Appendix D

Modeling Protocol

Modeling Protocol

for the

Charlotte-Gastonia-Rock Hill NC-SC

8-hour Ozone

Nonattainment Area

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1.0 Overview of 8-hour Ozone Modeling/Analysis Project

1.1. Policy Overview of the Ozone National Ambient Air Quality Standard

On July 16, 1997, the U. S. Environmental Protection Agency (USEPA) revised the national ambient air quality standard (NAAQS) for ground-level ozone. The 1-hour ozone NAAQS of 0.12 parts per million (ppm) averaged over a 1-hour period (40 CFR 50.9) was modified to an 8-hour ozone NAAQS of 0.08 ppm averaged over an 8-hour period (40 CFR 50.10). The USEPA was subsequently sued over the new NAAQS, and in May 1999, the U. S. Court of Appeals for the D. C. Circuit remanded the 8-hour ozone NAAQS back to the USEPA. In 2001, the USEPA proposed a response to the D.C. Circuit court's remand and reaffirmed the 8-hour ozone NAAQS, which became effective in 2003. On April 30, 2004, the USEPA then made nonattainment designations for the 8-hour ozone NAAQS with an effective date of June 15, 2004, based on air quality data from 2001 through 2003. The designations under the 8-hour ozone NAAQS began the implementation process. A major requirement is the development of a State Implementation Plan (SIP), due for submittal to the USEPA three years after the effective date of the nonattainment designations (June 15, 2007).

The new 8-hour ozone NAAQS is considered much more stringent than the previous NAAQS. The 1-hour ozone NAAQS was remanded one year from the effective date of the nonattainment designations. An exceedance of the 8-hour ozone NAAQS occurs when a monitor measures ozone above 0.084 ppm on average for an eight-hour period (per the rounding convention). A violation of this NAAQS occurs when the average of the annual fourth-highest daily maximum 8-hour ozone values over three consecutive years is greater than or equal to 0.085 ppm. This three-year average is termed the design value for the monitor. Figure 1-1 indicates the counties (based on 2001 through 2003 monitoring data) that had design values that violated the 8-hour ozone NAAQS. The USEPA designates nonattainment areas (Figure 1-2) based on these monitored exceedances and adjacent areas that could be contributing to the violation. Most nonattainment areas are based on Metropolitan Statistical Areas (MSA), although a few boundaries were based on smaller than a full MSA.

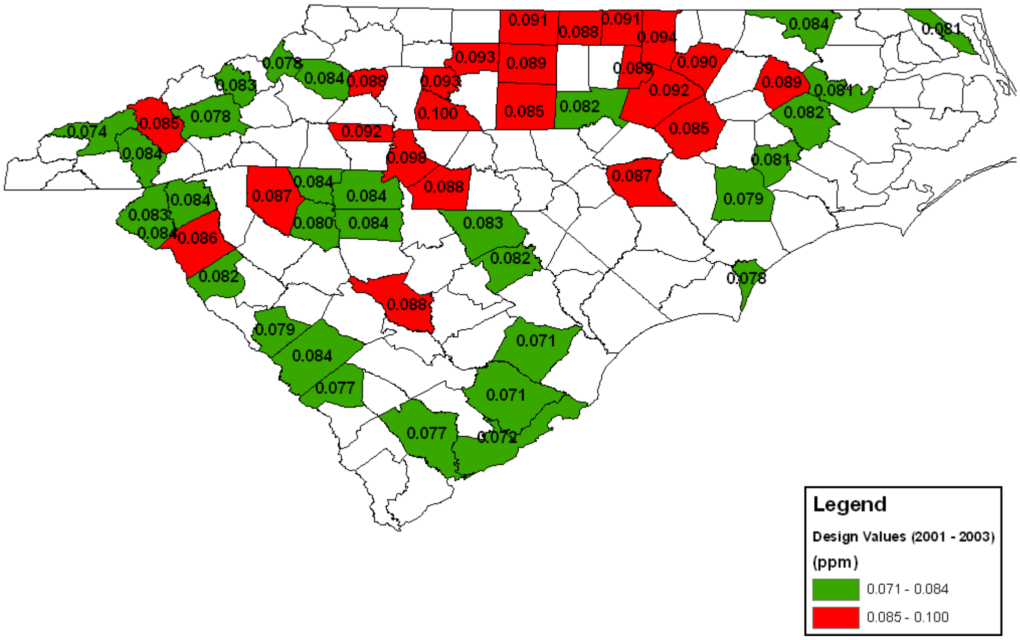

Figure 1-1: 8-hour ozone design values based on 2001 through 2003 monitoring data.

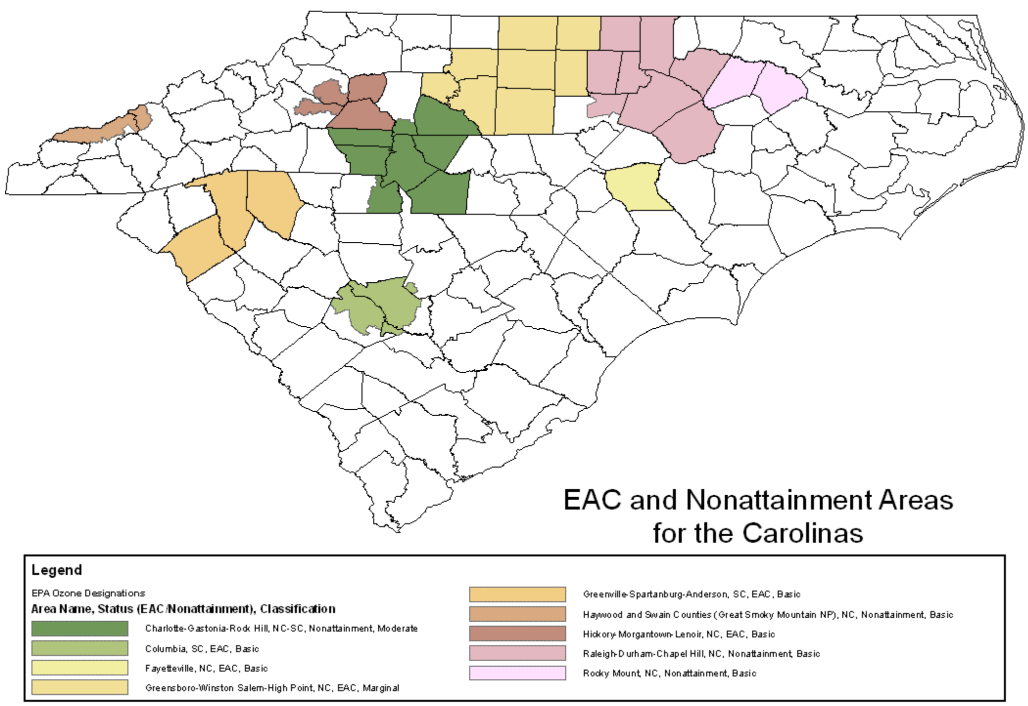

Figure 1-2: Map indicates the USEPA's final designation, with the notes indicating the areas that signed Early Action Compacts, and the area's classification.

1.2. Designations

Since the passage of the 1977 Clean Air Act Amendments (CAAA), areas of the country that violated the ambient NAAQS for a particular pollutant were formally designated as nonattainment for that pollutant. Five categories to define the degree of nonattainment were created for the 1-hour ozone NAAQS (section 181 of the 1990 CAAA). In order of severity, these categories were classified as marginal, moderate, serious, severe and extreme. The highest monitor design value in a nonattainment area was used to determine its classification, with the classification ultimately defining the attainment dates.

With the implementation of the 8-hour ozone NAAQS, there are two subcategories of designation. An area could be designated under section 172 of the 1990 CAAA (subpart 1) as "basic" and would have up to 5 years from designation to attain the NAAQS, or the area could be designated under section 181 (subpart 2) and classified as one of the five categories listed above with attainment dates based on the classification. Areas with a 1-hour ozone design value greater than 0.121 ppm were classified under subpart 2, and all other areas were classified under subpart 1.

Four North Carolina and two South Carolina areas subject to designation entered into Early Action Compact (EAC) programs that made provisions for states and local areas to achieve clean air earlier than the Clean Air Act (CAA) schedule. The four North Carolina areas that have entered into an EAC are Fayetteville area, Triad Area, Mountain Area, and Unifour (Greater Hickory) Area. The two EAC areas in South Carolina are the Columbia area and the Upstate (Greenville-Spartanburg-Anderson) area. The EAC areas in both states have all attained the 8-hour ozone NAAQS. Additionally, the Rocky Mount, Triangle and Great Smoky Mountain National Park nonattainment areas in North Carolina have also attained the 8-hour ozone NAAQS. Therefore, this modeling protocol will focus solely on the Charlotte-Gastonia-Rock Hill (hereinafter, Metrolina) 8-hour ozone nonattainment area. This area includes: Cabarrus, Gaston, Lincoln, Mecklenburg, Rowan, and Union Counties in North Carolina, part of Iredell County in North Carolina, and part of York County in South Carolina.

The Metrolina area has been classified as moderate under subpart 2 by the USEPA, with a maximum attainment date of June 15, 2010. The North Carolina Division of Air Quality (NCDAQ) and the South Carolina Department of Health and Environmental Control (SCDHEC) are committed to developing a comprehensive air quality control strategy to attain the 8-hour ozone NAAQS in the Metrolina area.

1.3. Participating Organizations

From the conceptual model of ozone formation, it is obvious that ozone is a regional problem, which causes SIP modeling to be a substantial undertaking that relies on the interaction of many groups that are affected by overall air quality and that impact the air shed of the affected states. It is imperative to include groups of "stakeholders" from industry, government, and the private sector represented during the modeling/analysis project. As each group involved brings its own perspective, knowledge, and experience to the modeling process, the ability to model and develop strategies for ozone reduction is greatly enhanced. The following organizations are invited to participate in developing the ozone SIP:

- NCDAQ
- SCDHEC
- Carolina Environmental Programs – University of North Carolina Chapel Hill
- Barons Atmospheric Modeling Systems
- University of North Carolina at Chapel Hill
- North Carolina State University
- Sonoma Technology, Inc.
- Mecklenburg County Department of Environmental Protection
- USEPA Region 4
- USEPA Office of Air Quality Planning and Standards
- USEPA Office of Research and Development
- North Carolina Department of Transportation
- South Carolina Department of Transportation
- North Carolina Department of Commerce
- North Carolina Department of Agriculture
- North Carolina State Energy Office
- Progress Energy
- Duke Energy
- Transcontinental Natural Gas Company
- Environmental Defense
- Sierra Club
- Charlotte Department of Transportation
- Furniture Manufacturing Representative
- Chemical Manufacturing Representative
- North Carolina Petroleum Council
- North Carolina Petroleum Marketers' Association
- Centralina Council of Governments
- Catawba Council of Governments
- Representatives from city and county governments in the nonattainment areas

Data and available expertise from participating agencies, organizations, and universities will be utilized in determining projected emissions and control strategies. All data and information will be reviewed and evaluated by the NCDAQ and SCDHEC. All stakeholders are invited to contribute emissions projections and control strategy information.

Both North Carolina and South Carolina will coordinate with various states and other parties as regional modeling is initiated to address the new ozone standards. Various other regional modeling applications, such as Southeastern States Air Resource Managers' seasonal ozone modeling and Visibility Improvement and Tribal Association of the Southeast (VISTAS) regional haze and fine particulate matter ($PM_{2.5}$) modeling, will also be considered. These interactions should provide a forum for discussing the latest improvements and refinements to air quality modeling.

1.3.1. Communication

Communication between the stakeholders is an integral part of completing the modeling/analysis project. Stakeholders need the opportunity to review and comment on documentation, control strategies, and modeling analysis. NCDAQ and SCDHEC will host periodic technical coordination meetings on the SIP process for their respective portions of the Metrolina nonattainment area. Consultation meetings on control strategy development and contingency plans will be held as necessary during the process. In general, as issues arise among the participants, special studies will be defined to help resolve all pertinent issues. Documentation will be developed concerning these issues, including methods of resolution and any remaining uncertainties, which will be submitted as part of each state's SIP.

Due to the far-reaching effects of the ozone attainment demonstration, it is important that all interested parties are kept informed on the progress of the modeling. Industries or organizations not directly represented on a modeling committee can monitor progress through the VISTAS website. NCDAQ, with involvement from SCDHEC, will also host several public meetings and focus groups with potentially impacted parties in order to get the most objective and comprehensive input in the development of the final control strategies.

1.3.2. Protocol Modification Procedures

The model configuration, as well as the source of input data and evaluation process, will be determined at the beginning of the process. In the event that the protocol needs to be revised to incorporate new tools or methodologies, an issue paper stating the need for modification will be developed and circulated to all organizations participating in the study. The issue paper will be discussed at the next scheduled technical coordination meeting. The revised protocol would then be developed and submitted to the USEPA for their review.

1.4. Schedule

NCDAQ and SCDHEC will follow the schedule outlined by the CAA, where a SIP is due for submittal by June 15, 2007. Using a 2009 modeling year, attainment will be demonstrated by at least June 15, 2010 or as expeditiously as practicable.

1.5. Selection of Future Year

A key decision from both a modeling and control strategy standpoint is the selection of the future year by which attainment will be modeled. The future modeling year has been chosen to meet the schedule previously put forth. The time line set by the CAA requires attainment of the 8-hour ozone NAAQS in a moderate area be met by June 15, 2010. Since this date is set prior to the completion of the 2010 ozone season, attainment of the NAAQS would have to be met by at least the end of the 2009 ozone season. NCDAQ and SCDHEC plan to use 2009 as the future year for attainment modeling, as it would coincide with future year modeling for the $PM_{2.5}$ SIP and VISTAS regional haze modeling effort.

