent on stable atmospheric conditions such as low level inversions which restrict the pollutants to the boundary layer. Two of the most important factors that affect human health are the concentration of ozone and duration of exposure.

### 1.1 Air Quality and Air Quality Index

Air Quality depends on the trace gas emissions from the biosphere, from human activities and the chemical reactions which govern the concentrations of trace species in the atmosphere. Air Quality is an assessment of extent of pollutants present in air in a given locality relative to permissible levels while Air Quality Index (AQI) is an index for reporting daily air quality. EPA (Environmental Protection Agency) of USA calculates the AQI for five major air pollutants regulated by the Clean Air Act: ground-level ozone, particle pollution (also known as particulate matter), carbon monoxide, sulfur dioxide, and nitrogen dioxide. For each of these pollutants, EPA has established national air quality standards to protect public health. Ground-level ozone and airborne particles are the two pollutants that pose the greatest threat to human health in USA. AQI as a yardstick ranges from 0 to 500 and higher the AQI value, greater the level of air pollution and greater the health concern. For example, an AQI value of 50 represents good air quality with little potential to affect public health, while an AQI value over 300 represents hazardous air quality. An AQI value of 100 generally corresponds to the national air quality standard for the pollutant, which is the level EPA has set to protect public health. AQI values below 100 are generally thought of as satisfactory. When AQI values are above 100, air quality is considered to be unhealthy at first for certain sensitive groups of people, then for everyone as AQI values get higher.

### 1.2 Spatial Temporal variability

Air pollution became a widespread problem in the United States (US) and, according to the Environmental Protection Agency (EPA), it is estimated that over 100 million individuals are routinely exposed to levels of air pollution that exceed one or more of their health-based standards [1]. The major air pollutants include oxides of sulfur and nitrogen, suspended particulate matter, oxides of carbon, hydrocarbons, lead. These gases are released into the atmosphere from either stationary sources such as industrial point sources or mobile sources like vehicular pollution. These pollutant gases will also produce secondary pollutant like surface Ozone, which has great oxidative capacity and is the primary component of urban smog. Criteria Pollutants Ozone and particulate matter ( $PM_{10}$  and  $PM_{2.5}$ ) are main focus now as they mainly drive the AQI (which is based on five criteria pollutants  $CO$ ,  $NO_2$ ,  $SO_2$ ,  $O_3$ ,  $PM$ ). These pollutants can affect our health in many ways, with irritation to the eyes, nose

and throat and more serious problems such as chronic respiratory disease and cardiovascular diseases. Understanding the long-term (yearly, decadal) trends of these criteria air pollutants is important for assessing chronic exposure to population and the efficacy of control strategies, emissions changes, and the year to-year influence of meteorology.

The air pollutant levels at any location can be explained by three factors: (a) the rate of emissions or production from all sources; (b) the rate of chemical or physical removal via reaction or deposition; and (c) the dispersion and transport of a chemical within, to, or from an area. These three factors are likely to be influenced by meteorological and anthropogenic factors such as temperature, precipitation, proximity to sources, or weekday – weekend emission activity differences. Meteorological conditions strongly influence air quality. These include transport by winds, recirculation of air by local wind patterns, and horizontal dispersion of pollution by wind; variations in sunlight due to clouds and season; vertical mixing and dilution of pollution within the atmospheric boundary layer; temperature; and moisture. The variability of these processes, which affects the variability in pollution, is primarily governed by the movement of large-scale high- and low-pressure systems, the diurnal heating and cooling cycle, and local and regional topography. Changes in climate affect air quality by perturbing ventilation rates (wind speed, mixing depth, convection, and frontal passages), precipitation scavenging, dry deposition, chemical production and loss rates, natural emissions, and background concentrations.

Further researches have shown that  $PM_{2.5}$  chemical composition and concentrations vary by location and source [2]. Particulates from different sources also have varying amounts of correlation with adverse health effects [3]. Most epidemiological studies which examine relationships between air pollution levels and human health needs spatial and temporal variation. Effects of changes under different possible emission scenarios are also important in determining pollutant distributions and future air quality risks.

### 1.3 Air Quality Management

The damages caused by air pollution in many countries are large and it is generally accepted that there is an urgent need for reducing the emissions to the atmosphere. The damages are caused by high ambient air concentrations and depositions of many chemical components. Among the most important components are acidifying constituents (sulfur and both oxidized and reduced nitrogen compounds), photochemical components (including ozone), particulate matter and toxic compounds, such as metals, organic compounds and others. The concentrations and depositions are dependent on (i) the total mass of pollutants emitted to the atmosphere and its spatial and temporal distribution (ii) transport and transformation processes in the atmosphere and (iii) deposition processes.

Assessments of emission reduction strategies must consider all the three factors and the complexity of these problems call for the use of atmospheric models. Average exposure of the ecosystem to concentrations and deposition, emission scenario studies and linkage to economical aspects and cost effectiveness are all examples of areas where the models are needed. Air Pollution is a good example of how models can play an important role in the decision making process toward protocols on emission reductions. Regional scale models quantifying the trans-boundary fluxes of air pollution between the European countries and deposition to ecosystems [4] have successfully been applied together with knowledge on ecosystem critical loads of acidity and the costs involved in emission reduction in order to find optimal solution for the reductions.



## 2. Air Quality assessment

Pollutants in the atmosphere undergo transportation and dispersion, whose characteristics are dependent on the prevailing atmospheric conditions. Pollutants can be transported across the continents due to globally circulating winds on time scale of months to years, e.g. intercontinental transport of dust from Sahara desert in Northwest Africa and the Gobi desert in East Asia and dispersed over a few hundreds of miles in a few days under the influence of local scale wind circulations. While wind is primarily responsible for transportation and dispersion, topography and atmospheric stability also play an important role. Horizontal and vertical motions arise due to atmospheric pressure gradients and stability conditions. Atmospheric pressure, defined as the weight of the air column above a point, varies due to differential surface heating. Heating and cooling of the earth surface is dependent on the type of surface, for e.g. water bodies have larger specific heat capacity and so takes longer time to get heated or cooled as compared to land surface. Different surfaces have different heating/cooling rates, e.g. asphalt surface gets heated/ cooled faster than vegetation surface; heating/ cooling at the surface causes lower/ higher density vertical columns leading to lower/ higher pressures. As air tends to move from denser to lighter regions, atmospheric wind gets established as movement from high pressure regions to low pressure regions. Similarly vertical motions are dependent on atmospheric stability. Heating at surface causes air to rise mixing with cooler and denser air at higher levels leading to instability and most of the mixing takes place in the lowest part of the atmosphere referred to as atmospheric boundary layer. This is characterized by turbulent fluctuations of wind velocity, temperature and moisture due to energy exchange with earth surface capped by an infinitesimal transition layer below the free atmosphere with lower/ higher stability conditions associated with stronger/ weaker vertical mixing. Since the pollutants originate near the earth surface, characteristics of the atmospheric boundary layer play an important role in the dispersion of pollutants. This is the reason why winter nights which are cooler with higher stability have stagnation of pollutants causing health hazards. Atmospheric dispersion on the scale of a few days (synoptic time scale) is influenced by the transient surface low and high pressure systems. Moderate to intense low pressure systems characterized by winds  $> 5\text{m/s}$ , mass convergence, higher instability and upward motions contribute to dispersion over wider horizontal extent ranging up to few thousand kilometers thus reducing the pollution effect through mixing with larger environment volume. Conversely, high pressure systems with calm winds, subsiding downward motion and higher atmospheric stability contain dispersion to smaller volume enhancing the pollution effects. These emphasize the role of atmospheric stability criteria and prevailing atmospheric circulation on the atmospheric dispersion of pollutants. In the absence of synoptic forcing, mesoscale and local circulations developed due to topography and land use variations and with synoptic forcing admixture of synoptic scale and mesoscale circulations control the pollutant dispersion.

Assessment of atmospheric dispersion requires precise information of meteorological parameters such as wind, temperature, humidity and stability at spatial and temporal resolutions as high as possible. Since meteorological observations are made at discrete spatial locations and at synoptic times (twice daily at 0000 and 1200 UTC), these data are to be generated at the required spatial and temporal resolutions. Weather prediction models provide the required quantitative information of the meteorological fields, which are used as input to a pollutant dispersion model to derive the spatial distribution. The integration of the weather prediction and dispersion models is the basis of the air quality models.

### 3. Meteorological Models - Numerical Weather Prediction

In view of the importance of meteorological variables in estimating atmospheric dispersion, a brief description of weather prediction using numerical models is provided here. Weather is defined as the state of the atmosphere at a given time and place, with respect to variables such as temperature, moisture, wind velocity, and barometric pressure where atmosphere is a gaseous envelop covering the Earth. Weather prediction is the application of science and technology to estimate the future state of the atmosphere (in terms of pressure, temperature, wind, rainfall etc) with reference to a specified region or location. Atmosphere is influenced by transient air movement and predicting that flow provides the status of weather conditions. Although different methods are available, numerical models alone provide quantitative weather forecasting. These models use a closed system of mathematical equations of dynamics developed from fundamental equations based on conservation of mass, momentum and water vapor along with equation of state and thermodynamic energy equation for temperature in differential form and use of numerical methods to solve them to produce future state of atmosphere starting from an observed initial state. To solve these equations numerically, the study region is to be formulated as of rectangular form with equally spaced horizontal intersecting grid in the horizontal direction and enough number of vertical levels as suitable for numerical solution. Due to constraints of mathematical formulation, numerical set up and the computational resources, the horizontal grid resolution is often restricted to a few kilometers. Since atmospheric modeling includes both the dynamical and physical parts, the physical processes of atmospheric radiation, planetary boundary layer, convection, cloud microphysics and surface physics are to be parameterized as these processes occur on scales smaller than the resolvable scales of domain resolution. For the system to predict the weather for a certain area it needs initial conditions and boundary conditions as adjacent areas affect the area of interest. It is known that observations are available at non-uniform locations and are sparser than the model resolution; the atmospheric variables are to be interpolated to the model grid using objective methods. Errors in the observations, interpolation to model grid, limitations in the representation of physical processes and errors due to numerical methods of solution all lead to uncertainties in weather forecasting and increase of errors with the progress of prediction. Rapid advances in computational resources have lead to the design and development of atmospheric models as applicable for real time weather forecasting of various weather phenomena with scales of few kilometers to thousands of kilometers. There are many meteorological models available for weather prediction and the mainly used are the WRF, MM5, RAMS. Brief description of these models as follows.