1.6. Organization of Air Quality Modeling Protocol

The remainder of the protocol documentation is broken down into nine additional sections as follows:

- Section 2 provides a conceptual description of ozone formation in the Carolinas.
- Section 3 presents details of the ozone episode selection process.
- Section 4 details the models that will be used during this modeling project.
- Section 5 describes the model grid specifications.
- Section 6 discusses the emission inventory development.
- Section 7 lays out the quality assurance plan and procedures.
- Section 8 details the tools and procedures for model performance evaluation.
- Section 9 discusses how the control strategies will be designed.
- Section 10 focuses on the model attainment test and supplemental analyses.
- Section 11 lists the references.
- Appendices follow the final section.

2.0 Conceptual Description of Ozone Formation

To fully understand the complexity of the ozone formation across North and South Carolina, one must first examine the interactions between the biogenic and anthropogenic emissions sources within North and South Carolina and throughout the surrounding region, as well as the geographical orientation, topography, and the meteorological patterns that develop over each of the Carolinas on a typical summertime day. All of these interacting components play a pivotal role in the day-to-day air quality response across the state. On a few select days each summer that often occurring together in episodes, these components work together to produce 8-hour ozone concentrations in excess of the NAAQS. The frequency and duration of these high ozone episodes in an individual summer season are significantly impacted by global scale meteorological patterns and climate deviations.

2.1. General Geography and Topography throughout the Carolinas

The geographic orientation and the topography of the Carolinas help create a climate of great variation and unpredictability for the centrally located Metrolina Area. Both states lie along the South Atlantic Coast in proximity to the warm waters of the Gulf Stream. A semi-permanent subtropical ridge centered to the east, the Bermuda High, contributes an abundance of moisture through much of the summer and fall seasons. Anomalies in its mean position greatly affect conditions needed to produce or even abate ozone production over a wide area extending well beyond the borders of each state.

In addition, the mean positions and strengths of the Bermuda High and Gulf Stream allow for abundant atmospheric moisture influx during all seasons of the year and allows for a variety of weather, from tropical storms to ice and snow events. Effects of each of these features on the overall climate of the Carolinas are often offset by a warm, dry west-to-northwest ("down-sloping") continental flow from over the high terrain of the Appalachians, usually following the passage of a frontal system or surface trough (or "trof") trailing from a strong polar jet stream low sliding over the Appalachians from the Great Lakes into the Mid Atlantic regions. Often this flow helps develop a weak, but broad, surface low pressure just to the east of the mountains, known as the "lee-side trof." Flow patterns around this feature often affect production and/or transport of ozone. Despite the fact that South Carolina contains only a tiny fraction of the mountainous terrain that is so abundant in North Carolina, these "down-sloping" flow patterns affect ozone production across portions of the state in much the same manner.

2.2. North Carolina Geography and Topography

North Carolina is situated in the middle of the Northern Hemisphere and is slightly closer to the Tropics than to the Arctic region. This mid-latitude location on the globe is characterized by mild winters, extended warm-humid summers, and varied spring and fall seasons. This mid-latitude location also allows for extended hours of daylight during the summer season with the sun nearing its zenith at noon on the summer equinox. This near vertical positioning of the midday sun and long duration of the daylight hours are important aspects that help define the overall ozone formation and air quality potential in North Carolina.

With respect to the oceans and landmasses of the Northern Hemisphere, North Carolina is nestled along the southern portion of the Atlantic Seaboard of North America with the Atlantic

Ocean to the east and the continental United States (US) to the west. From the coastal regions of North Carolina, the elevation gradually slopes upward across the Coastal Plain, the Sandhills, and the Piedmont before rapidly increasing to the highest elevation peaks of eastern North America in the Mountains. The proximity to the warm waters of the southern Atlantic and the Gulf Stream allows for abundant atmospheric moisture influx during all seasons of the year and allows for a variety of weather from tropical storms to ice and snow events. This moisture influx is often offset by a dry west to northwest down-slope flow over the high terrain of the North Carolina Mountains from the continental US. The geographic orientation and the topography of North Carolina ultimately creates one of the most difficult to predict and variable climates in the western Northern Hemisphere.

2.3. South Carolina Geography and Topography

South Carolina is situated in the middle of the Northern Hemisphere roughly between 33º and 34º N latitude and is closer to the Tropics than to the Arctic region. This mid-latitude location on the globe is characterized by mild winters, extended warm and humid summers, and varied spring and fall seasons. This proximate location allows for extended hours of daylight during the summer season, with the solar elevation nearing zenith by noon on the summer equinox. This near vertical positioning of the midday sun and long duration of the daylight hours greatly affect the development of optimal ozone formation conditions.

With respect to the oceans and landmasses of the Northern Hemisphere, South Carolina is nestled along the southern portion of the Atlantic Seaboard of North America, with the Atlantic Ocean to the east and the breadth of the continental United States to the west. From the coastal regions of South Carolina, the elevation rises in a gentle upgrade traveling westward away from the seacoast. Terrain is fairly flat across the Coastal Plain (known locally as the "Lowcountry"), somewhat hilly inland through the Sand Hills and Piedmont regions, and rapidly increases to a maximum of approximately 1000 meters (m) in altitude along the Blue Ridge in the extreme northwestern portion of the state bordering North Carolina and Georgia. With only a small coverage of elevated mountainous terrain, high ozone concentrations associated with valley inversions are rare in South Carolina.

2.4. Precursor Pollutants and Air Quality Landscape of the Carolinas

Ozone forms through the reaction of oxygen with nitrogen oxides (NO_x) and volatile organic compounds (VOCs). Since both NO_x and VOC emissions are needed for ozone formation, they are often referred to as ozone precursors. To fully comprehend the States' ozone problem, NCDAQ and SCDHEC first started with an examination of the precursors to ozone.

Due to the generally warm and moist climate of the Carolinas, vegetation abounds in many forms, and forested lands naturally cover much of the state. The biogenic sector is the most abundant source of VOC emissions in both North and South Carolina and accounts for approximately 90% of the total VOC emissions. The overwhelming abundance of biogenic VOC emissions makes the majority of North and South Carolina a NO_x limited environment for the formation of ozone. Despite an industrial and urbanization trend during the past several decades with increasing amounts of anthropogenic NO_x and VOC emissions, the majority of the urbanized and populated regions of the Carolinas are still mostly NO_x limited.

During extremely stagnant atmospheric conditions, the center most portions of North Carolina's largest metropolitan cities occasionally demonstrate some VOC limited characteristics for ozone formation. This is due to the limited amount of biogenic VOC emissions and prevalence of mobile (on-road and non-road) based NO_x emissions in the urban cores. With major metropolitan areas far fewer and much less urbanized in South Carolina, VOC limited conditions rarely occur in South Carolina.

2.4.1. Metrolina Modeling: North Carolina Conceptual Description

North Carolina's most populous metropolitan regions are located in the central portions or the Piedmont of the state. The three largest cities (Charlotte, Greensboro, and Raleigh) form a partial crescent extending from the southwest to the northeast. This combination of metropolitan regions is often referred to as the Piedmont Crescent. A network of interstate highways interconnects these three largest cities and further extends into adjoining states in a general southwest to northeast pattern. In a similar southwest to northeast orientation, a major interstate highway also passes through the western portion of the Coastal Plain and connects a string of medium-sized cities (Lumberton, Fayetteville, Smithfield, and Rocky Mount). One additional interstate highway travels from the southeastern coast westward through the Piedmont Crescent and then continues westward across the Mountains. Major state highways are more random in orientation, but generally converge into the Piedmont Crescent and the major cities in a spoke-like fashion. The mobile-based NO_x emissions follow these highway networks with the highest emissions occurring in or near the city centers. The industrial point sources with both anthropogenic NO_x and VOC emissions are also generally located in close proximity to the cities and the major road networks. Finally, North Carolina's largest NO_x emissions sources, coal-fired electric generating units, are spatially scattered around the state but are most heavily concentrated near the state's center.

By combining each of the major emission source categories [Biogenic VOCs, Mobile (highway and non-road) based NO_x, and Industrial NO_x and VOCs], the highest concentrations of precursor pollutants for ozone formation are focused throughout the Piedmont Crescent described in the previous paragraph. Therefore, the greatest potential for ozone formation under ideal weather conditions is also in this central portion of North Carolina. Over multiple years and a wide variety of meteorological conditions, this increased potential for ozone formation in central North Carolina is realized and demonstrated by the calculated 8-hour ozone design values. The highest of these design values are indeed located very near the two largest cities of this Piedmont Crescent, Charlotte and Raleigh. Of the 2002-2004 8-hour ozone design values, all of the design values in excess of the NAAQS are located within or just downwind of the Piedmont region.

High ozone conditions and 8-hour ozone design values exceeding the NAAQS have also been recorded in the higher elevations or ridge tops of the North Carolina mountains. This is a generally rural region removed from the significant anthropogenic sources of precursor pollutants in North Carolina and throughout the Southeast. At these remote locations, the major contributor to the higher ozone conditions is regional transport of anthropogenic precursor pollutants and ozone. This same principle applies to the small area of elevated terrain in South Carolina along the Appalachian escarpment. The regional transport phenomenon is described in detail in Section 2.5.

2.4.2. Metrolina Modeling: South Carolina Conceptual Description

South Carolina experiences its greatest concentration of urbanization in only a few widely scattered places across a fairly symmetrical political geography. The main areas of concern for potential ozone violations are in the region around its capital city, Columbia, and in the "Upstate," a broad southwesterly extension of North Carolina's aforementioned Piedmont Crescent, encompassing parts of Anderson, Greenville, Spartanburg, Cherokee, and York Counties (together making up the Interstate 85 corridor). It is prudent to note that the term "urbanization" is quite general in its interpretation in describing the Upstate region, in view of the fact that combining the population of these counties in their entirety (both urban and rural) still barely exceeds 1 million residents. The major concentration of industrialization and urbanization in South Carolina actually occurs in the Charleston area, which, by virtue of favorable coastal geography and meteorology, has never been of concern for ozone formation.

Like its northern neighbor, South Carolina's landscape is transected by a spoke-like network of Interstate highways, the majority connecting mainly rural agricultural areas and small cities with the state capital, Columbia (the state capital), as its hub. Four out of the five Interstate routes also extend through North Carolina, the only exception being the east-west oriented Interstate 20, though a large portion of its traffic either originates, or terminates in North Carolina (via Interstate 95 and other primary routes).

Along with the aforementioned Interstate 85 corridor, a second major north-south interregional highway, Interstate 95, parallels the coast at various distances, only coming into contact with very minor urbanization around Florence in the northeastern part of the state (the Pee Dee region). For this study, the Interstate 77 corridor through northern York County will be of special interest, as it is the only interstate highway running directly between the city of Charlotte and its southern suburbs across the state line into South Carolina.

Use of these highways for interstate commerce concerns is quite heavy, with mobile source emissions patterns, much like in North Carolina, of these routes being monitored very closely. As would be expected, higher concentrations lie close to their mutual convergence in and around Columbia and in the Upstate area. This is evident in that these two areas are the only locations within the boundaries of the state to record 8-hour ozone design values in excess of the NAAQS for 2002-2004.

In contrast to North Carolina, the major cities in South Carolina, being much smaller in scale, rarely contain the majority of large stationary anthropogenic NO_x and/or VOC sources, such as the boilers of coal steam electric generation plants (EGUs), within the spheres of their air sheds. These sources are generally scattered about the state at random, usually near coastal harborages and inland waterways. They may or may not be in close proximity to an Interstate or any other heavily traveled major route in the US Federal / SC DOT maintained highway system.

2.5. Meteorological Characteristics

Almost all high ozone episodes occurring in the Southeastern US will have some common meteorological characteristics, including warm temperatures, lower relative humidity, little or no precipitation, and relatively light winds. These conditions are nearly universally indicative of regional high pressure patterns causing large-scale sinking (subsiding) air at various levels of the atmosphere. The differences in the position, strength, and movement of these high pressure areas, along with differences in various mid-to-upper level wind patterns, allow staff to discern six meteorological scenarios, or "regimes," in which high ozone episodes are likely to occur in the Carolinas. These meteorological regimes are discussed in the following paragraphs.

2.5.1. Scenario #1: Eastern US Stacked High Scenario

Conditions that have traditionally lead to large-scale exceedances of the 8-hour ozone NAAQS result from the development of a broad surface high-pressure area sprawled over the eastern third of the United States, with a large mid-to-upper level high-pressure area centered over the Plains and/or Great Lakes States. The mid-to-upper level ridge serves to block the movement of fronts into the Eastern United States during the ozone season. This often results in abnormally hot temperatures, little precipitation, and the buildup of elevated concentrations of ozone and its precursors over much of the Midwest, Northeast, and the interior of the South Atlantic States, especially North and South Carolina. As the mid-to-upper level ridge slowly slides eastward, it situates itself overtop of the surface high-pressure at the western extent of the mean Bermuda High position, creating a "stacked high" over much of the Eastern US. The resulting large-scale subsidence leads to very low vertical mixing heights prohibiting dispersion of precursor pollutants. The stagnant air mass from the "stacked high" scenario is prime for high ozone episodes in the Eastern US. A weak surface trough can develop to the east of the Mountains during this scenario producing a south-southwesterly flow across portions of the Carolinas. The presence of the trough can enhance ozone concentrations along and just east of the trough axis because of surface convergence and pooling of precursor pollutants in this region. The lack of significant precursor pollutant transport can create large ozone concentration gradients across the region.

An example of these conditions, resulting in extreme ozone exceedances over a wide swath of North and South Carolina, is demonstrated in the June 11, 2002 Daily Weather Map, Figure 2-1. The presence of an upper level high-pressure area directly atop a surface high-pressure area in the Eastern US can clearly be seen.

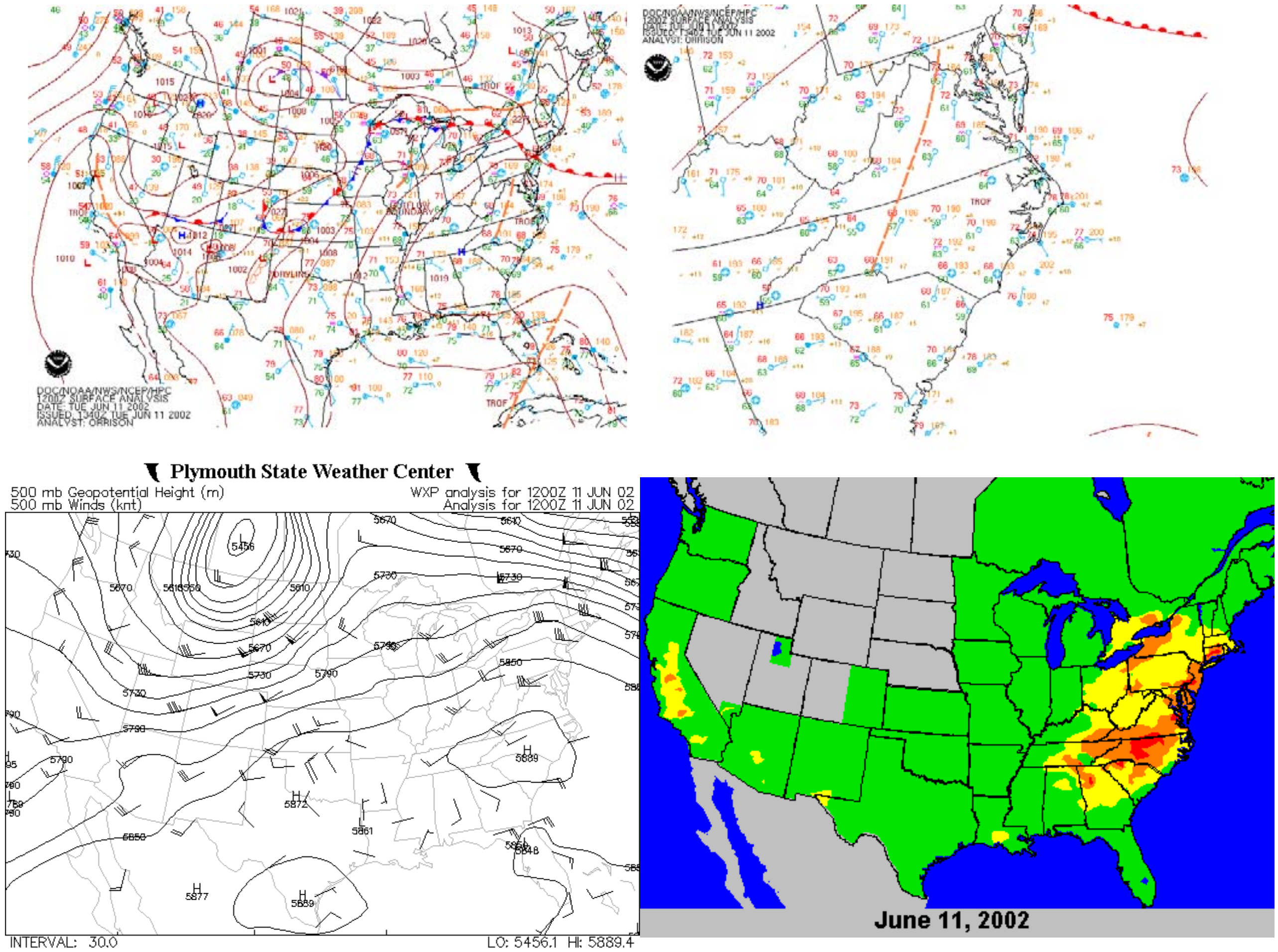

Figure 2-1: Daily Weather Maps for June 11, 2002, example of an Eastern Stacked High

2.5.2. Scenario #2: Common Back-Door Frontal Approach Scenario

The most frequently occurring meteorological scenario is characterized by the movement of cold fronts toward the Carolinas and the presence of high-pressure to the south or southwest of the area. Cold fronts often move toward the Carolinas during the summer months but are typically too shallow to move completely through the region. They commonly become east west oriented and stall out as far south as southern Virginia or the northern sections of North Carolina. Sometimes high pressure to the north forces the surface boundary to retrograde into the region from the north and/or northeast. These situations are known as back-door fronts. Because both vertical and horizontal momentum is generally weak along these boundaries, and because they tend to dissolve, merge with the lee-side trof, or retreat back to the northeast as a warm front in time, they tend to create surface wind shifts that cause pollutants to re-circulate over the same areas repeatedly. The back-door regime is characterized by a weak upper-level flow pattern, a down sloping westerly surface flow to the south of the boundary, and maximum temperatures that range from the mid to upper 90's and dew points approaching the upper 60's to mid 70's.

Widespread exceedances of the 8-hour ozone NAAQS may occur in all areas, save the far eastern coastal regions of the Carolinas, during these conditions.

An example of this scenario that resulted in widespread exceedances in both Carolinas can be seen in the June 4, 2002 Daily Weather Map, Figure 2-2. Note the presence of a warm front that has just passed through North Carolina to the north.

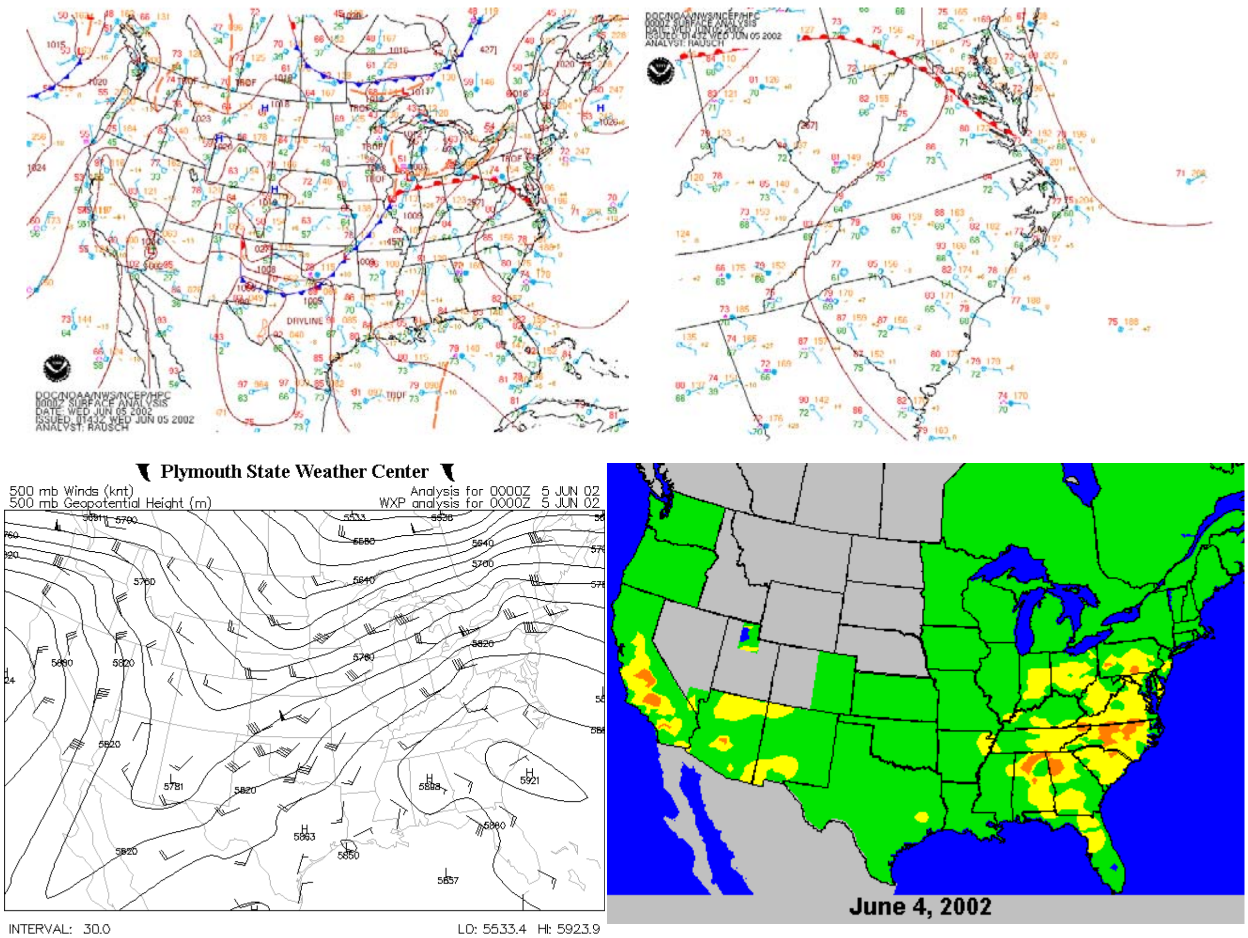

Figure 2-2: Daily Weather Maps for June 4, 2002, example of a Frontal Approach.

2.5.3. Scenario #3: (Post Back-Door) Canadian High Scenario

A third meteorological scenario, with some similarities to Scenario #2, that sometimes results in high concentrations of ozone across the Carolinas is characterized by a surface high-pressure area building in from the north following the passage of an anomalously strong "Back-door" front. Since this type of boundary has little upper-level support, a mid-to-upper level ridge over the Mid-Mississippi Valley region may be able to build east into the Carolinas. The position of the mid-to-upper level ridge produces a northerly flow aloft throughout this scenario. As the Canadian-borne surface high-pressure builds into the Carolinas, it brings with it milder and drier air by means of a north-northeasterly breeze. These conditions can lead to scattered exceedances of the 8-hour ozone NAAQS across the Carolinas. Temperatures are typically in the low to mid 80's (with dew points in the mid 50s to low 60's) during the beginning of this type of scenario. However, high temperatures may eventually reach the upper 80's to low 90's (with dew points in the upper 60's to low 70's) as the center of the surface high-pressure slides into the Carolinas and the wind field slackens. An example of these conditions from August 10, 2002, is shown in Figure 2-3.

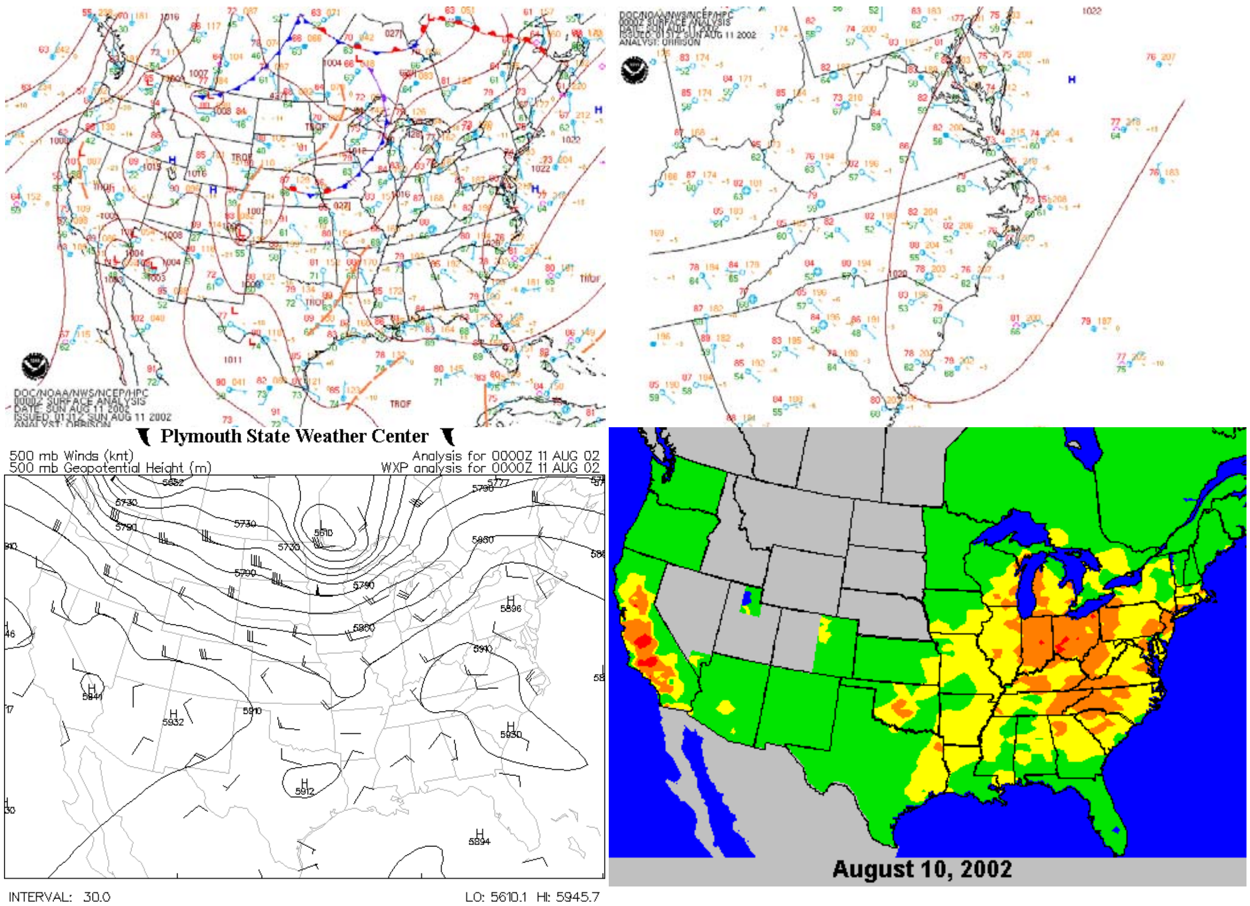

Figure 2-3: Daily Weather Maps for August 10, 2002, example of a Canadian High.