#### 3.1 WRF modeling system

Weather Research and Forecasting (WRF) modeling system was developed and sourced from National Center for Atmospheric Research (NCAR), as the next generation model after MM5, incorporating the advances in atmospheric simulation suitable for a broad range of applications. It has two cores, NMM and ARW which are developed independently and have differences in dynamics, methods of solution and physical schemes. Here a description of ARW model is presented as it is widely used for air quality modeling studies. ARW (Advanced Research WRF) model has versatility to choose the domain region of interest; horizontal resolution; interactive nested domains and with various options to choose parameterization schemes for convection, planetary boundary layer (PBL), explicit moisture;

radiation and soil processes. ARW is designed to be a flexible, state-of-the-art atmospheric simulation system that is portable and efficient on available parallel computing platforms and a detailed description was provided by Skamarock et al. (2008) [5]. The model consists of fully compressible non-hydrostatic equations and the prognostic variables include the three-dimensional wind, perturbation quantities of pressure, potential temperature, geopotential, surface pressure, turbulent kinetic energy and scalars (water vapor mixing ratio, cloud water etc). The model equations are formulated using mass-based terrain following coordinate system, and solved in Arakawa-C grid using Runge-Kutta third order time integration techniques. The model has several options for spatial discretization, diffusion, nesting and lateral boundary conditions. The ARW Solver is the key component of the modeling system, which is composed of several initialization programs for idealized, and real-data simulations, and the numerical integration program. ARW supports horizontal nesting that allows resolution to be focused over a region of interest by introducing an additional grid (or grids) into the simulation with the choice of one-way and two-way nesting procedures. ARW model system was used in this study for its accurate numerics, higher order mass conservation characteristics and advanced physics.

### 3.2 MM5 modelling system

MM5 is a regional mesoscale model used for creating weather forecasts and climate projections. MM5 modeling system software is mostly written in Fortran and has been developed at Penn State and National Center for Atmospheric Research (NCAR) as a community mesoscale model with contributions from users worldwide. MM5 is a limited-area, non-hydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale atmospheric circulation [6]. The model is supported by several pre and post-processing programs, which are referred to collectively as the MM5 modeling system [<http://www.mmm.ucar.edu/mm5/>].

### 3.3 RAMS modeling system

Regional Atmospheric Modeling System (RAMS) is a highly versatile numerical code developed by scientists at Colorado State University for simulating and forecasting meteorological phenomena, and for depicting the results. [<http://rams.atmos.colostate.edu/rams-description.html>].

## 4. Air Pollution Dispersion modeling

Air pollution models are the only method that quantifies the deterministic relationship between emissions and concentrations/depositions, including the consequences of past and future scenarios and the determination of the effectiveness of abatement strategies. Air pollution measurements give information about ambient concentrations and deposition at specific locations and times, without giving clear guidance on the identification of the causes of the air quality problem. This makes air pollution models indispensable in regulatory, research, and forensic applications. The concentrations of substances in the atmosphere are determined by 1) transport, 2) diffusion, 3) chemical transformation, and 4) ground deposition. Transport phenomena, characterized by the mean velocity of the fluid, have been measured and studied for centuries. For example, the average wind has been studied by man for sailing purposes. The study of diffusion (turbulent motion) is more recent.



Among the first articles that mention turbulence in the atmosphere, are those by Taylor (1915, 1921) [7,8].

Pollutants in the atmosphere get transported longer distances by large scale atmospheric wind flows and dispersed in the atmosphere by small scale turbulent flows and mix with environment. Dispersion is difficult to understand and estimate due to presence of different scales of eddies and their complex interaction. Atmospheric dispersion models shall include the physical and chemical processes of transportation, transformation and dispersion of pollutants in the atmosphere to provide estimates of pollutant concentrations with the information of emission sources and concentrations. Current models are designed to compute the pollutant concentrations using information of characteristics of emission sources, emission rates, terrain variations, meteorological variations and background concentrations. These dispersion models use mathematical based concepts of dispersion and diffusion with proper treatment of complex terrain and land use. The pollutants concentrations in the atmosphere constantly change influenced by weather conditions. Meteorological parameters play an important role in the atmospheric dispersion as transport is controlled by large scale wind flows and dispersion by atmospheric stability, vertical mixing and local mesoscale winds. A proper design and application of the dispersion models can be used for identification of contributors through establishment of source- receptor relationships, assessment of air quality compliance with government norms, planning of new facilities, management of emissions at sources, prediction of high concentration episodes, providing information for risk assessment and management. Above all these, modeling information saves cost of continuous monitoring over large areas and for longer times. All the model estimations are to be evaluated to understand the uncertainties due to inaccuracies in emission strength, meteorological input data, physics of dispersion concentration estimations and analysis before assessment of health effects.

There are two modeling approaches, following Lagrangian and Eulerian mechanics. In the Lagrangian approach, the path of an air parcel (or puff) is followed and the changes tracked along the trajectory path. Lagrangian modeling was mostly used for transport of SO<sub>2</sub> over large distances and longer time-periods [9, 10, 11, 12]. In Eulerian method, the 3-dimensional atmosphere is divided into grid cells, both in horizontal and vertical directions, and the time changes of the properties are identified at each grid cell. Eulerian modeling was adopted for urban area studies on ozone [13]; for SO<sub>2</sub> [14] and for regional scale sulfur [15, 16]. As such Eulerian modeling was used only for specific episodes of a few days. Hybrid approaches, in which particle-in-cell methods were employed, were used by Friedlander and Seinfeld (1969)[17], Eschenroeder and Martinez (1970)[18] and Liu and Seinfeld (1974)[19]. It may be stated that prior to 1980, Lagrangian models were generally used for transport studies of sulfur and other particulate matter whereas Eulerian models were adopted for episodic events of secondary pollutants such as ozone. After 1980, the basic concepts were fine tuned with development and use of 2-D and 3-D global troposphere models. AERMOD and CALPUFF computer packages were developed for simulation of non-reactive chemicals (e.g., SO<sub>2</sub>). AERMOD is a steady-state Gaussian plume model which uses wind field derived from surface, upper-air, and onsite meteorological observations combined with terrain elevations and land use. CALPUFF is a non-steady state Lagrangian puff dispersion model with advantage of realistically simulating the transport in calm and stagnant conditions and over complex terrain, and coastal regions with sea/land breezes. AERMOD is suitable for short-range simulations whereas CALPUFF is appropriate for both long-range and short-range simulations.

There are different types of modelling approaches available and they are photochemical modelling, Plume Rise models, particle models, Deposition Modules, Odor models and Statistical models and a brief description as follows.

#### 4.1 Photochemical modeling

These photochemical models are large-scale air quality models that simulate the changes of pollutant concentrations in the atmosphere using a set of mathematical equations characterizing the chemical and physical processes in the atmosphere. These models are applied at multiple spatial scales from local, regional, national, and global. Some examples of photochemical models are to be CMAQ, CAMX, UAM, WRF/Chem etc.

The Community Multi-scale Air Quality (CMAQ) modeling system has been designed for air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation [<http://www.epa.gov/asmdnerl/CMAQ/index.html>]. CMAQ was also designed to have multi-scale capabilities so that separate models were not needed for urban and regional scale air quality modeling. CMAQ modeling system simulates various chemical and physical processes that are thought to be important for understanding atmospheric trace gas transformations and distributions.

The Comprehensive Air quality Model with extensions (CAMx) is a computer modeling system for the integrated assessment of gaseous and particulate air pollution [<http://www.camx.com/>]. This model is designed to simulate air quality over many geographic scales; treat a wide variety of inert and chemically active pollutants like Ozone, inorganic and organic PM<sub>2.5</sub>/PM<sub>10</sub>, Mercury and toxics and to provide source-receptor, sensitivity, and process analyses.

The Urban Airshed Model (UAM) modeling system, developed and maintained by Systems Applications International (SAI), is the most widely used photochemical air quality model [<http://uamv.saintl.com/>].

#### 4.2 Plume rise models

The simplest way of estimating smoke concentrations is to assume that plumes diffuse in Gaussian pattern along the centerline of a steady wind trajectory. Plume models usually assume steady state conditions during the life of the plume, which means relatively constant emission rates, wind speed, and wind direction. For this reason, they can be used only to estimate concentrations relatively near the source or for a short duration with restrictions to the influence of topography or land use. Most air pollution models include a computational module for computing plume rise i.e., the initial behavior of a hot plume injected vertically into a horizontal wind flow, e.g., PRIME in AERMOD and HYSPLIT.

#### 4.3 Particle models

Particle model simulates the source by the release of many particles over the duration of the burn. The trajectory of each particle is determined as well as random component that mimics the effect of atmospheric turbulence. This allows a cluster of particles to expand in space according to the patterns of atmospheric turbulence rather than following a parameterized spatial distribution pattern, such as common Gaussian approximations. These models tend to be the most accurate way of simulating concentrations at any point in time but restricted to individual point sources with simple chemistry or sources that have

critical components such as toxins that must be tracked precisely. These models use Lagrangian coordinates for accurate depiction of place of each time of particle movement e.g. HYSPLIT.

#### 4.4 Deposition modules

Many air pollution models include the computational module for computing the fraction of the plume deposited at the ground as a consequence of dry and wet deposition phenomena.

#### 4.5 Odor modeling

Odor models include algorithms to simulate instantaneous or semi-instantaneous concentrations, since odors are instantaneous to human sensations. The mechanisms of dispersion of odorous chemicals in the atmosphere are the same as the dispersion of other pollutants. In multiple pollutants emission, the relationship between concentrations of individual chemicals and odor is not well defined and odor must be characterized in terms of an odor detection threshold value for the entire mixture of odorous chemicals in the air.

#### 4.6 Statistical models

Statistical models are techniques based on statistical data analysis of measured ambient concentrations. These are non-deterministic, as they do not establish nor simulate a cause-effect, physical relationship between emissions and ambient concentrations. These models are used in air quality forecast and alarm systems and receptor modeling. Statistical techniques have been used to forecast air pollution trends a few hours in advance for the purpose of alerting the population. Receptor models are mathematical or statistical procedures for identifying and quantifying the sources of air pollutants at a receptor location. Receptor models use the chemical and physical characteristics of gases and particles measured at source and receptor to both identify the presence of and to quantify source contributions to receptor concentrations e.g., Chemical Mass Balance (CMB) Model.

Basically there are two approaches for the computation of pollutants dispersion in the atmosphere. One is the offline approach, in which meteorological fields are first simulated and dispersion models use these meteorological data for dispersion and deposition computations with no feedback between pollutant concentrations and meteorological fields. In the online approach, the meteorology and dispersion models are run simultaneously, with exchange of information both ways at each time step. Both these methods have their own advantages, offline method more frequently used for primary pollutants such as mercury, PM<sub>2.5</sub> etc and online approach for secondary pollutants such as ozone. We briefly describe here outlines of HYSPLIT offline model and WRF/Chem online model as results from dispersion studies over the Mississippi Gulf coast region with these two models carried out at TLGVRG, Jackson State University under a NOAA supported research program are presented in later sections.