2.5.4. Scenario #4: Modified Canadian High

The fourth meteorological scenario, initially, is very similar to Scenario #3 above. Canadian-borne surface high-pressure builds into the Carolinas delivering lower dew points and milder temperatures with a light north-northeasterly wind. This cool down is short-lived, however. As the high-pressure center moves south, a light southwesterly flow dominates, temperatures soar, and dew points increase. A mid-to-upper level ridge slowly sprawls eastward across the country, resulting in a very weak flow aloft. An example of these conditions from July 8, 2002, is shown in Figure 2-4.

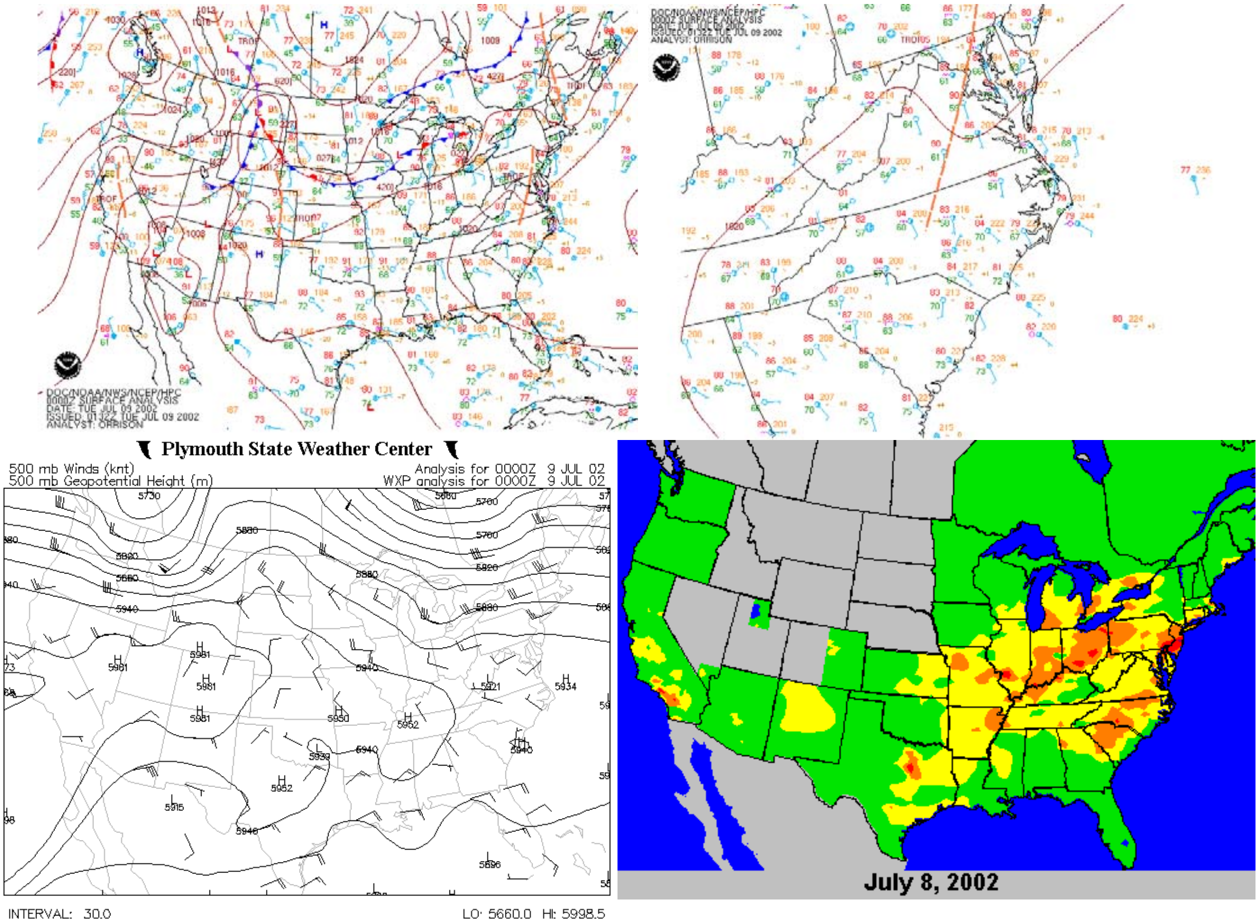

Figure 2-4: Daily Weather Maps for July 8, 2002, example of a Modified Canadian High

2.5.5. Scenario #5: Continental High in a Progressive Pattern Scenario

Meteorological scenarios other than the four already identified can result in high ozone concentrations, but these situations are usually limited to one day in duration. Single-day ozone episodes can occur during a progressive meteorological pattern in parts of both Carolinas. This scenario is characterized by a surface high-pressure area that moves across the continent into the Southeastern United States. This associated air mass ushers dry, near-cloudless weather into the Carolinas for a very short period (usually one or two days) as it pushes out into the Atlantic Ocean. This often results in isolated 8-hour ozone exceedances of the NAAQS, especially in the urban areas of the Carolinas, on the day(s) that the surface high pressure area is transitioning across the region.

This scenario is very rarely seen during the core ozone season across the Carolinas; though some parts of North Carolina and extreme Upstate South Carolina may experience it in anomalous years. This is due to the extreme difficulty true frontal boundaries have moving southeast across the Appalachians in the summer months. Without the benefit of strong westerly (Mid-Latitude) winds aloft, these fronts normally become diffuse and die out over the rugged terrain of Western North Carolina, Tennessee, and Northern Georgia. The shallow continental surface highs behind them, being too weak to push the fronts further south, are shunted eastward into the Mid-Atlantic region. As it is, the "Typical Progressive Pattern" more commonly develops in the spring and fall months when the polar jet stream exerts much more influence in synoptic conditions over the South Atlantic States. Surface ridges are active enough during normal periods in these seasons to penetrate southward over even the highest of the Appalachian mountain ranges.

2.5.6. Scenario #6: Tropical Cyclone Influence

During the latter half of the ozone season, when the mid-to-upper level flow is very weak along the South Atlantic Coast, tropical systems working their way across the Atlantic Ocean may approach the North and South Carolina coastlines. If the storm maintains enough strength and distance from the coast, its outflow aloft can greatly enhance subsidence in the mid-to-upper levels around its periphery, resulting in warm, dry air across a wide area far inland from the coast. Temperatures may rise far above seasonal norms, under nearly cloud-free skies as a result of this extreme subsidence regime.

Though this occurs infrequently and rarely causes elevated ozone in inland areas on its own, the influence from a tropical cyclone can modify all five of the previously stated scenarios by enhancing ozone production and stagnation. The resulting combination can cause even more significant and widespread ozone rises than would otherwise occur in any of the scenarios alone. An example of these conditions from September 4, 2002, is shown in Figure 2-5. It is worthy to note such a modification to the five previously identified scenarios.

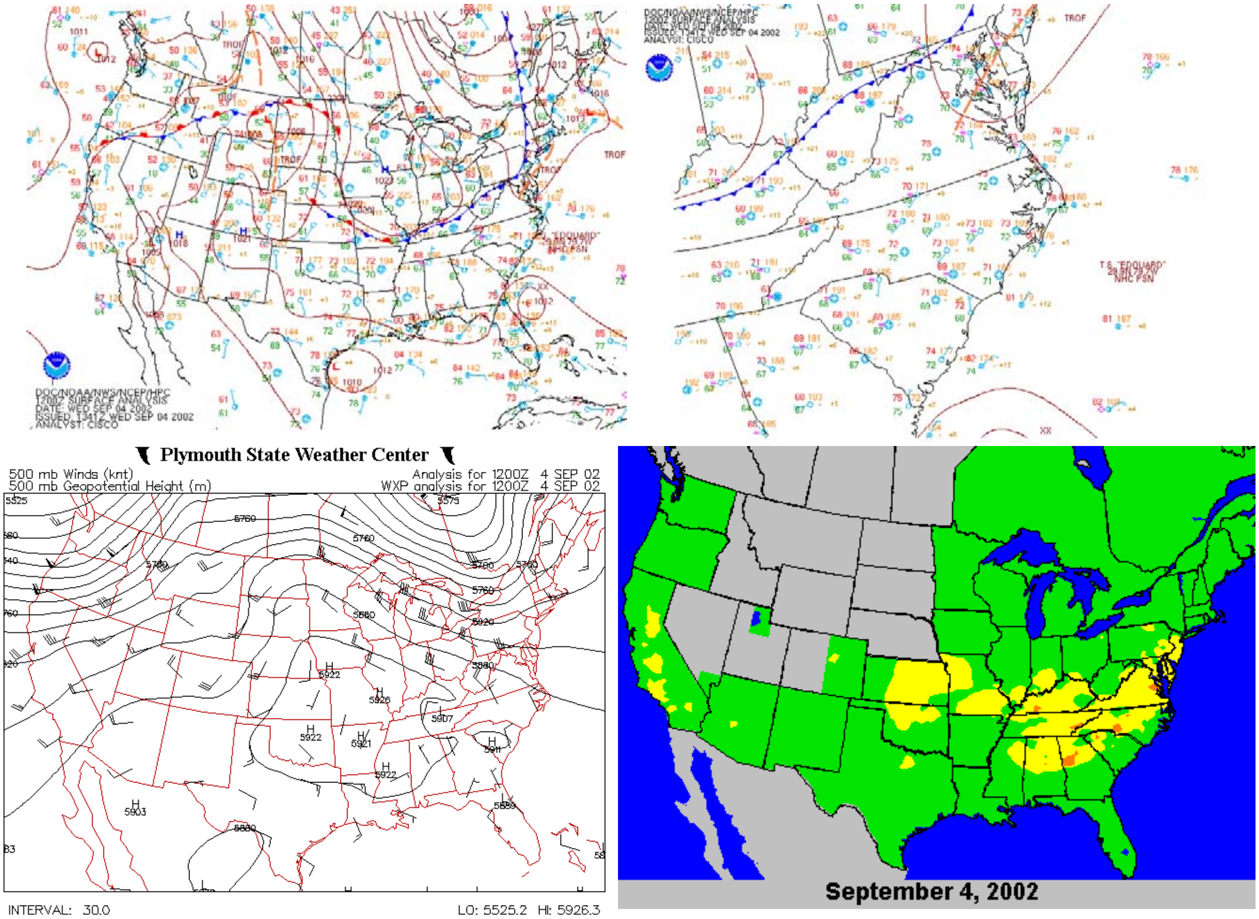

Figure 2-5: Daily Weather Maps for September 4, 2002, example of a Tropical Influence.

2.6. Regional Transport and Recirculation

Even in the 21st century, South Carolina is still mainly a rural agrarian state with only a few small cities that are considered any part of a US Census Bureau-designated Metropolitan Statistical Area (MSA). North Carolina, though possessing more urbanization than South Carolina (especially in the Piedmont Crescent) is also largely rural in nature. Just outside the borders of the Carolinas, however, is a collection of large metropolitan regions. Many of these concentrated urbanized areas are among the largest in the Continental United States. These metropolitan regions have similar emissions profiles and frequencies of high ozone concentrations leading to exceedances of the 8-hour ozone NAAQS. It is reasonable to conclude that precursor pollutants, as well as formed ozone, can be transported from any of these larger metropolitan regions into the Carolinas with an appropriate wind flow orientation from one or more of these regions. In addition to the local precursor pollutant influences already discussed in Section 2.2, regional transport of precursor pollutants and ozone is an important factor in producing ozone exceedances across the region.

A closer study of observed meteorological data in the lower portions of the atmosphere and observed air quality concentration data from across the southeastern United States further supports the importance of regional transport of ozone concentrations into North and South Carolina. The NCDAQ and SCDHEC have performed a number of studies of boundary-layer characteristics over the region using NOAA-developed profiling and trajectory analysis tools, as well as a ground-based radar profiler system located in the Charlotte area. These tools allow meteorologists and planners on both staffs to use gridded climate data to plot detailed analyses of the winds from near the surface upward to an identifiable subsidence or trapping inversion that is a common characteristic observed during the majority of the high ozone episodes in the Carolinas.

The atmospheric depth from the surface to this subsidence inversion is also the usual extent of the afternoon convective mixed layer. Wind speeds throughout this mixed layer are fairly uniform during the midday and afternoon hours when ozone concentrations are at a maximum throughout the Southeast. Many of these analyses identify several large metropolitan areas in close proximity to North and South Carolina as potential source regions for precursor pollutants and ozone transport during the typical daytime ozone production period.

Overnight, the convective mixing is greatly diminished because of the lack of solar radiation and surface heating. The loss of the convective mixing also results in the wind profile becoming stratified from the surface to the subsidence inversion with the lowest winds speeds at the surface. With little or no surface wind, some other atmospheric mechanism is needed to support regional transport during the nighttime hours. It is not uncommon for a low-level jet to form above the surface and beneath the subsidence inversion during the height of a high ozone episode in the Carolinas. The low-level jet is generally oriented southwesterly in the lee of the Blue Ridge escarpment, reaching a maximum intensity during the middle of the overnight period. Data from National Weather Service radiosonde soundings and other wind profilers throughout the Southeast and Mid-Atlantic suggest that the spatial extent of the low-level jet phenomenon can extend across multiple states. Figure 2-6 is a classic example of a low-level jet as observed by the Charlotte wind profiler during a high ozone episode on June 27, 2003. The dark red wind barbs indicate the core of the low-level jet at 500 meters above the ground around 2:00 a.m.Eastern Daylight Time (EDT) or 6:00 a.m. Universal Time (UTC).

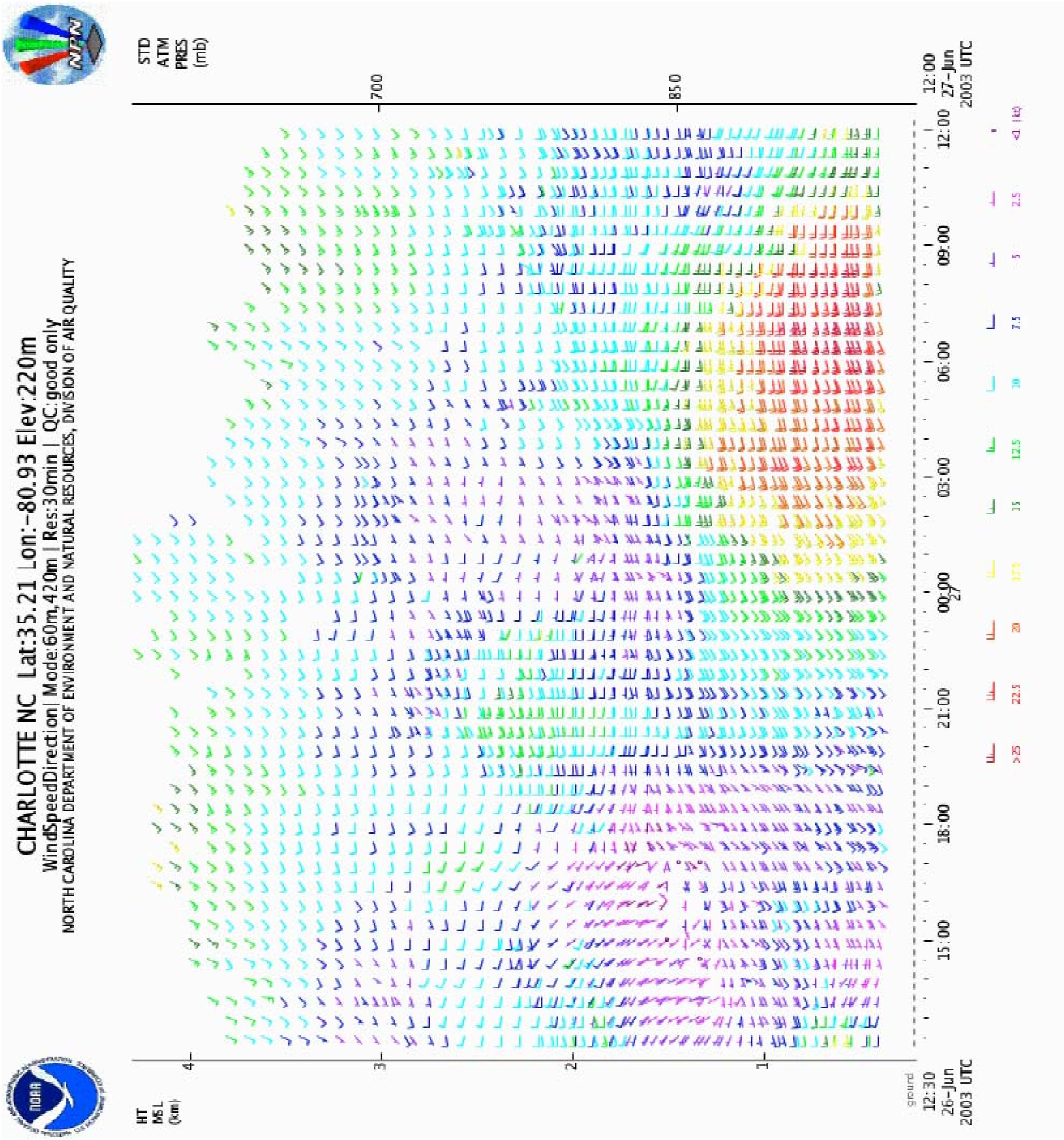

Figure 2-6: Charlotte Wind Profiler for June 27, 2003. The dark red barbs indicate the core of the low-level jet at 500m.

The low-level jet phenomenon is a well-documented and researched contributor to regional transport of precursor pollutants and ozone (Clark et al., 2003). The NCDAQ operates several ozone monitoring sites at the ridge tops or peaks of several mountains and also at multiple levels of a television transmission tower in the center of the state. Even though elevated terrain is lacking within the borders of South Carolina, the SCDHEC also operates an ozone monitoring site in the mountainous region straddling the border region with Georgia and North Carolina in the far northwestern corner of the state. These higher altitude or elevated monitoring sites extend sufficiently above the nocturnal surface inversion, or stable layer, into the residual layer of the atmosphere where these low-level jets occur. Consistently during high ozone episodes across the region, ozone concentrations remain elevated at these sites (throughout the duration of the overnight low-level jet) long after concentrations at lower elevation monitors nearby have abated. As the daytime convective mixing is initiated the next morning, the regionally-transported pollution aloft is mixed downward to the surface, further adding to the local influences driving the total ozone response.

The regional transport discussion would not be complete without recognition of recirculated pollution around the entire Southeast and Mid-Atlantic region. As many of the meteorological scenarios explained earlier progress, winds in the lower and middle atmosphere can shift around in a variety of directions. In the most frequent scenarios, winds transition from one direction to another in a clockwise fashion during the extent of the complete synoptic cycle or scenario. This clockwise shifting of the winds is a key characteristic of eastward-moving high pressure systems in the Northern Hemisphere.

In a large recirculation pattern, plume(s) of precursor pollutants and formed ozone may leave the Carolinas one day, travel across multiple states, then return to the very air shed from where they started within a matter of days. Throughout the journey of air parcels in this type pattern, precursor pollutants and ozone are constantly being exchanged and added to the air parcels from each source sector and metropolitan region along the way, irrespective of any geo-political boundaries. Recirculation can also occur on much smaller scales and within state boundaries. In such smaller scale recirculation patterns, precursor pollutants and ozone from two neighboring metropolitan regions can exchange back and forth over a series of days, especially as a strong area of high-pressure moves from west to east across the region.

While still a form of regional transport, there are not clearly defined originating source regions or destinations during a recirculation event. Figure 2-7 provides a back trajectory analysis of a regional scale recirculation event centered over western North Carolina.

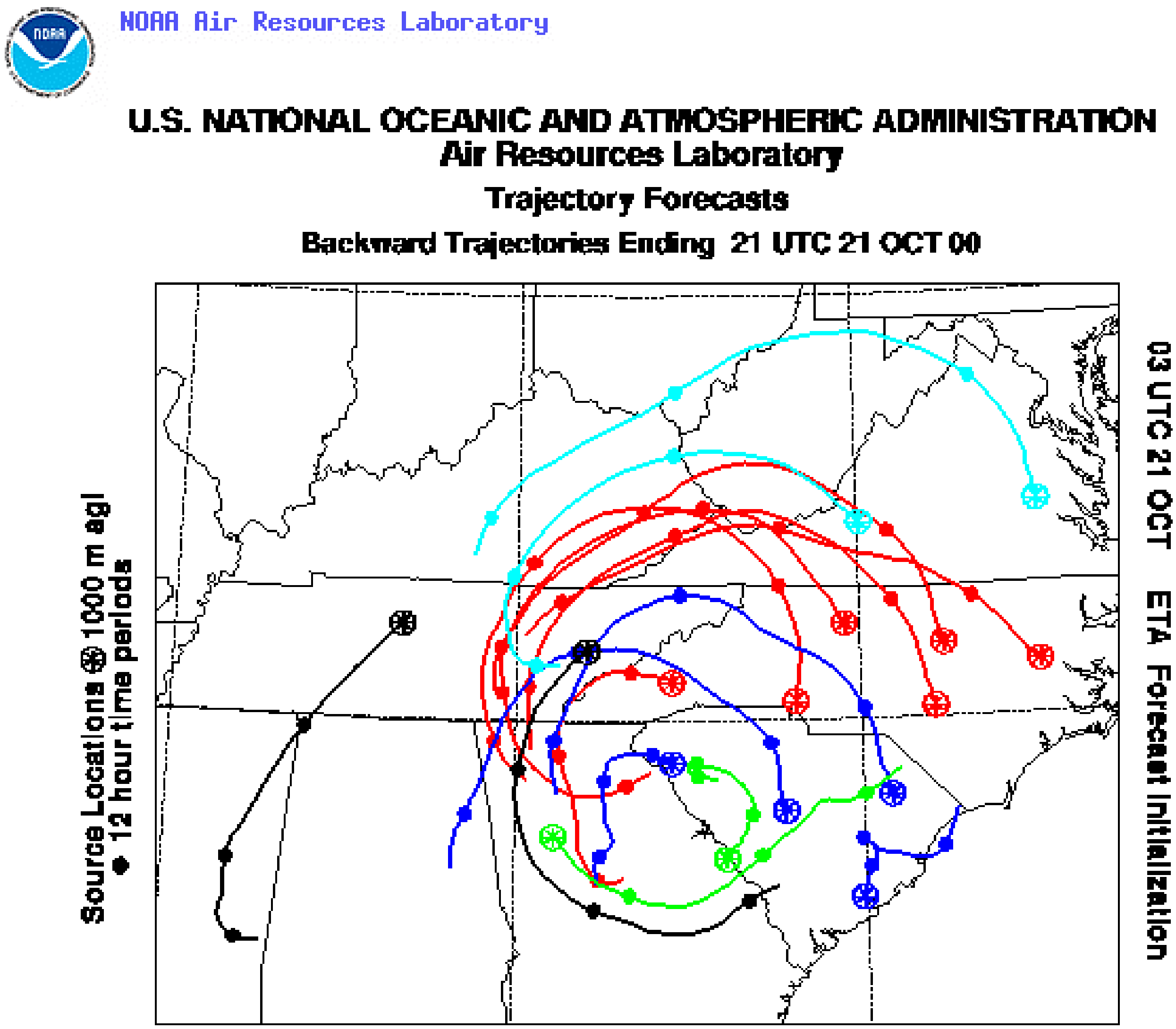

Figure 2-7: Back Trajectory Analysis of Recirculation.

3.0 Ozone Episode Selection

A crucial step to SIP modeling is the selection of episodes to model. Several considerations need to be weighed before settling on not only which days to model, but how many days for each episode need to be modeled. This section details the guidance and process by which episodes were selected for the 8-hour Ozone SIP modeling package.

3.1. Overview of USEPA Guidance on Ozone

The USEPA's final draft guidance on 8-hour ozone modeling (EPA, 2005) sets out specific criteria for the selection of episodes to model for attainment of the 8-hour ozone NAAQS. First, episodes should include days encompassing a variety of meteorological conditions, including varying wind directions, where maximum 8-hour ozone values exceed 84 parts per billion (ppb). Second, episodes should be selected that contain days where values peak sufficiently close (within ± 10 ppb) to the current design value (DVB). Third, episodes should be chosen around days for which there are extensive air quality and meteorology measurements, including measurements aloft, measurements of indicator species and/or precursor measurements. Finally, a modeling period of a sufficient number of days should be selected to ensure robust attainment tests at violating monitoring sites.

In addition to these primary criteria, the USEPA also suggests a set of secondary criteria that may be used in the selection of episodes. These criteria allow states to give preference to previously modeled episodes. This is a very valuable consideration, as the USEPA points out, since it can save modeling resources and effort. The USEPA also recommends selecting episodes that occur during the period corresponding to the current design value, which for a five-year design value would be the period from 2000 to 2004 (three-year design values would encompass the period from 2001 to 2003). Additional considerations include selecting episodes maximizing the number of days and sites observing a violation, include weekends and holidays, and include those meeting primary and secondary criteria in other nonattainment areas, when participating in regional modeling. Using the aforementioned USEPA criteria, NCDAQ and SCDHEC systematically examined the data available to determine the best episodes for modeling.

3.2. Episode Selection

With the advances in computing speed and storage-capacity technologies, and with the aid of regional modeling efforts, NCDAQ and SCDHEC intend to move toward the modeling of the peak ozone season for the 8-hour ozone SIP. By modeling the peak season, several criteria are covered, including the modeling of weekends and a sufficient number of days to ensure a robust modeled attainment test. Modeling the peak ozone season will also accomplish the goal of evaluating the myriad of meteorological conditions that influence ozone concentrations.

To determine an appropriate time period to model, an examination of the 8-hour ozone maxima monitored across the Metrolina area was initiated for each ozone season from 1997 through 2004. This was done in order to determine which season yields the most days at or above the 85 ppb ozone standard. The same seasons were then re-examined to first tabulate design values at each monitoring site using the recently suggested three-year design values and five-year weighted design values at each monitoring site; and second, to determine the number of days each monitoring site observed a value within 10 ppb of its design value. The five-year weighted design values were derived by taking a running average of the three-year design values within the five-year window. For example, the 2000-2004 weighted average is calculated by averaging the 1999-2001, 2000-2002, and 2001-2003 design values at each monitoring site, whereby the fourth high from 2002 is weighted three times, the fourth high from 2001 and 2003 is weighted twice, and the fourth high from 2000 and 2004 is weighted once. Thus, Table 3-1 displays a count of the number of days in which the center year (e.g., 2002) of the design period (e.g., 2000-2004) contains peak ozone concentrations within 10 ppb of the five-year weighted design value for all monitor sites in the Metrolina area. Table 3-2 presents results for the number of days within 10 ppb of the three-year design values, again, for all monitoring sites in the Metrolina area.