#### 4.7 HYSPLIT model

HYSPLIT (Hybrid Single-Particle Lagrangian Integrated Trajectory) model version 4, developed jointly by National Oceanic and Atmospheric Administration (NOAA) Air Resources Laboratory (ARL) and Australian Bureau of Meteorology, is a computational tool designed to produce air parcel trajectories, and to carry out simulations on different spatial and time scales from local, regional and long-range transport, dispersion, and deposition of

air pollutants [20]. The model can take inputs of meteorological data from any of the Mercator, Lambert and Polar map projections but the data is required on grids and at regular time intervals. The model handles the input data from different resolutions, interpolates to an internal terrain following sub-grid and performs the calculations using data from fine to coarse resolutions and also from different map projections, e.g. starting from a Mercator or Lambert conformal regional grid and switching to Polar stereographic global grid. The trajectories and the pollutant dispersion and concentrations are calculated using Lagrangian mechanics in which advection and diffusion are calculated independently and has computational advantages with single point source emissions without constraints on resolution as compared to the application of Eulerian method for complex emission scenarios requiring solutions at all grid points of a region. Hysplit model computes the trajectories based on Lagrangian approach which is the advection of each particle in time following three dimensional velocity fields. In this model, dispersion and deposition can be computed using either puff or particle model or a hybrid in which both puff and particle approaches are adopted. In puff model, pollutant puffs are released from the source at regular intervals with each puff containing an appropriate fraction of the pollutant mass. The puff expands in time according to the atmospheric dispersion and advected following the trajectory. The puffs will split into new smaller puffs when their size exceeds the meteorological grid. The expansion within grid cell represents dispersion due to sub-grid scale turbulence and puff splitting represents grid scale process. Concentrations are calculated on the grid following a defined spatial distribution within the puff. In the particle model, cluster of particles are released from the source which will expand in space and time following the atmospheric dispersion. Advection of each particle will have a component related to in situ atmospheric turbulence. Concentrations are calculated as a sum of all the particles in a grid cell. By default, Hysplit model uses a hybrid approach in which puff and particle dispersions are incorporated in the horizontal and vertical representations respectively, which has the advantages of using puff model for better representation of horizontal distribution limiting the number of particles and better particle representation in the vertical where large discontinuities are possible. Both the horizontal puff and vertical particle dispersions use turbulence velocity components obtained from meteorological data. Regardless of the approach, atmospheric stability, atmospheric mixing and rate of pollutant dispersion are necessary for simulating pollutant dispersion. Atmospheric stability is estimated from wind and temperature parameters, horizontal and vertical mixing coefficients are estimated from velocity deformation and the coefficients of heat respectively, and the dispersion is computed as dependent on the mean and turbulent velocity components. Concentrations are summed up at each time step at all the grid points. This methodology clearly indicates the importance of the input meteorological data towards best representation of the vertical atmospheric structure. This model is simple to use with menu driven operations with the computations requiring only a few minutes operable on both windows and Linux based computer systems. The current version 4.9, suitable for Windows, was released on February 24, 2009 and Beta version suitable for IBM AIX and Linux servers was released on August 25, 2009.

#### 4.8 WRF/Chem model

The Weather Research and Forecasting - Chemistry model (WRF/Chem) is a new generation regional air quality modeling system developed at NOAA (National Oceanic and Atmospheric Administration) [21]. This model uses the Eulerian mechanics, in which



meteorology and chemistry variables are predicted at all the grid points at each time step. Although the computations are time consuming, it is most suited for prediction of air quality which requires full and continuous interaction of chemical species with meteorological parameters. This modeling system has two modules for meteorology and chemistry. For meteorology part, ARW mesoscale weather prediction model described in section 3 is used. The chemistry module treats the processes of dry deposition, coupled with the soil/vegetation scheme; aqueous phase chemistry coupled to some of the microphysics and aerosol schemes; biogenic emissions; anthropogenic emissions; gas-phase chemical reaction calculations; photolysis schemes; and aerosol schemes with different choices. The air quality component of the model is fully consistent with the meteorological component; both components use the same transport scheme, the same horizontal and vertical grids, the same physics schemes and the same time step for transport and vertical mixing. The model is consistent with all conservative transport done by the meteorology model. The resolution of the model is flexible, ranging from a few kilometers to hundred kilometers. This modeling system is suitable as coupled weather prediction/ dispersion/ air quality model to simulate release and transport of primary pollutants such as particulate matter and the prediction of secondary pollutants such as ozone. The model can be run on parallel processing computer platforms to save computational time. The current version is 3.2.1 released on August 18, 2010.

## 5. Air Quality modelling over Mississippi Gulf Coast

Pollutant contamination in the environment is a serious environmental concern for US Gulf coast region as of many other coastal habitats elsewhere. The Mississippi coastal region is environmentally sensitive due to multiple air pollution problems originating as a consequence of several developmental activities such as oil and gas refineries, operation of thermal power plants, rapidly increasing traffic pollution etc. The Mississippi Delta encompasses the largest area of coastal wetlands in the United States and supports one of the most extensive developments of petroleum extraction of any coastal area in the world. This area has been experiencing ecological impacts from energy development related human activities for more than hundred years. Coastal wetlands are vital for protecting developed areas from storm surges, providing wildlife and fish habitat, and improving water quality. Mississippi Gulf Coast area has sensitive ecosystems like National Forests, State parks, wildlife management and refuge areas, conservation areas or wildlife sanctuaries. The growth of industrial and commercial operations has created a need for air pollution dispersion models that can handle complex meteorological conditions of the coastal environment. Differential heating, strong thermal gradients along the land-sea interface and topographic friction cause localized mesoscale phenomena such as land-sea breeze circulations, sea breeze induced convection and formation of thermal internal boundary layer. The horizontal and vertical extents of the land-sea breeze, the internal boundary layer and their spatial heterogeneity under varying synoptic meteorological settings typify the complex dispersion patterns in the coastal region. The Thermal Internal Boundary Layer (TIBL) limits the region of vertical mixing, heating/convection and the low-level circulation characteristics which influence the coastal area dispersion. These spatio-temporal effects are to be included in the dispersion assessment for realistic air quality estimations using appropriate meteorological and dispersion models.

During the recent past years, air quality modeling studies have been carried out under varied meteorological conditions using sophisticated mesoscale models and observational



assimilation techniques which have shown significant success [22-31]. At Jackson State University, we have conducted several studies on multi-scale simulation of meteorological fields for wind, temperature, humidity, and planetary boundary layer (PBL) turbulence utilizing ARW mesoscale weather prediction model (described in section 3.1). The simulated high resolution meteorological fields were integrated with HYSPLIT dispersion model (described in section 4.7) for studies on the source- receptor relationships of mercury and PM<sub>2.5</sub> pollutants. Similarly WRF/Chem model (described in section 4.8) was used to study the evolution of surface ozone over MS Gulf coast region and Jackson city urban metropolitan region. We present here the results from our studies which indicate the importance and usefulness of offline models for study of primary pollutants (Hg and PM<sub>2.5</sub>) and online models for surface ozone.

### 5.1 Case study of PM<sub>2.5</sub>

The Mississippi Gulf Coast is a typical coastal urban terrain featuring several industries that have been identified as emission sources of PM<sub>2.5</sub> and its precursor gases. A case study was undertaken to assess the WRF-HYSPLIT modeling approach towards assessment of source-receptor relationships of PM<sub>2.5</sub> over MS Gulf Coast [32]. For this study, measurements of PM<sub>2.5</sub> sulfate and nitric acid collected as 6-h samples during 17-20 June 2009 at the two selected locations, Harrison County School (30.5N, 89.1W) and Wiggins Airport (30.8N, 89.13W) were used. During this period, the concentrations of PM<sub>2.5</sub> sulfate and HNO<sub>3</sub> at Harrison and Wiggins were in the range of 5–8  $\mu\text{g m}^{-3}$  for sulfate and 1.5–3  $\mu\text{g m}^{-3}$  for HNO<sub>3</sub>. The experimental study constituted two parts, simulation of atmospheric fields using WRF model and deriving back trajectories and forward deposition concentrations using HYSPLIT model. WRF model was used to produce the necessary atmospheric fields for 24-h periods with the outputs were stored at 1-h interval as needed for input to dispersion model. Model-simulated atmospheric flow fields were validated by comparison with the North American Mesoscale (NAM)-12 km regional analysis as they are critically important for computation of back trajectories and forward dispersion. The model simulated wind flow showed anti-clockwise circulation agreeing with NAM analyses. The onset and extent of sea breeze along the coastal regions was well simulated. HYSPLIT model, driven by meteorological inputs from ARW model, was used to produce 24 numbers of back trajectories at 1-h intervals to identify the sources along the paths of trajectories. The back trajectories, drawn from each observation site (Figure 1) shown that the air parcels were mostly confined to heights below 1.0 km within the planetary boundary layer and had paths in the quadrant between south and west, all pointing the origination of parcels from land on west-side and from sea on south-side (i.e.) Gulf of Mexico. Specifically, Watson, Cajun, and Morrow power plants were identified to be possible land sources as located within the path of back trajectories. HYSPLIT model was run in the forward mode, driven by the ARW model-generated atmospheric fields at 1-h interval and the hourly emission rates, starting from each of the three identified coal-fired power plants to produce the 24-h atmospheric dispersion separately for SO<sub>2</sub> and NO<sub>x</sub> with the hourly emission rates derived from EPA annual emissions data. The forward 24-h atmospheric dispersions from the three sources for SO<sub>2</sub> (Figure 2) showed the dispersion to be towards east/northeast under the prevailing wind flow of southwesterly/westerly relative to the observation sites. The pattern of the pollutant dispersion was a slowly expanding plume due to the low magnitude of the wind speed (2–5 m/s). The contributions from each of the three power plants to the two

observation sites have shown that Big Cajun and Morrow plants contributed to a smaller extent  $<0.235 \mu\text{g m}^{-3}$  for Wiggins location while none of three sources contributed for the observations at Harrison although these two sites are only 65 km apart. These results lead to the conclusion that increasing activity in diesel-powered heavy duty vehicles (ship) over the Gulf of Mexico (as 60% of US energy imports are from this area) and ports around, diesel oil emissions from this area may also contribute to precursors  $\text{SO}_2$  and  $\text{NO}_x$  of  $\text{PM}_{2.5}$ . The source attribution from the Gulf of Mexico could also be due to the diurnal Gulf breeze; with the night time land breeze carry the land-borne precursor pollutants on to the sea and daytime Gulf breeze would bring back the pollutants from the sea to the land region, thus representing the Gulf of Mexico as a virtual pollutant source. Although the case study does not concern with an episodic event, it brings out the result that the integrated modeling approach does not produce spurious results.

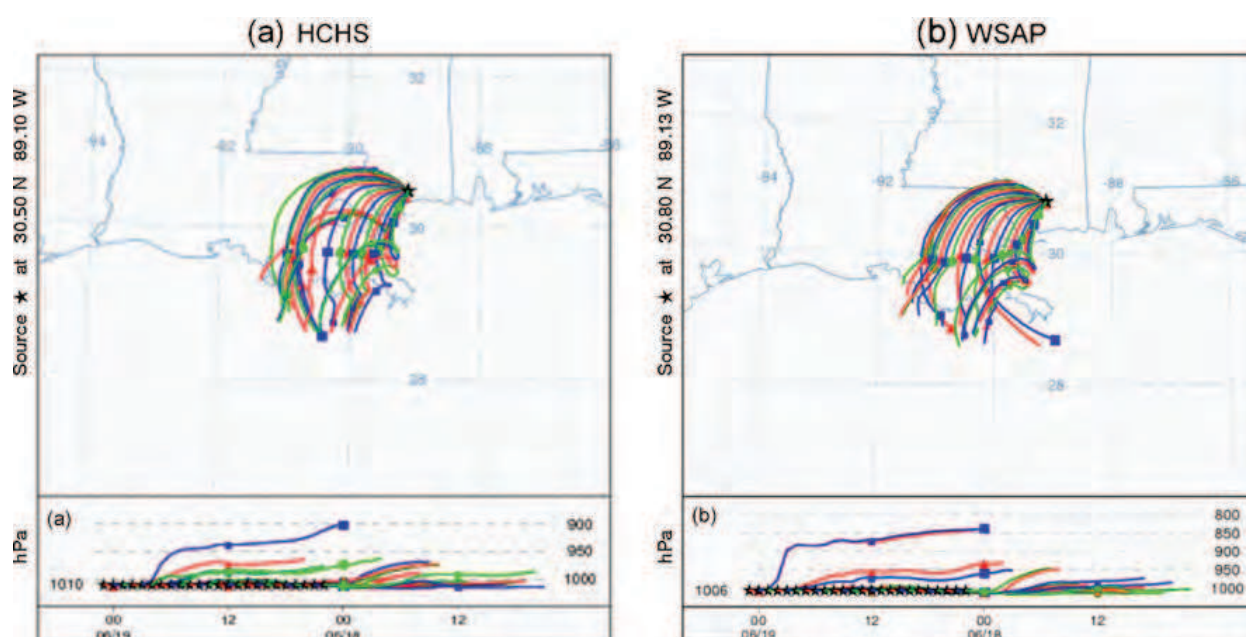


Fig. 1. Computed back trajectories at 1-h intervals for the 24-h period ending 0100 UTC on 19 June 2009 from the observation sites at (a) HCHS (left) and (b) WSAP (right). Top portion shows the horizontal path, and the bottom portion shows the vertical path of the trajectories.

## 5.2 Case study of Mercury

Mercury is known to be a potential air pollutant in the MS Gulf coast region in addition to  $\text{SO}_x$ ,  $\text{NO}_x$ , CO and Ozone. An episode of high mercury concentration, with RGM value of  $75 \mu\text{g/m}^3$  at 1600 UTC of 5 May 2008 observed at the Grand Bay NERR location on Mississippi Gulf Coast (30.41N, 88.4W) was selected as a case study. WRF-ARW model was used to simulate the atmospheric fields at 4 km resolution and with the outputs stored at 1-h interval. The ARW model derived 10m wind flow over the study region was validated with EDAS- 40km analysis. WRF model produced sea breeze with upward vertical motions adjacent to the coast and downward vertical winds in the northeastern and central parts of the land region relatively stronger than EDAS fields. The HYSPLIT model was used to simulate Lagrangian back trajectories from NERR site for the 12-hour period ending at 1600 UTC 5 May 08 with each of inputs from EDAS 40 km, ARW 36 km and ARW 4 km data

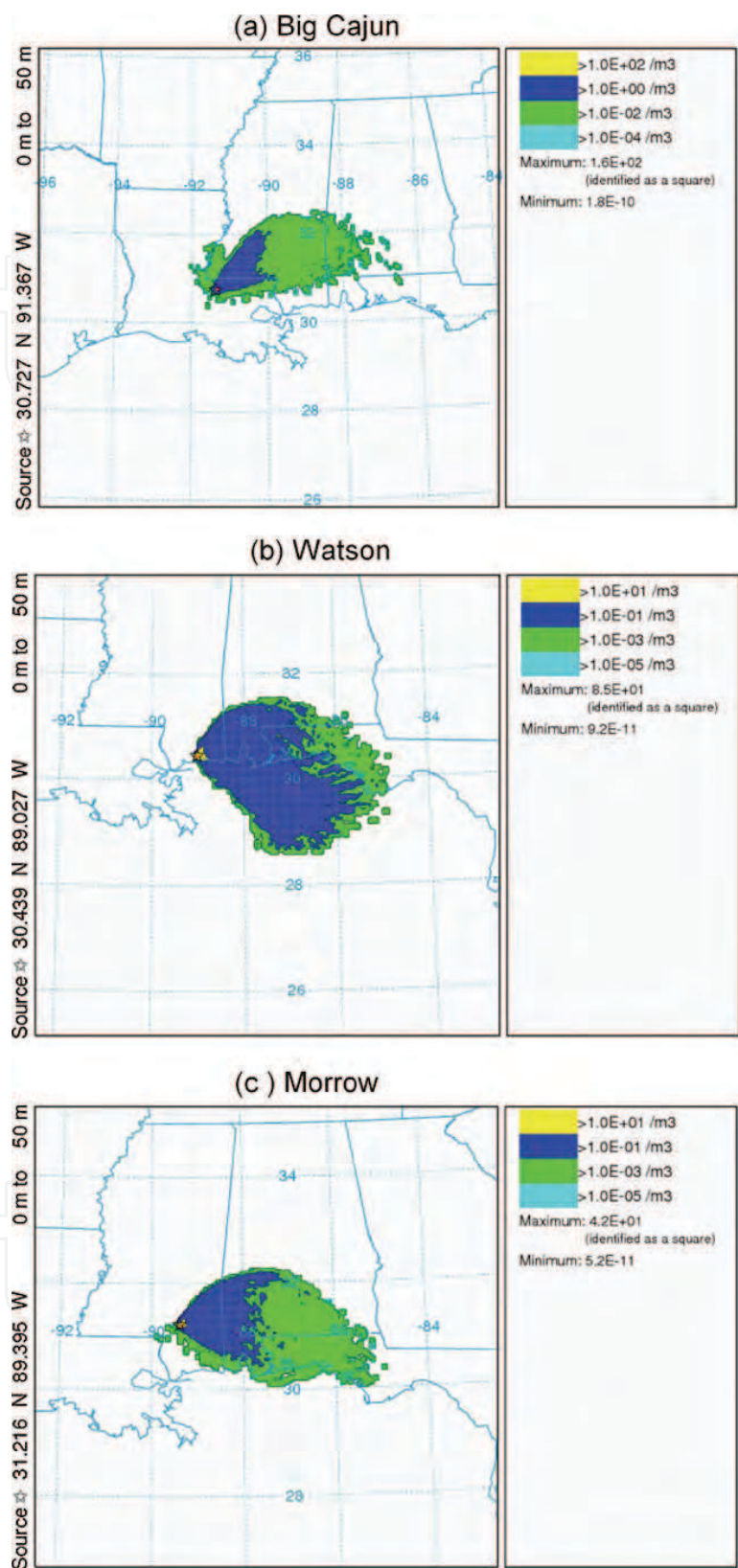


Fig. 2. HYSPLIT-generated SO<sub>2</sub> concentration ( $\mu\text{g m}^{-3}$ ) averaged between 0 and 100 m levels and integrated for 24-h period between 0100 UTC of 18 June 2009 and 0100 UTC of 19 June 2009 sourced from the three identified coal-fired power plants.



(Figure 3). These back trajectories have shown that the air parcels originated towards north-northwest to north and the height of the parcels to be below 100 m level. The trajectories from ARW 4 km data were more towards east and realistic corresponding to mesoscale circulations and associated turbulence and vertical motion fields in the coastal region. The mean trajectory paths indicated four important sources i.e., Charles R Lowman (31.489N, 87.9W) and Barry (30.84N, 88.09W) power plants located in Alabama State and Jack Watson (30.44N, 89.026W) and Daniel (30.64N, 88.59W) power plants located in Mississippi State. The HYSPLIT model produced 24-hour ground level (0 -25 m) RGM concentration patterns with inputs from both the EDAS 40-km analysis (Figure 4) and the high resolution ARW 4km (Figure 5) data were compared. The deposition concentrations with ARW model have shown that Barry plant chiefly contributed with multiple peaks at different times during the day and with the highest concentration occurring 4 hours earlier than the actual measured peak and minute contributions from Daniel and Lowman plants. With EDAS data, Lowman and Daniel plants were identified to contribute chiefly. The concentration values with ARW fields were roughly one order higher than those obtained with EDAS fields. The representation of the wind field in the EDAS and the ARW data lead to major differences in the transport of the RGM from these two nearby sources (Barry and Daniel) in the two simulations. The multiple peaks in the simulated concentrations using ARW data was due to the diurnal circulation at the coast found in the ARW simulations indicating the impact of the sea- land breeze type mesoscale phenomena causing frequent plume transitions. This study helped to establish the sources and their relative contributions to the moderate mercury episode concentrations at NERR observation site using the integrated ARW-HYSPLIT modeling approach.

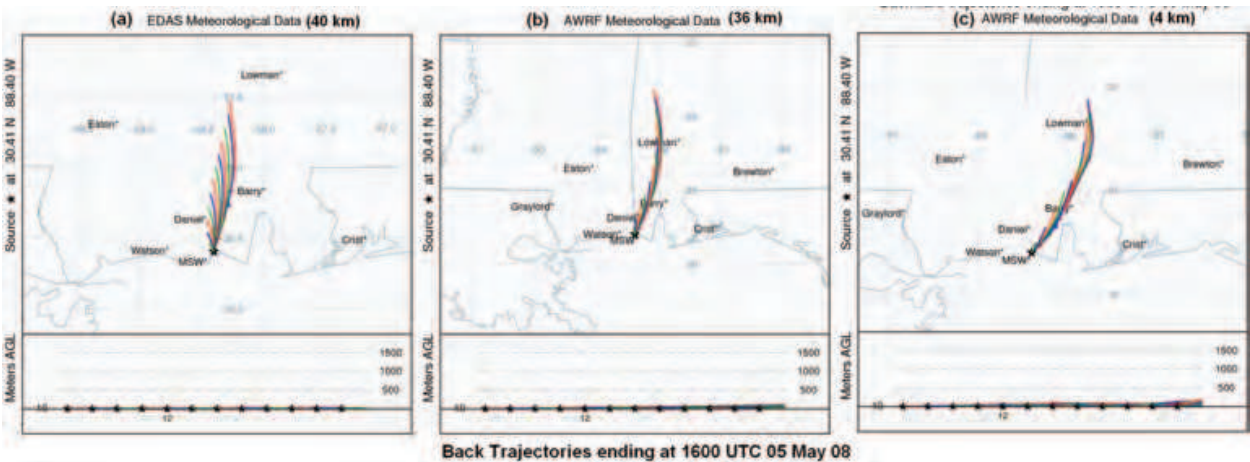


Fig. 3. Back trajectories produced by HYSPLIT model using EDAS-40 km (left); ARW-36km (middle) and ARW-4 km (right).