Table 3-1: Total Number of Days within 10ppb of the 5-year DVB for Metrolina Monitors

Site Name	County	1995-1999	1996-2000	1997-2001	1998-2002	1999-2003	2000-2004
Monroe	Union					10	34
Enochville	Rowan	14	19	22	8	8	22
Crouse	Lincoln	15	26	10	15	13	25
Rockwell	Rowan	9	18	23	5	13	15
Arrowood	Mecklenburg	5	15	18	7	9	27
County Line	Mecklenburg	28	22	15	6	6	14
Garinger	Mecklenburg	12	17	12	7	6	18
York	York, SC	15	17	22	16	14	32
Total		98	134	122	64	79	187

Grey shading indicates incomplete data for DVB calculation.

Table 3-2 Total Number of Days within 10ppb of the 3-year DVB for Metrolina Monitors

Site Name	County	1996-1998	1997-1999	1998-2000	1999-2001	2000-2002	2001-2003	2002-2004
Monroe	Union			21	10	10	33	8
Enochville	Rowan	14	19	25	9	6	33	8
Crouse	Lincoln	15	30	10	19	10	25	9
Rockwell	Rowan	9	18	22	5	11	13	4
Arrowood	Mecklenburg	5	14	17	10	9	29	28
County Line	Mecklenburg	10	22	13	6	5	14	8
Garinger	Mecklenburg	11	15	14	7	6	18	7
York	York, SC	17	16	23	19	13	32	9
Total		81	134	145	85	70	197	81

Grey shading indicates incomplete data for DVB calculation.

The results of these evaluations indicated that, overall, the 2002 ozone season contained, generally, the most exceedance days for the individual monitoring sites, as well as the most days within 10 ppb of the calculated design values. When 2002 was not the highest year, it was generally either the second or third highest, for either design value convention. The only other years that consistently ranked high for this criterion were 1998 and 1999. Further examination of the past eight ozone seasons reveals that 1998, 1999, and 2000, have the greatest number of days exceeding an ozone concentration of 84 ppb (Table 3-3).

Table 3-3: Total Number of Days with Observations Greater than 84ppb for Metrolina Monitors

Site Name	County	1997	1998	1999	2000	2001	2002	2003	2004
Monroe	Union			14	4	3	17	1	0
Enochville	Rowan	11	23	30	12	15	28	7	1
Crouse	Lincoln	4	19	6	15	9	21	5	0
Rockwell	Rowan	11	31	34	7	17	22	6	1
Arrowood	Mecklenburg	9	21	19	5	5	12	1	1
County Line	Mecklenburg	22	43	33	16	10	22	4	3
Garinger	Mecklenburg	18	27	18	12	9	21	4	4
York, SC	York	2	6	7	1	0	15	0	0
Total		77	170	161	72	68	158	28	10

Grey shading indicates incomplete data.

To narrow the period for episode selection further, other criteria were examined. One of USEPA's secondary criteria suggests consideration of episodes drawn only from 2000 – 2004, as this period corresponds to the most current design value. By selecting 2002, our base case year would be the same as our base line (typical) year, centered in the middle of the five-year 2000 – 2004 period. This would mean the 2002 emissions inventories would not have to be adjusted to correspond to a different base case year during modeling efforts. Differences between the base case and base line (typical) inventories are explained in Section 6. Additionally, the selection of 2002 as the base case season also fulfills the secondary criteria, which suggests that states give preferential treatment of previously-modeled episodes. Through NCDAQ's and SCDHEC's work with the Visibility Improvement, State and Tribal Association of the Southeast Regional Planning Organization (VISTAS RPO), the 2002 calendar year has already been modeled as the base-case year for regional haze reduction goals.

Though VISTAS modeling is geared mainly towards Regional Haze and $PM_{2.5}$ demonstrations on a regional scale, the modeling can still be applied to ozone. The VISTAS modeling employs "one atmosphere" modeling, or modeling of all atmospheric constituents including particulate matter (PM) and ozone. This modeling is done in parallel to capture interactions between various compounds. Since ozone, along with $PM_{2.5}$ and regional haze, is being modeled as part of VISTAS modeling efforts, its data can easily be extracted from the modeling results.

3.3. The Representativeness of the 2002 Ozone Season

2002 was an active year with numerous poor air quality episodes. Across the Carolinas, high ozone values generally coincide with high PM values since both need similar atmospheric condition to accumulate. The 2002 season was examined to verify that it was representative of the nature of ozone formation in North Carolina (as stated herein as inclusive of York County South Carolina) to further support its use in modeling.

3.3.1. The Overall 2002 Ozone Season

The months of May through September 2002 were typical of the meteorology one would expect for an active ozone season, namely warmer and drier than average. Temperatures were 1 – 2 degrees Fahrenheit (ºF) warmer than average across the state and throughout the Mid-

Atlantic States, which can be seen in Figure 3-1. Precipitation values were four to six inches below normal (Figure 3-2) or 75-90% of normal (Figure 3-3) for most of the Carolinas. The dry conditions were also present for much of the coastal Mid-Atlantic States. The warmer and drier conditions led to lower soil moisture (Figure 3-4) throughout much of the East coast, which reduced the evaporation of moisture into the air, and thus lowered dewpoint temperatures. With less available moisture in the atmosphere, cloud cover was decreased, leading to more sunlight, increased photochemistry, and higher levels of ozone produced across the Carolinas.

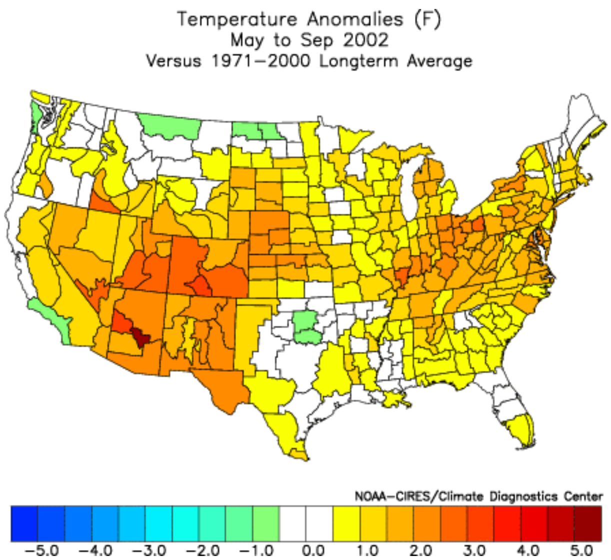

Figure 3-1: Temperature Anomalies (ºF) during the 2002 ozone season, compared to the most recent 30-year climate average.

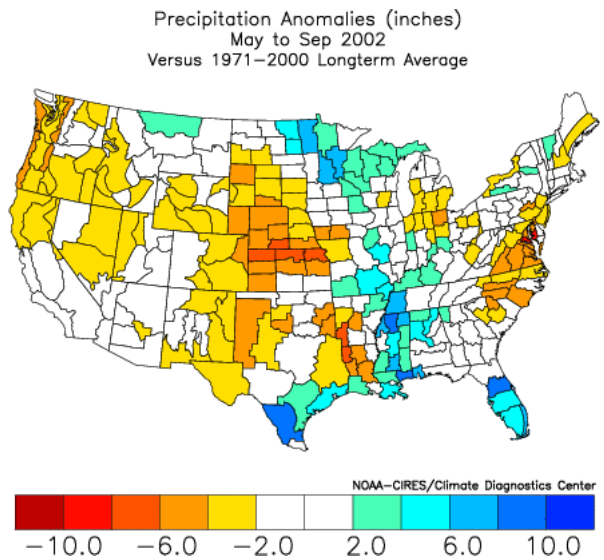

Figure 3-2: Precipitation Anomalies (inches) during the 2002 ozone season, compared to the most recent 30-year climate average.

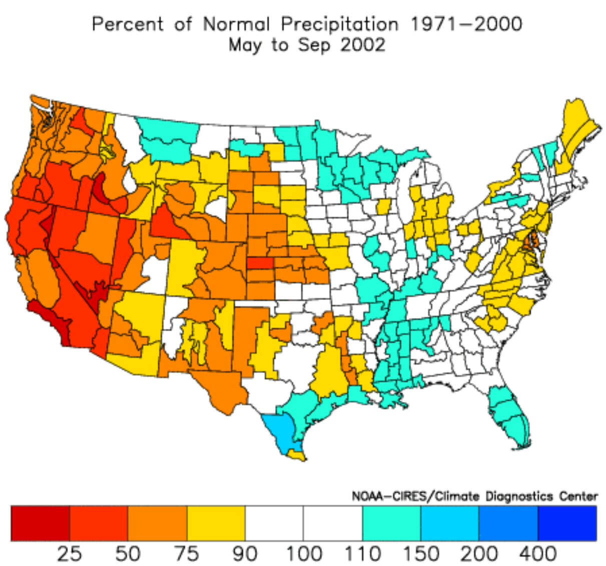

Figure 3-3: Percent of Normal Precipitation during the 2002 ozone season, compared to the most recent 30-year climate average.

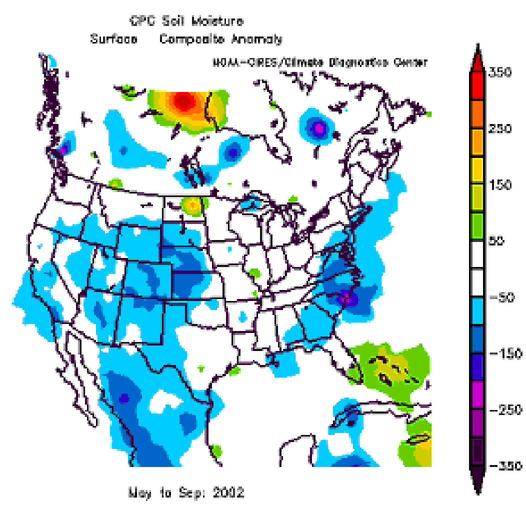

Figure 3-4: Soil Moisture Composite Anomaly (tenths of inches) for the 2002 ozone season, as compared to the most recent 30-year climatological average.

With below normal precipitation and soil moisture, varying levels of drought were observed throughout much of the Eastern US during the summer of 2002. Figure 3-5 shows the Palmer Drought Index for the May - September 2002 timeframe. The Palmer Drought Index uses 0 to denote normal, and drought conditions are shown in terms of negative numbers; for example, minus two (-2) is moderate drought, minus three (-3) is severe drought, and minus four (-4) is extreme drought, and so on. Values in central North Carolina, including the Metrolina area were below -4, indicating extreme drought conditions.

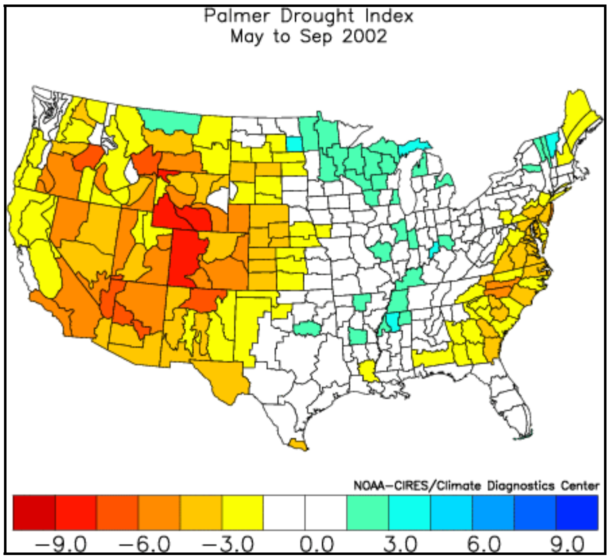

Figure 3-5: Palmer Drought Index. Negative values indicate long-term drier than normal conditions.

2002 Meteorological data collected at the Charlotte-Douglas Airport (CLT), the official National Weather Service observation station serving the Metrolina area, mirror the results of the regional analysis. At CLT, the mean temperature was 74.8 ºF compared to the average mean of 74.6 ºF, or only 0.2 ºF above normal. However, the observed mean maximum temperature was 85.6 ºF, versus a normal 84.5 ºF. The observed mean low temperature was actually cooler than average; 64.0ºF versus 64.7 ºF.

Reduced minimum temperatures, as well as the greater departures in daytime temperatures, were a product of the dry conditions prevalent over the southeast. Less cloud cover and lower dew points both lead to lower nighttime temperatures and increased daytime temperatures. Evidence of low moisture in the air can be seen in the average relative humidity for June, July, and August, where the mean relative humidity at CLT was approximately 5.5% below normal.

The number of days in excess of 90 ºF recorded at CLT was also above climatological norms, with a total of 50 days above 90 ºF in 2002, compared to a normal of 37 days. This is important to note, as repeated days where temperatures peak at or above 90 ºF generally correlate well with high ozone events in the Metrolina area.

The observed rainfall during the 2002 ozone season in the Carolinas was reflective of the drought conditions seen in the overall regional analysis. Rainfall at CLT was 14.48 inches during the core season, much below the 30-year average of 18.36 inches. Below normal precipitation is another indication of decreased cloud cover, which in turn leads to more sunlight (increased UV), enhanced photochemical transformation of precursory pollutants, and thus, higher amounts of ozone.

3.3.2. The 2002 Ozone Season Month-By-Month

Mean temperatures for the month of May 2002 were close to normal across most of the Southeastern US (Figure 3-6). May also proved to be relatively mild for the Metrolina area, where the mean maximum temperature for CLT was 0.7 degrees below normal. The month was considerably drier than normal for most states along the southeast coast, North and South Carolina included, with reported precipitation of 75% to 90% of their normal values (Figure 3-7). Even with local rainfall amounts highly variable across the Carolinas, however, CLT actually received near normal amounts.