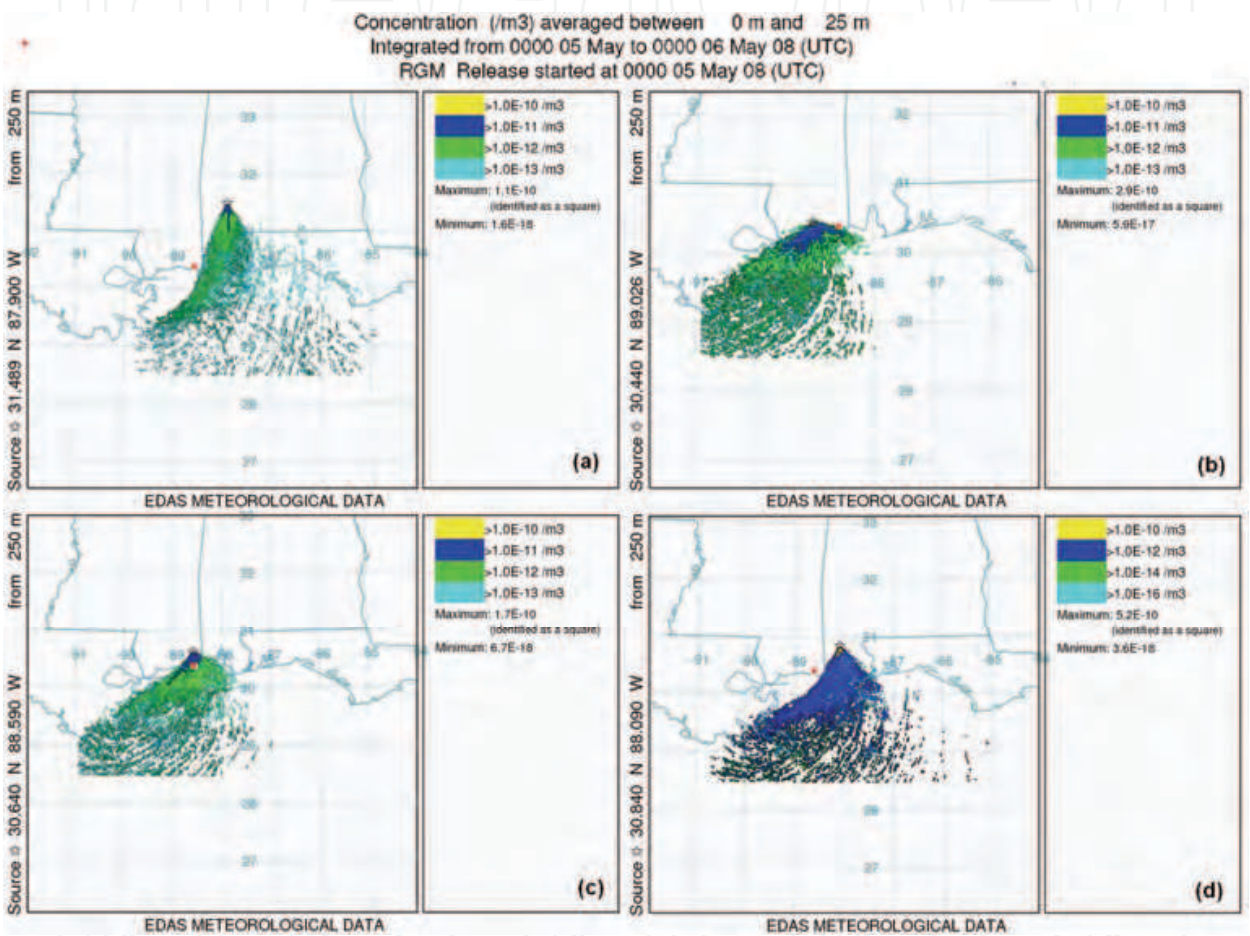


Fig. 4. Atmospheric dispersion as predicted by HYSPLIT model using EDAS-40 km data from the four different sources of Lowman (upper left), Watson (upper right), Daniel (bottom left) and Barry (bottom right).



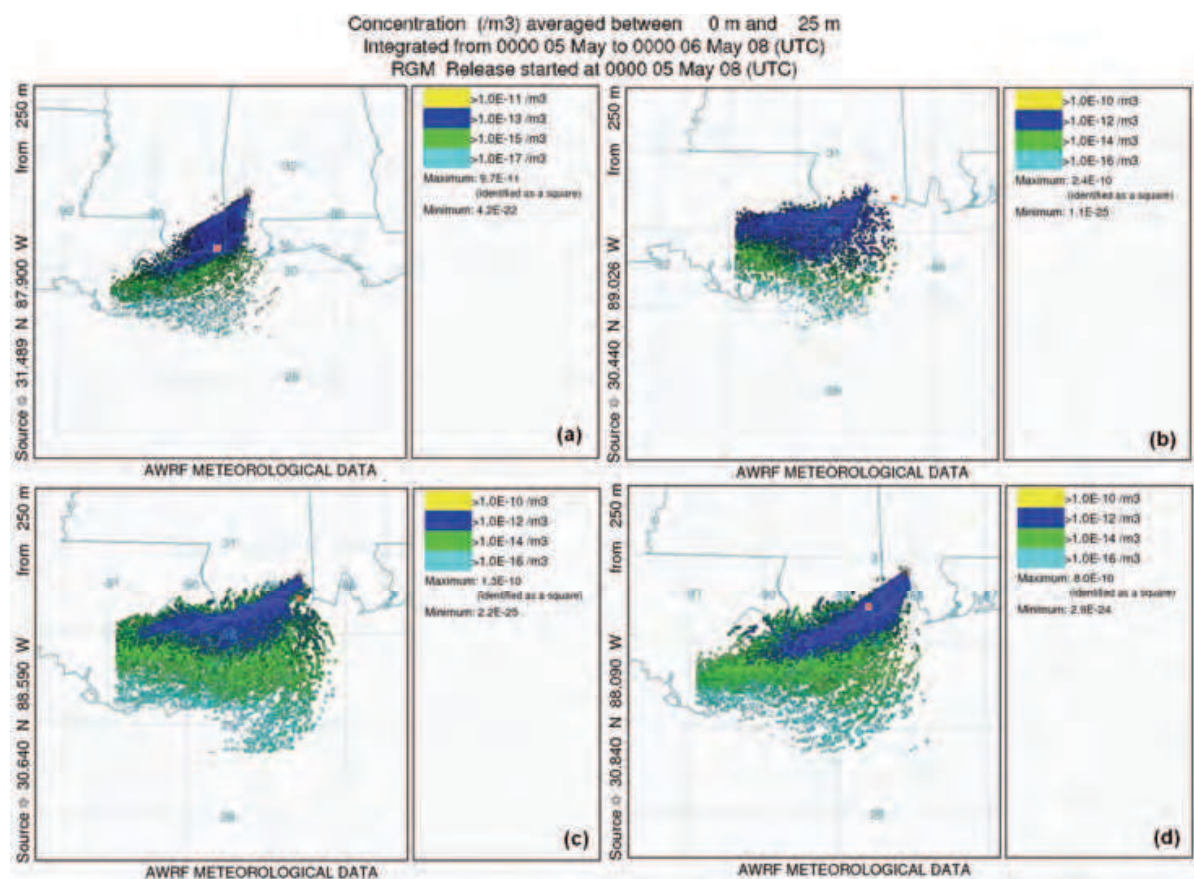


Fig. 5. Atmospheric dispersion as predicted by HYSPLIT model using ARW- 4 km data from the four different sources of Lowman (upper left), Watson (upper right), Daniel (bottom left) and Barry (bottom right)

5.3 Case study of surface ozone over Jackson metropolitan area

As per US EPA (United States Environmental Protection Agency), urban air quality in US with reference to ozone is a growing concern due to its oxidative capacity which will have great impact on the environment. Large number of people are likely to be exposed to the unhealthy ozone concentrations when ground-level ozone gets accumulated in urban metropolitan areas under certain weather conditions [33] and quantitative atmospheric dispersion models will be of great help to provide effective decision support systems for planners and administrators. We made an attempt to study the evolution of surface ozone and other precursor emissions like NO<sub>x</sub> and CO over southeast parts of US in general and Jackson, MS urban area in particular. We were motivated to take up this study to assess the performance of WRF/Chem in the simulation of a moderate ozone episode over an urban locality in which the atmospheric flow patterns are strongly influenced by local terrain and land cover patterns and the results from this study would provide useful information of urban air pollutants to air quality regulatory agencies and health administrators. WRF/Chem model was adapted to have nested four domains with the horizontal resolution of 36-12-4-1 km (Figure 6), with the innermost 1 km domain covering Hinds County. The chemistry was initialized with idealized profiles of anthropogenic emissions data which consists of area type emissions on a structured 4-km grid and point type emissions at latitude and longitude locations. WRF/Chem model was used to simulate the spatial and

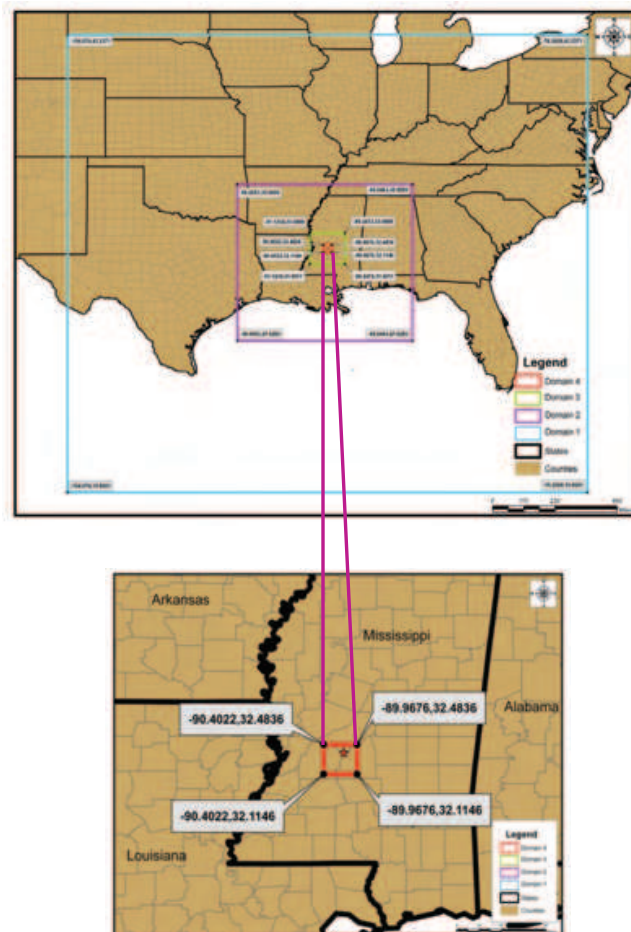


Fig. 6. Model domains. Innermost domain covering the study region of Jackson, MS is shown as red square. Observation site is shown as star.