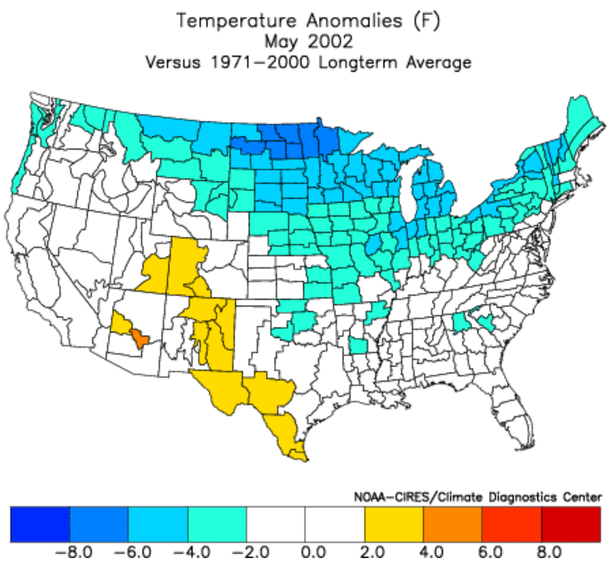

Figure 3-6: This map shows the Temperature Anomalies (ºF) during May 2002, as compared to the most recent 30-year climate average.

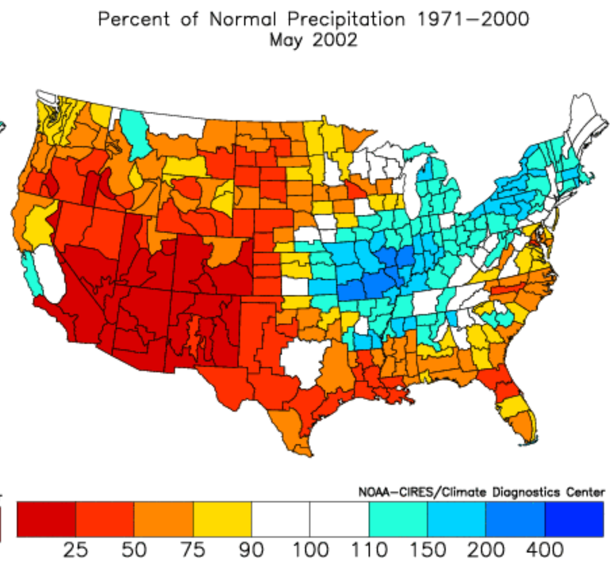

Figure 3-7: This map depicts the Percent of Normal Precipitation during May 2002, as compared to the most recent 30-year climate average.

The mean temperatures for June were approximately 2ºF to 4ºF above normal from the Piedmont of North Carolina back into the Midwestern US. However, the remainder of the Southeastern US experienced temperatures rather near climatological norms (Figure 3-8). During June, the Raleigh-Durham area experienced its highest maximum temperatures of the summer, over 6 ºF above normal. However, maximum temperature departures at CLT were not as extreme, at around 1.8 ºF above normal. Precipitation was 50% to 75% of normal for most of the southeast and less than half that of normal in south central North Carolina and parts of South Carolina (Figure 3-9). Moderate to severe drought persisted, with the more extreme conditions occurring around the Metrolina area.

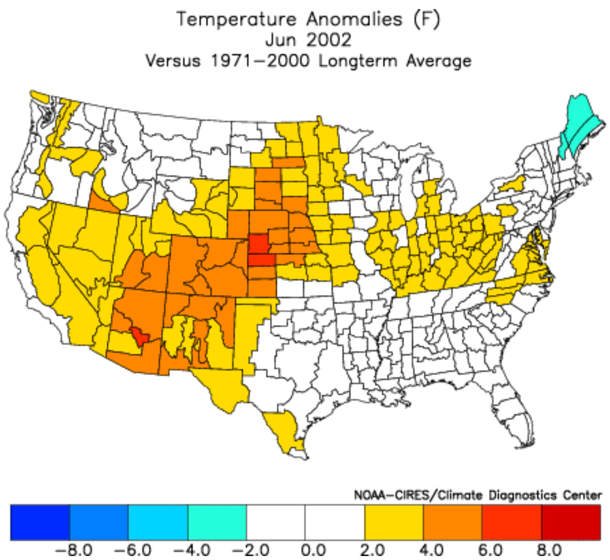

Figure 3-8: This map shows the Temperature Anomalies (ºF) during June 2002, as compared to the most recent 30-year climate average.

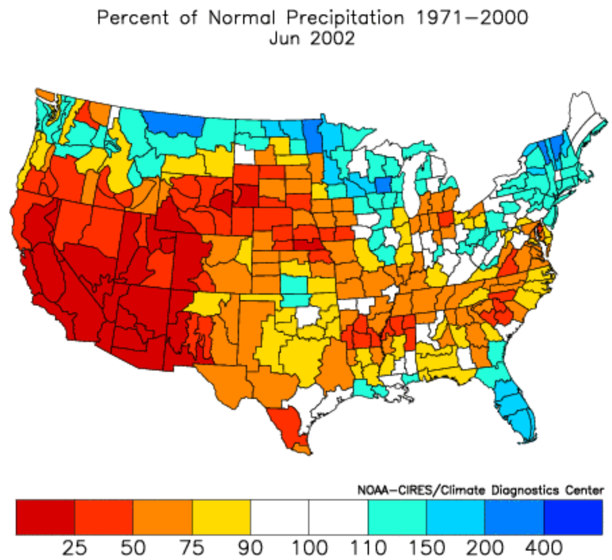

Figure 3-9: This map depicts the Percent of Normal Precipitation during June 2002, as compared to the most recent 30-year climate average.

Mean temperatures in July 2002 were 1ºF to 2ºF above normal throughout the mid-Atlantic region, with greater above-average temperature departures located across the northern half of the US (Figure 3-10). CLT had maximum temperatures reaching approximately 3º F above average. Rainfall continued to be below normal from eastern Georgia through North Carolina (Figure 3-11). Charlotte rainfall was approximately one-third of normal for the month.

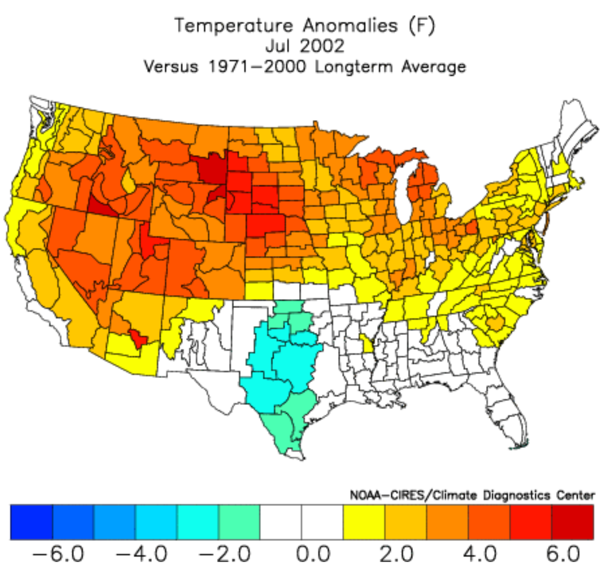

Figure 3-10: This map illustrates the Temperature Anomalies (ºF) during July 2002, as compared to the most recent 30-year climate average.

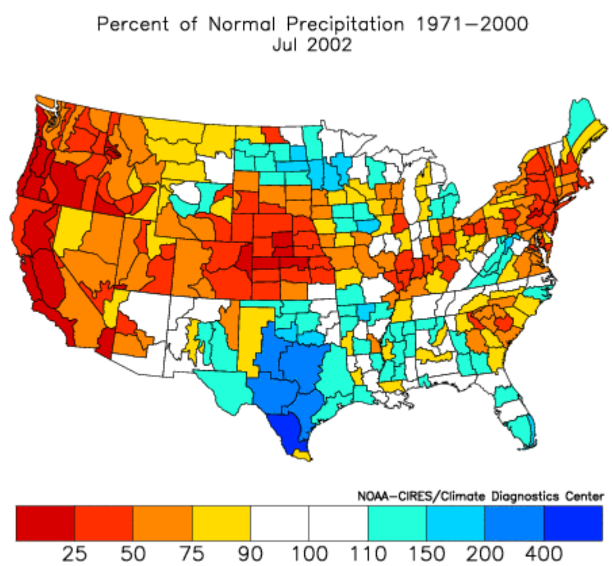

Figure 3-11: This map shows the Percent of Normal Precipitation during July 2002, as compared to the most recent 30-year climate average.

Temperatures in August were slightly above normal in most of the eastern third of the country, with some locations experiencing temperatures significantly above normal (Figure 3-12). The mean maximum temperature at CLT followed this trend, averaging out at 1.4 ºF above normal. Precipitation along the South Atlantic Coastal states, including the Carolinas was above normal due to the influence of tropical systems moving across the region (Figure 3-13). However, long-term drought continued to persist for the remainder of the East Coast of the US throughout the month.

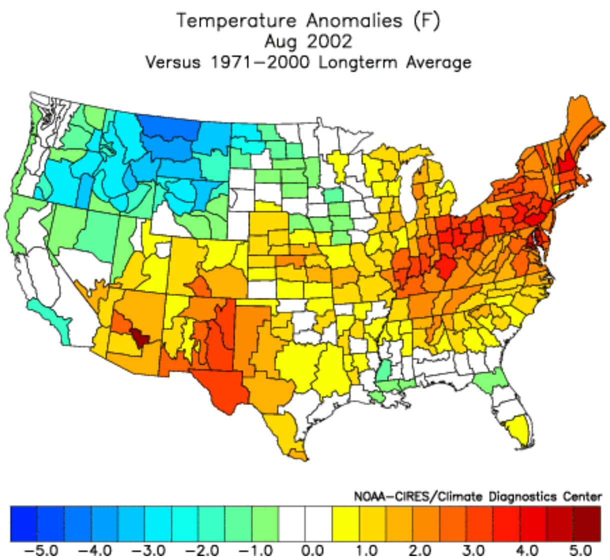

Figure 3-12: This map depicts the Temperature Anomalies (ºF) during August 2002, as compared to the most recent 30-year climate average.

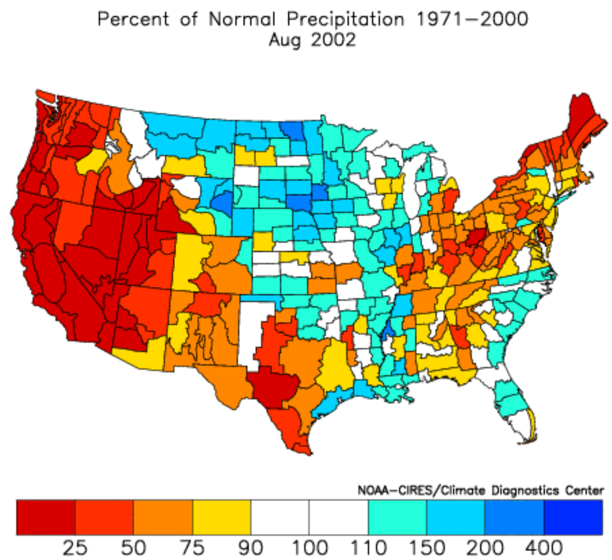

Figure 3-13: This graphic illustrates the Percent of Normal Precipitation during August 2002, as compared to the most recent 30-year climate average.

Mean temperatures in the central Carolinas were generally 1ºF to 2ºF above average throughout September 2002, with most of the US east of the Rockies significantly above climatological averages (Figure 3-14). Mean maximum temperatures at CLT, however, were actually slightly below average. As in August, the influence of nearby tropical systems caused September to be wetter than normal across the area between the Mississippi River and the Appalachian Mountains (Figure 3-15). The rainfall total at CLT was close to the climatological norm for the month even as the Piedmont region of North and South Carolina continued to hang on to drought conditions due to long-term precipitation deficits.

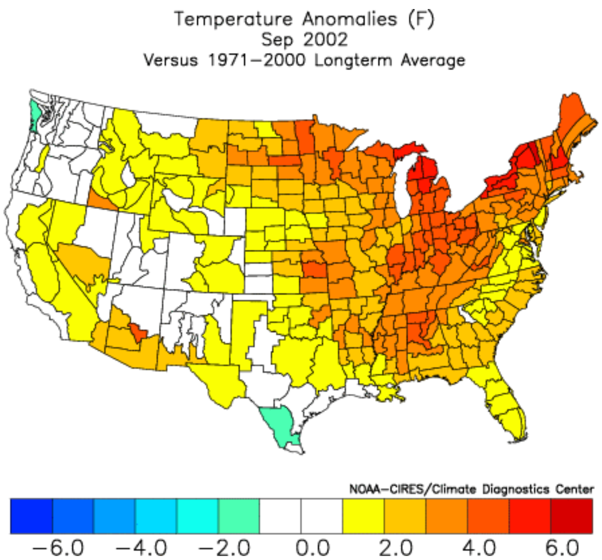

Figure 3-14: This image shows the Temperature Anomalies (ºF) during September 2002, as compared to the most recent 30-year climate average.

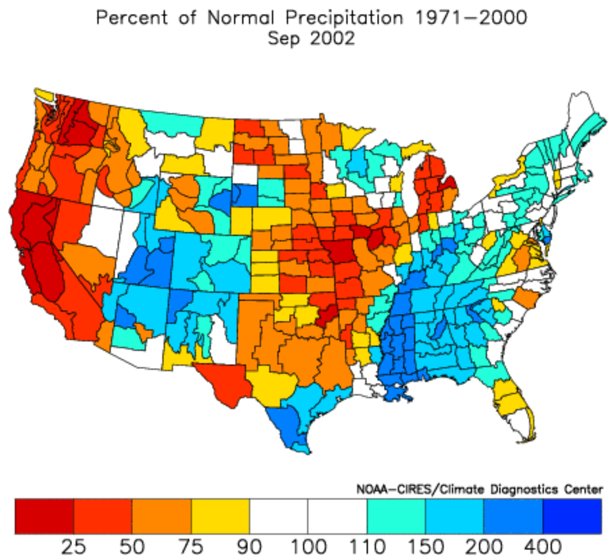

Figure 3-15: This map depicts the Percent of Normal Precipitation during September 2002, as compared to the most recent 30-year climate average.