temporal variations of surface ozone and other precursor pollutants CO (Carbon Monoxide), NO (Nitric oxide), NO<sub>2</sub> (Nitrogen dioxide) and HONO (Nitrous acid). The simulated time series at the specific location (32.38578 N, 90.141006 W) inside Jackson city during 7 PM 6 June to 7 PM 7 June 2006 showed that surface ozone gradually decreased from 7 PM onwards reaching minimum around midnight and stays nearly constant till dawn and gradually increased from dawn to noon reaching a maximum of 50 ppb around 1 PM. The model simulated the time variations and the time of attainment of maximum same as of observations with slight underestimation. The vertical variation of the model simulated ozone at peak time showed that the magnitude of ozone is nearly constant up to 900 hPa level, decreases rapidly up to 800 hPa level and then gradually increases upward. This means that there is good mixing of O<sub>3</sub> in the PBL region extended up to 900 hPa level as common for a summer afternoon. The time series of CO and NO<sub>2</sub> showed a maximum around midnight followed by gradually decrease and with increasing trends at certain times of daytime. The maximum during the first parts of the night could be attributed to these accumulations, decrease during later half to their dispersion and the increasing trends to the reaction between NO with VOC leading to NO<sub>2</sub> and other products. The occurrence of NO maximum at 11 AM, 2 hours prior to ozone maximum indicates the mechanism of NO<sub>2</sub> splitting as NO and O and the formation of O<sub>3</sub> through the amalgamated reaction of O and O<sub>2</sub>. Similar explanation holds good for CO, as O<sub>3</sub> is produced in the troposphere by the

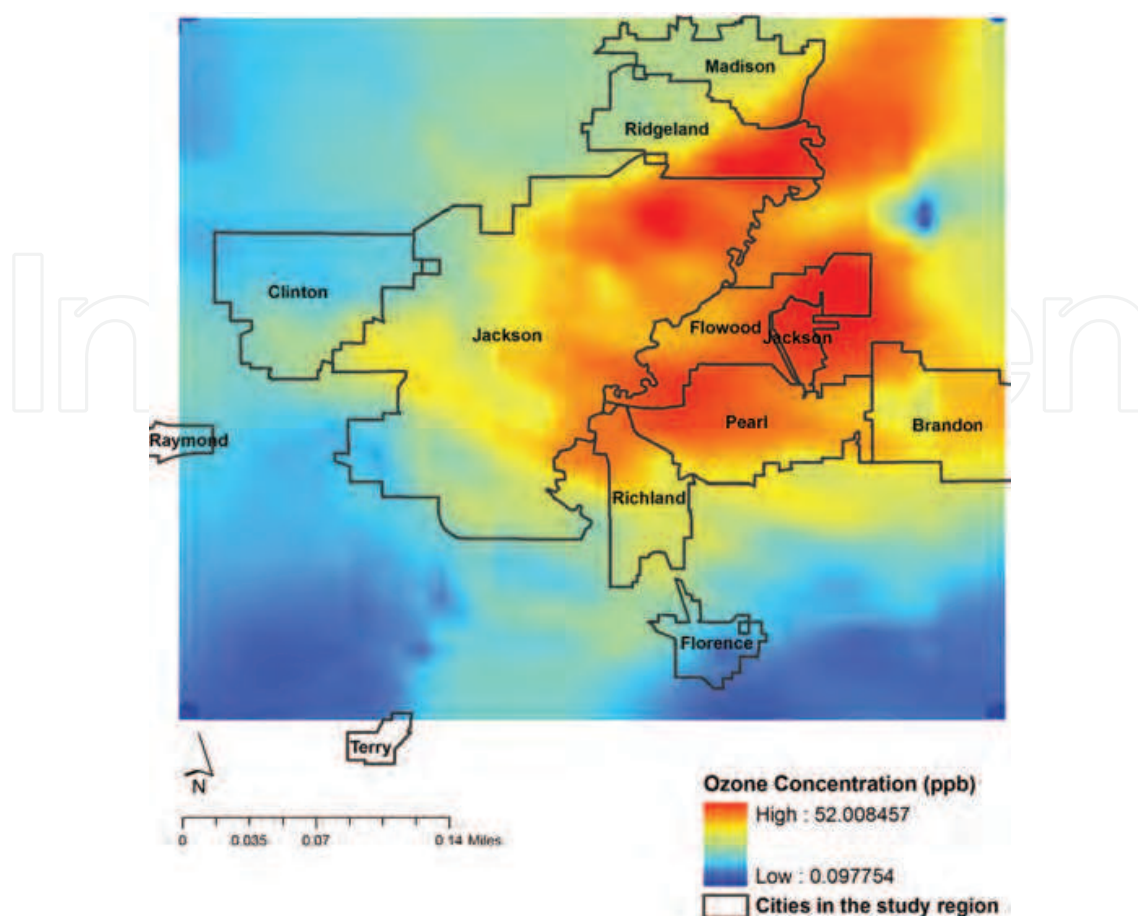


Fig. 7. Spatial distribution of model simulated surface ozone (ppbv) “over domain 4 covering Jackson city and neighbourhood at 1 PM CDT 7 June 2006.

photochemical oxidation of hydrocarbons in the presence of nitrogen oxides ( $\text{NO}$  and  $\text{NO}_2$ ). The time series of HONO showed a maximum between 10-12 AM indicating contributions from nearby combustion sources and its decrease after 12 noon could be due to its breakdown through reactions with  $\text{NO}$  and  $\text{OH}$  in the presence of sunlight. All these indirectly supports formation of ozone as it leads production of  $\text{NO}$  and  $\text{OH}$ . The spatial distributions of  $\text{O}_3$  corresponding to the peak time at 1 PM (Figure 7) showed that the central, east and northeast parts of model domain, covering the regions of Jackson, Flowood, Pearl and parts of Ridgeland and Madison have the maximum concentrations whereas the western and southern parts covering Clinton, Raymond and Florence were less affected. This spatial pattern indicates the maximum as associated with the identified urban locations due to mobile traffic and combustion sources. The spatial distributions of  $\text{NO}$ ,  $\text{NO}_2$ , HONO and  $\text{CO}$  are similar indicating that mobile and combustion sources in Jackson, Ridgeland and Madison were contributing to the production of  $\text{O}_3$  through chemical reactions. Back trajectories drawn from the observation site showed the air parcels to originate from west and south, where the road-ways are located which confirm that the pollutants of mobile origin are chiefly responsible for the production of ozone in sunlight hours. This study is important as ozone and other pollutant species were simulated at 1 km resolution over Jackson urban metropolitan region providing important information for assessment, management and mitigation of urban pollutants.



#### 5.4 Case study of surface ozone over MS Gulf Coast

A regional scale study was undertaken to simulate the surface ozone in the central Gulf coast using WRF/Chem model. A moderately severe ozone episode, with ozone values exceeding 80 ppbv that occurred during 8-11 June 2006 was selected for a case study [34]. The model was configured with three two-way interactive nested domains (36-12-4 km resolution) and 31 vertical levels (Figure 8) with the inner finest domain covering the Mississippi coast. The default profiles for chemical species available with the model were used as the initial pollutants. The model simulated meteorological fields and ozone distributions were compared with available observations for validation. Several sensitivity experiments with different planetary boundary layer and land surface model schemes which revealed that YSU PBL scheme in combination with NOAA land surface model provided best simulation of meteorological fields in the lower atmosphere over the MS Gulf Coast region [35]. The patterns of simulated surface ozone and NO<sub>2</sub> concentrations with different PBL and land surface physics have shown variations. While the patterns of ozone were similar with the YSU and MYJ PBL formulations, MYJ PBL produced relatively shallow mixing layers as compared to moderately deep mixed layer development with YSU and ACM schemes. As of soil schemes, 5-layer soil model simulated relatively deeper mixed layers than NOAA LSM. The simulated ozone patterns with ACM PBL scheme were different from other PBL schemes as it produced localized higher concentrations over northern Mississippi, eastern Louisiana and west Florida coast (Figure 9). The peak ozone concentration were  $\geq 65$  ppbv with ACM PBL over the northern parts of Mississippi river and west Florida coast located to the south of Alabama. The convergence in the surface flow along the coast and along Mississippi river in runs with ACM PBL and RUC LSM caused high ozone formation in these areas. The combination of YSU PBL and NOAA land surface schemes gave best simulations for all the meteorological and air quality fields with least BIAS, RMSE and highest correlation values due to better simulation of PBL height, wind speed, temperature and humidity.

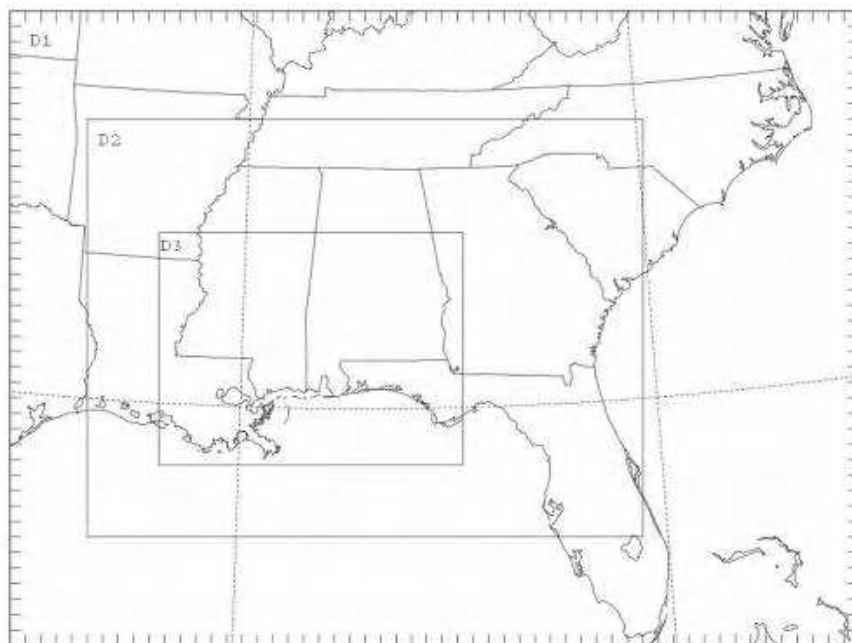


Fig. 8. Modelling domains used in WRF/Chem. Outer domains D01, D02 are coarse with resolutions 36 and 12 km and the inner finer domain (D3) is of resolution 4 km.

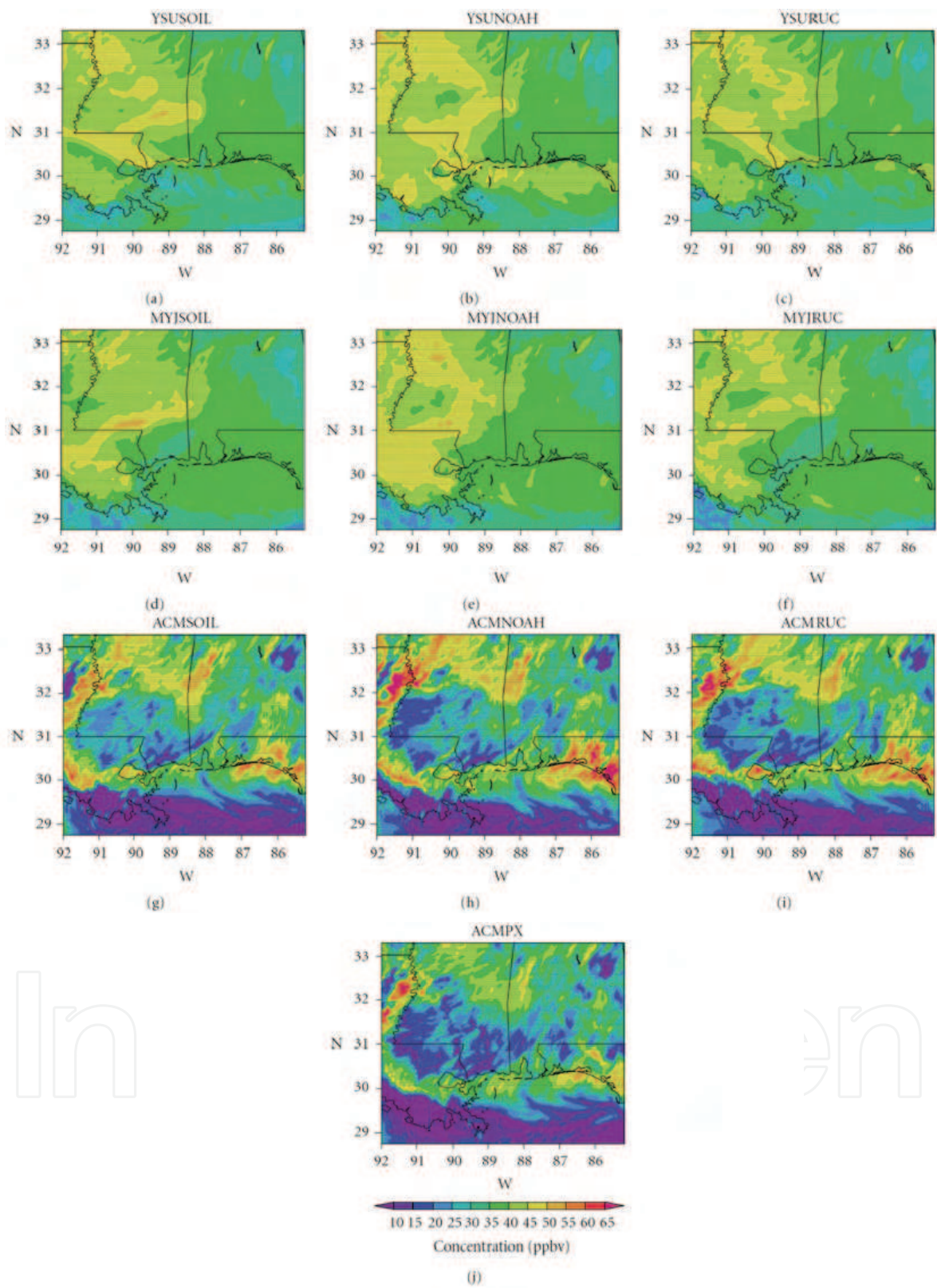


Fig. 9. Simulated ozone concentration (ppbv) in the model fine domain at the lowest level (30m) from experiments with different PBL and LSM options at 10 CST 9 June 2006 for the experiments YSUSOIL, YSUNOAH, YSURUC, MYJSOIL, MYJNOAH, MYJRUC, ACMSOIL, ACMNOAH, ACMRUC and ACPX.



## 6. Applications of Geographic Information Systems (GIS)

Geographical Information System (GIS) is a powerful tool that facilitates linking spatial data to non-spatial information [36]. With its embedded relational database component, the system assists in storing, mapping and analyzing geo-referenced data in an organized structure [37]. The database and the geographical base form the two major components of the GIS system that helps in visualizing the data in a map format. Unlike the reports generated by stand alone applications, which summarize the tabular data, these maps illustrate the geographical connections among the spatial variables and visually communicate geo-specific information to a decision maker.

The conceptual approach of GIS not only provides the capability of querying the spatial data but also, with its inbuilt analytical tools, translates the existing spatial patterns into measurable objectives. These analytical capabilities of GIS offer a dynamic dimension to 'Spatial Analysis' factor in determining the principles of behavior or illustrating the inter-relationships among spatial and non-spatial data.

Understanding these relationships or dependencies in a spatial phenomenon is the major crux of any field; health, environment, geology, hydrology, air pollution studies, agronomy and many others. With its framework, GIS facilitates the integration of various field-specific applications into its interface and allows integrated ways to conduct research and develop new analytical approaches to relate their information to the terrestrial activities. These abilities (providing fully functional data processing environment) distinguish GIS from other information systems as it results in enhancing the applications with productive findings that are broadened and deepened in a geographic location.

To build a spatial data model, GIS Systems support three basic types of data (1) Vector Data: a) Events or Points: Pattern expressed as points in space, b) Lines: Patterns expressed as networks and c) Polygons: Patterns expressed as analytical units with defined closed boundaries, (2) Raster data: a) Grid-cell data and (3) Image: a) Satellite Imagery, photographs.

The spatial analysis modeling process involves interpreting and exploring the interactions, associations and relationships among these data types specific to a geographic location. The exploratory process in developing the spatial model is composed of a set of procedures.

- To identify/map the various data layers and describe the attributes associated with the spatial pattern (Representation model)
- To explore/model the relationships, association or interactions between the data layers identified in representation model (Process Model)

While representation model involves deriving necessary input datasets, in most of the cases, the datasets needs to be reclassified by setting a common measurement scale to the attribute variables by giving weight age depending on their influence. Numerous interactions/relationships between various data components of a region can be captured by the wide range of spatial analytical modeling tools like Suitability analysis, Distance analysis, Hydrological analysis, Surface analysis. Depending on the type of interaction, the spatial model makes use of these analyses in designing the process.

Another dynamic tool GIS offers is the geo statistical analyst tools that include numerous techniques in exploring and modeling the relationships in the spatial data. The inclusion of interpolation methods provides a powerful environment to the users to assess the quality of their analysis. Many disaster mitigation spatial problems are addressed using the Network Analyst tool as required by different research applications. The capabilities of Network

Analyst tool allows to dynamically model realistic conditions and facilitates in examining the flows within and between the natural and man-made networks.

The broad range of many analyst tools, with their modeling and analysis features, not only makes the GIS applications penetrate through number of research fields (from environment, transportation, community *etc.*) but also exploring associations and relations ships between these fields.

### 6.1 GIS in air pollution studies

The quality of air is a very important factor in projecting or representing the status of environment and health of any region. Air pollution studies that analyze the quality of air provide strategic information to the decision making process and play a significant role in the implementation of the policies that influence the air quality of a region. Most of the air pollution models, in their pollutant distribution simulations, consider the physical characteristics of the pollution such as wind direction, speed, temperature *etc.*, in determining the air pollution trajectory. Integrating these models with GIS presents a geographic dimension to the air quality information by relating the actual pollution concentrations to the plant and human life in that location. With its numerous analyst tools, GIS can demonstrate the relationship of poor air quality and occurrences of deficient human and environmental health [38]. GIS can portray the spatial correspondence between the air quality and the disease statistics in the area that is potentially impacted [39]. In this process, GIS can explore:

- The relative spatial phenomenon of the pollutant with respect to the geographical distribution in terms of location, extent and distance.
- The spatial extent of the pollutant dispersion and its intensity at any geographical location under the impact zone
- The socio-economic characteristics of the populations affected by these pollutants
- The data visualization from various perspectives by classifying and reclassifying the data by determining the class breaks.

Examining the relationships between high pollution concentrations across various demographic thematic layers helps in identifying *hotspots* that are in need of special investigation or monitoring. Data visualization, illustrating such information through a map provides an insight in a more dynamic way that helps the authorities to plan their future strategies.

The output generated from an air pollution dispersant model (Figure 10), illustrates the mercury pollution concentrations in the Gulf Coast region. The intensity and spatial dispersion of the pollutant are presented in a scientific terminology as units and latitude/longitude. The format of this scientific information generated by these models may not be suitable for directly integrating the data into the policy making process. The relevance of this information to a spatial location has to be derived and its implications need to be presented in a format that relates to the socio-economic or health characteristics of the people living in that region. The gap of presenting the scientific format from a geographical dimension can be filled by integrating these outputs with Arc GIS tools. Viewing the same data across various demographic themes projects the vulnerable populations under the impact zone and assists the authorities in making informed choices.

Figure 11 illustrates the HYSPLIT output shown in Figure 10 in a GIS environment. The output of HYSPLIT is obtained in the format of ASCII with relevant data on latitude, longitude and the mercury concentrations at various points in the dispersion trajectory.

Using data management and 3D Analyst tools, the ASCII file is converted into a point data and a TIN (Triangular Irregular Networks) file is created from this vector data. By interpolating the cell Z-values (Mercury concentrations) using natural neighbors method, the TIN is converted to a Raster file. The final mercury dispersion raster file is then mapped over the Gulf Coast states.

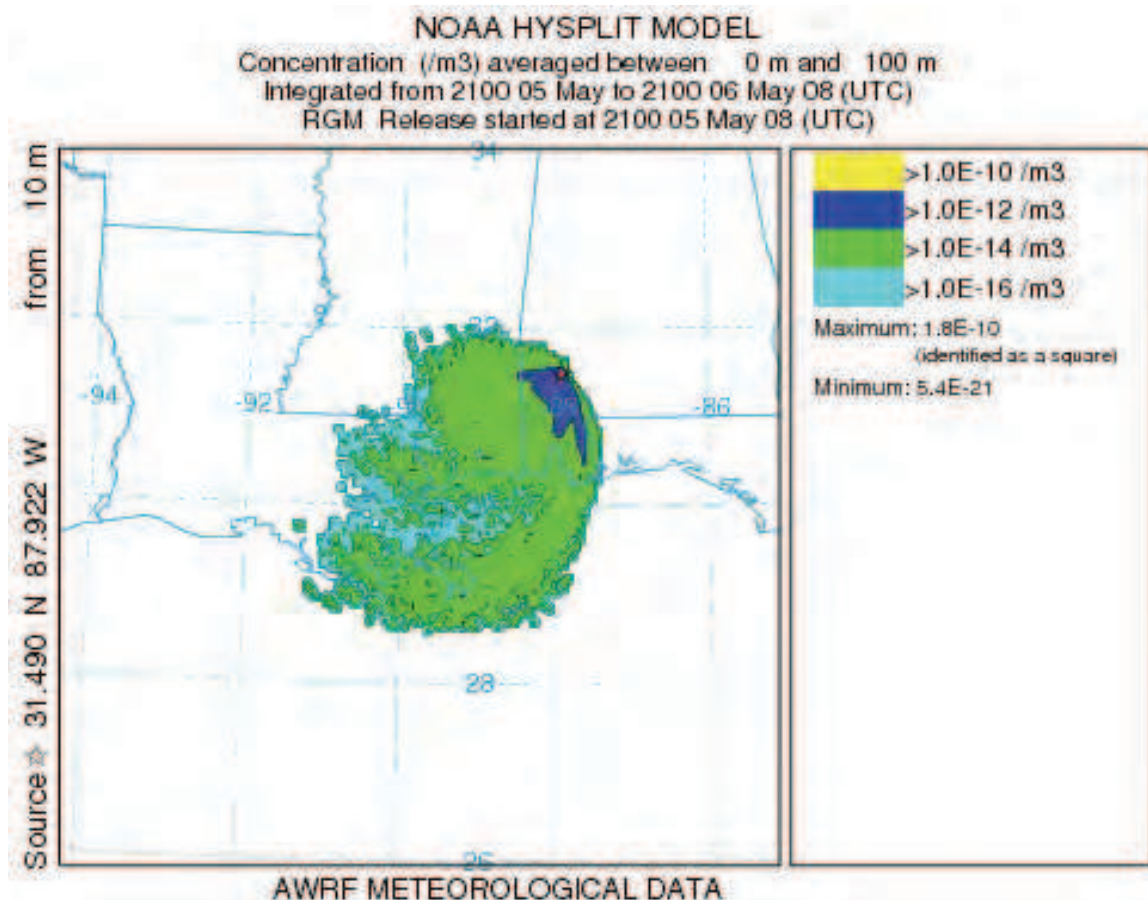


Fig. 10. Output generated from the HYSPLIT model developed by NOAA

Figure 11 describes that parts of Mississippi, Louisiana and Alabama were impacted by the emissions from the Barry Generating Plant in Alabama. The mercury dispersion raster file is overlaid on the classified demographic thematic layer (dark to light color indicates high to low dense population) shows most of the tracts that are under the impact zone are densely populated.

The impact of severe pollution zones: red (very high) and yellow (high) colors, on vulnerable populations (age above 65 years and less than 5 years) are presented in Figure 12 and Figure 13.

Integrating HYSPLIT model output with classified demographic GIS data gives a clear visual representation of the spatial location of highly dense vulnerable populations under impact zone. It assists in projecting the age of the vulnerable population (which in this case ages less than 5 years) under the risk due to the pollution impact.

A spatial phenomenon or a relation can be developed by examining the health statistics of these tracts against the pollution levels they are being exposed. Such spatial phenomenon may reveal hidden facts and can be a significant contribution in designing the policy strategies.



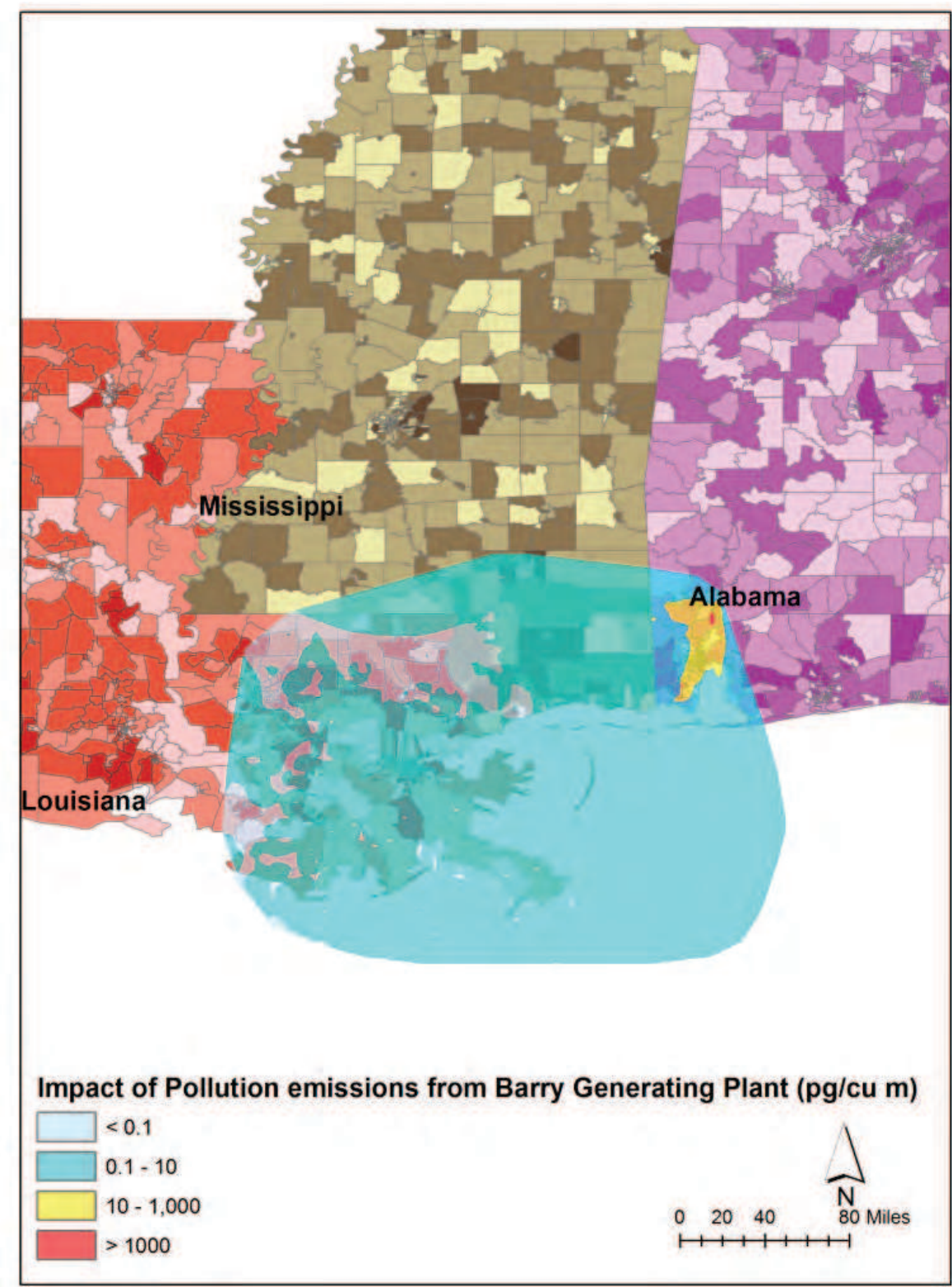


Fig. 11. Representation of HYSPLIT output in GIS environment

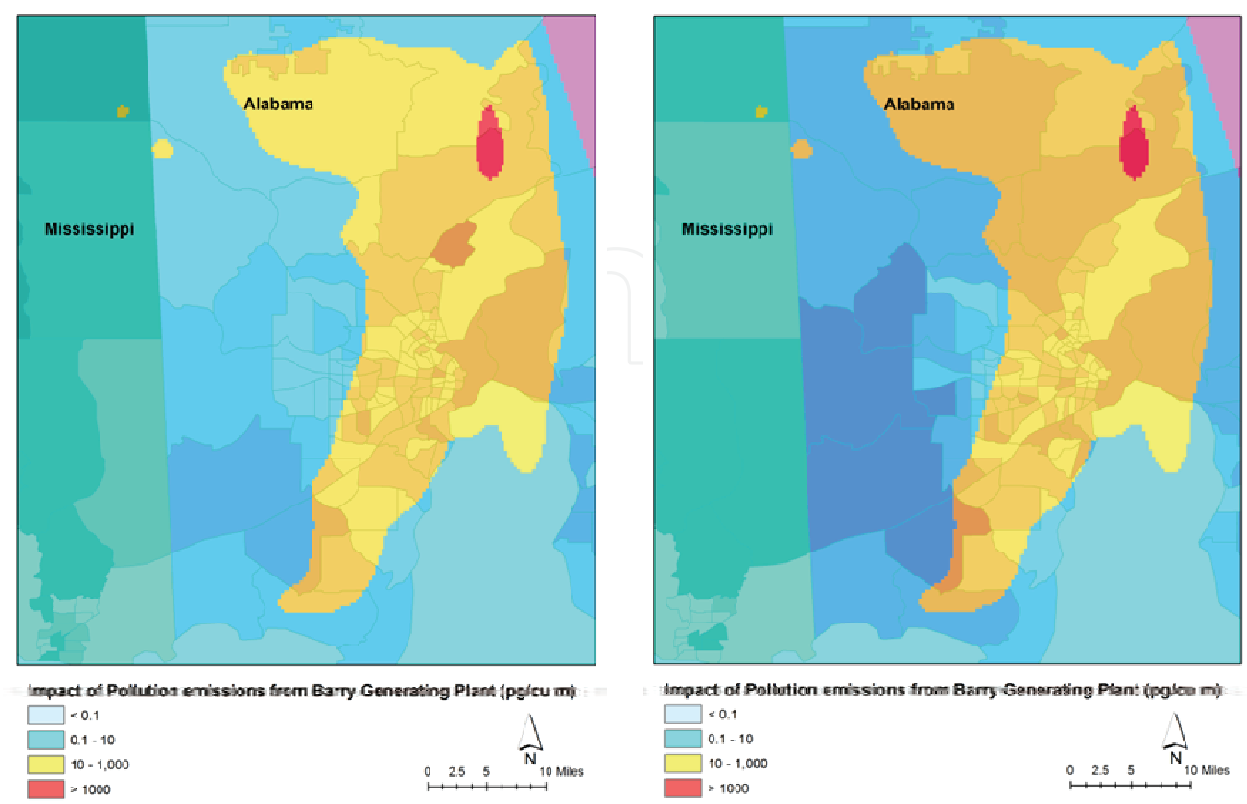


Fig. 12. Population of age above 65 under the impact of Barry Plant-mercury emissions.

Fig. 13. Population of age less than 5 years under the impact of Barry Plant -mercury emissions.

The demographic age classification under the impact zone of 10-1000 pg/m<sup>3</sup> of mercury concentration (yellow color) can be well interpreted from the figures 12 and 13. The GIS functionalities facilitate in estimating the actual numbers: tracts, along with vulnerable population numbers, falling under the impact zone (Table 1). For convenience, four classes of populations were made based on density (i.e.) >1200, 800-1200, 400-800 and <400.

Age \ Population	Population		
	High density population (>1200) (no. of tracts)	Medium density population (800-1200) (no. of tracts)	Low density population (400-800) (no. of tracts)
5 years and below	1797(1)	15761(13)	11665 (28)
65 years and above	1640 (1)	5710 (6)	22652 (38)

Table1. Numbers of area tracts and population affected from pollutant dispersion

The pollutant dispersion region covered approximately 92 tracts in which about 338,439 habitants live. From the data in Table 1, it may be inferred that elders with 65 years and more are the most affected in the two categories of high and low density population concentrations whereas more children below 5 years were affected in the category of 800-1200. This emphasizes the need to detailed analysis using GIS to clearly understand the relative age groups affected, in this case due to pollution. Presenting such statistical



information through GIS mapping leads to risk assessment and provides an idea of not only the areal extent of pollutant influence but also its impact on demographic data lines.

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Leading air quality professionals describe different aspects of air pollution. The book presents information on four broad areas of interest in the air pollution field; the air pollution monitoring; air quality modeling; the GIS techniques to manage air quality; the new approaches to manage air quality. This book fulfills the need on the latest concepts of air pollution science and provides comprehensive information on all relevant components relating to air pollution issues in urban areas and industries. The book is suitable for a variety of scientists who wish to follow application of the theory in practice in air pollution. Known for its broad case studies, the book emphasizes an insightful of the connection between sources and control of air pollution, rather than being a simple manual on the subject.

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