In summary, the 2002 ozone season was slightly warmer than normal across the Carolinas. Precipitation ended up below normal, with greatest departures from May through July. The influence of tropical systems brought above normal rainfall for August and September. Despite the rainfall, overall drought conditions persisted for the entire ozone season, with the abnormally dry conditions impacting the ozone response in a number of ways. In general, below normal rainfall correlates to less cloud cover and a decrease in soil moisture. Low soil moisture led to lower dew point temperatures from reduced evapotranspiration, further contributing to the reduction of cloud cover over the course of the season. With more incoming solar radiation that would have otherwise been absorbed by cloud cover, higher daytime maximum temperatures occurred over a broad area. The combination of these factors promoted more ozone conversion in the ambient air as compared to a more climatologically-normal summer with wetter conditions.

3.4. Episode Classification

As shown climatologically, 2002 potentially provides an excellent year as a basis for attainment modeling. Following this line of logic, 2002 should provide equally adept as a basis year for the evaluation of various control strategies for maintaining the NAAQS for ozone. However, further study was necessary to identify enough of a variety of episode periods occurring during the 2002 season to justify this supposition. To perform this evaluation, methodology was developed to correlate periods of elevated ozone that occurred in the Metrolina area during the 2002 ozone season with each of the six meteorological scenarios presented in Section 3. The following sub-sections outline the episode classification methodology and procedures, as well as the resultant determinations, in further detail.

3.4.1. Procedures for Episode Classification

Ambient monitoring data from the Metrolina area was used to determine the days during the 2002 season that an exceedance of the 8-hour NAAQS for ground-level ozone occurred. These days were then grouped into individual episodes and evaluated using the selection criteria discussed in Section 2. A further analysis of each ozone episode, which used several sources of air quality and meteorological data to determine the diversity and severity of the identified episodes throughout the 2002 ozone season, was performed.

Ambient ozone data from 2002 for the entire eastern US, gathered from graphics provided by USEPA's AIRNOW website archive, was then examined, wherein focus was placed on 8-hour peak ozone concentrations. The ability to visually inspect the data provided easy assessment of the spatial and temporal distribution of ozone throughout the Carolinas, as well as other areas of the eastern US. The visual inspection of the ambient ozone data made it possible to easily determine whether the event was regional, sub-regional, or local in nature.

In addition to the ambient data plots, several surface and upper air meteorological datasets were examined to assess the atmospheric conditions contributing to the build-up of ozone in each episode. Local Climatological Data sheets obtained from NOAA's National Climatic Data Center (NCDC) were used to collect diurnal (daily) temperature, precipitation, and wind speed and direction data. Daily Weather Maps from NCDC were then used to determine the approximate location of surface fronts, troughs, and ridges, as well as daily peak temperatures and total daily precipitation.

Prognostic model analysis charts derived from the NOAA Weather Research and Forecast Model's North American Mesoscale module (WRF/NAM, formerly called Eta) were used to assess conditions such as wind fields, temperatures, moisture, and the location of ridges and troughs. These charts were used as an enhancement in the classification of high ozone episodes from the 2002 season in relating them to previously defined meteorological scenarios. The combination of the spatial ozone plots with the meteorological charts went further in illuminating instances where the potential for recirculation, a contributor to high ozone episodes, may exist.

3.4.2. Episode Classification of the 2002 Ozone Season

All days with ozone exceedances at any monitoring site in the Metrolina Area were considered in the episode classification process. There were a total of 38 days in 2002 with an exceedance of the 8-hour NAAQS at one or more monitors in the Metrolina areas. These days were divided into episodes based on the distribution of measured ozone and the meteorological conditions that occurred throughout the period of exceedance. In all, there were 13 different high ozone episodes during the 2002 ozone season.

All episodes have some common characteristics. Warm temperatures, little or no precipitation, and relatively light winds are needed to produce ozone. Typically, these conditions are characteristic of a surface high pressure area. The differences in the position, strength, and movement of the surface high pressure areas, along with differences in the mid-to-upper level wind patterns, allow us to discern several meteorological scenarios in which ozone episodes are likely. These meteorological scenarios were previously discussed in Section 2.4.

An initial analysis of ambient data and Daily Weather Maps was used to place each of the 13 ozone episodes into one of the five meteorological scenarios. A list with the number of monitors exceeding the 8-hour ozone NAAQS in each of the three major metropolitan areas was compiled and reviewed (See Table 3-4). This information was used to exclude those episodes from each category that did not have sufficient spatial or temporal distribution to justify further study. Nine episodes could be considered "widespread," with three eastern stacked high episodes, three frontal approach episodes, three Canadian high episodes, and one modified Canadian high episode, as well as four instances of tropical influence. (Note: Some episodes contained two scenarios, such as a stacked high followed by a frontal approach.) A more detailed analysis of each of these nine episodes was made using all sources of air quality and meteorological data to select the episodes that would best meet the modeling objectives.

Table 3-4: Ozone Exceedance Days During 2002

Episode	**Meteorological Scenario**	**Number of Monitors Exceeding 8 Hour NAAQS in the Metrolina Area**
05/24	3	3
05/25		6
06/03	2	3
06/04		4
06/05		1
06/10	1	7
06/11		7
06/12		6
06/13		7
07/01	1	2
07/02		7
07/03		5
07/04		3
07/05	2	3
07/06		2
07/08	4	8
07/09		5
07/16	1	5
07/17		8
07/18		5
07/29	1 (B)	2
07/31	2	1
08/01	5→2	3
08/02		6
08/05	2 (T)	1
08/06		1

Table 3-4: Ozone Exceedance Days (Continued)

08/09	3	6
08/10		7
08/11		7
08/12		6
08/13		4
08/21	3	2
08/22		2
08/23	1	6
09/04	2 (T)	2
09/05	3 (T)	3
09/06		1
09/11	2 (T)	1

Note: The Metrolina has a network of eight monitors.

Meteorological Scenarios:

1- Eastern Stacked High
2- Frontal Approach
3- Canadian High
4- Modified Canadian High
5- Progressive Continental High
B- High pressure in Bermuda high configuration
T- Tropical system present ‘near’ North Carolina

The aforementioned selected episodes provide a wide range of conditions that will provide the basis for a thorough analysis of the variety of factors that lead to ozone exceedances in North and South Carolina. Control strategies can be tested under conditions that range from short duration ozone peaks above the 1-hour ozone NAAQS to extended periods of widespread exceedances of the 8-hour ozone NAAQS. These episodes also range from exceedances that were multi-regional to exceedances confined primarily to the Carolinas. For a brief summary of each episode, please see Appendix A.

In summary, the wide variety of episodes in 2002 makes it an appropriate season to model ozone for the Metrolina attainment demonstration. Additionally, the episode characterization process identifies the period of May 15 through August 31 as containing the most significant episodes of the 2002 ozone season. NCDAQ and SCDHEC plan to conserve computational and staff resources by modeling this slightly narrower period rather than the entire ozone monitoring season of April to October. This will in no way compromise the desire to capture every high ozone scenario for complete evaluation of control strategies.

4.0 Models and Modeling Configurations

NCDAQ and SCDHEC intend to utilize the same configuration of regional meteorological, emissions processing, and photochemical air quality models used by the VISTAS PM/regional haze modeling study. The underlying science behind each component of the overall modeling system are identified and discussed briefly in this section. Although the configuration of each of the modeling components has been selected as the culmination of intensive study by VISTAS, there remains the possibility that certain algorithms and parameter settings may still be updated prior to the running of the final annual 2002 base case simulation and subsequent model performance testing.

The NCDAQ and SCDHEC modeling team will remain in close contact with the VISTAS, as well as other RPO regional modeling initiatives throughout the Metrolina attainment modeling study, to determine appropriate refinements to the model codes, input databases, and post-modeling analysis procedures. Notable limitations of the models, relevant to their intended purpose in this attainment modeling analysis, will also be evaluated in detail.

4.1. Recommended Models

Based on extensive research of available documentation of the VISTAS Regional Haze modeling analysis, it has been determined by NCDAQ and SCDHEC that the Metrolina attainment modeling should utilize the following suite of models:

- **MM5:** The Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Meteorological Model (MM5) is a nonhydrostatic, prognostic meteorological model routinely used for urban- and regional-scale photochemical, fine particulate matter, and regional haze regulatory modeling studies.

- **SMOKE**: The Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system is an emissions modeling system that generates hourly gridded speciated emission inputs of mobile, nonroad mobile, area, point, fire, and biogenic emission sources for photochemical grid models.

- **CMAQ:** USEPA's Models-3/ Community Multiscale Air Quality (CMAQ) modeling system is a "One-Atmosphere" photochemical grid model capable of addressing ozone, particulate matter, visibility, and acid deposition at regional scale for periods up to one year.

4.2. MM5 – Mesoscale Prognostic Model

Over the past decade, researchers at the Pennsylvania State University (PSU) and the National Center for Atmospheric Research (NCAR) have collaborated in the refinement and extension of the PSU Mesoscale Meteorological Model leading to the current version of the system, MM5 (version 3.6, MPP). Originally developed in the 1970s at PSU and first documented by Anthes and Warner (1978), the MM5 modeling system has maintained its status as a state-of-the-science model through enhancements provided by a broad user community (e.g., Chen and Dudhia, 2001; Stauffer and Seaman, 1990, 1991; Xiu and Pleim, 2000). The MM5 modeling system is routinely employed in forecasting projects as well as refined investigations of severe weather. Utilization of MM5 within air quality applications is also a common practice. In recent years, the MM5 modeling system has been successfully applied in continental scale annual simulations for the years 1996 (Olerud et al., 2000), 2001 (McNally and Tesche, 2003), and 2002 (Johnson, 2003). Due to its ongoing scientific development worldwide, extensive historical applications, broad user community support, public availability, and established performance record compared with other applications-oriented prognostic models, MM5 has been selected as the preferred meteorological model for this effort. This section provides an overview of the MM5 and its data input requirements.

4.2.1. MM5 Overview

The non-hydrostatic MM5 model (Dudhia, 1993; Grell et al., 1994) is a three-dimensional, limited-area, primitive equation, prognostic model that has been used widely in regional air quality model applications (Seaman, 2000). The basic model has been under continuous development, improvement, testing, and has been openly peer-reviewed for more than 20 years (Anthes and Warner, 1978; Anthes et al., 1987). It has been used world-wide by hundreds of scientists for a variety of mesoscale studies, including cyclogenesis, polar lows, cold-air damming, coastal fronts, severe thunderstorms, tropical storms, subtropical easterly jets, mesoscale convective complexes, desert mixed layers, urban-scale modeling, air quality studies, frontal weather, lake-effect snows, sea-breezes, orographically induced flows, and operational mesoscale forecasting.

MM5 is based on the prognostic equations for three-dimensional wind components (u – zonal wind component, v – meridional wind component, and w – vertical wind component), temperature, water vapor mixing ratio, and the perturbation pressure. Use of a constant reference-state pressure increases the accuracy of the calculations near steep terrain. The model uses an efficient semi-implicit temporal integration scheme and has a nested-grid capability that can use up to ten different domains of arbitrary horizontal and vertical resolution. The interfaces of the nested grids can be either one-way or two-way interactive. The model is also capable of using a hydrostatic option, if desired, for coarse-grid applications.

MM5 uses a terrain-following non-dimensionalized pressure, or "sigma," vertical coordinate similar to that used in many operational and research models. In the non-hydrostatic MM5 (Dudhia, 1993), the sigma levels are defined according to the initial hydrostatically-balanced reference state so that the sigma levels are also time-invariant. The gridded meteorological fields produced by MM5 are directly compatible with the input requirements of "one atmosphere" air-quality models using this coordinate (e.g., CMAQ). MM5 fields can be easily used in other regional air quality models with different coordinate systems (e.g., Comprehensive Air Quality Model with Extensions - CAMx) by performing a vertical interpolation, followed by a mass-conservation re-adjustment.

Distinct planetary boundary layer (PBL) parameterizations are available for air-quality applications, both of which represent sub-grid-scale turbulent fluxes of heat, moisture and momentum. These parameterizations employ various surface energy budget equations to estimate ground temperature based on the insolation, atmospheric path length, water vapor, cloud cover, and longwave radiation. The surface physical properties of albedo, roughness length, moisture availability, emissivity and thermal inertia are defined as functions of land-use for numerous categories via a look-up table. One scheme uses a first-order eddy diffusivity formulation for stable and neutral environments and a modified first-order scheme for unstable regimes. The other scheme uses a prognostic equation for the second-order turbulent kinetic energy while diagnosing the other key boundary layer terms.

Initial and lateral boundary conditions are specified from mesoscale three-dimensional analyses performed at 12-hour intervals on the outermost grid mesh selected by the user. Additional surface fields are analyzed at three-hour intervals. A Cressman-based technique is used to analyze standard surface and radiosonde observations, using the National Meteorological Center's (NMC) spectral analysis as a first guess. The lateral boundary data are introduced into MM5 using a relaxation technique applied in the outermost five rows and columns of the most coarse grid domain.

A major feature of the MM5 is its use of state-of-science methods for Four Dimensional Data Assimilation (FDDA). The theory underlying this approach and details on how it has been applied in a variety of applications throughout the country are described in depth elsewhere (Stauffer and Seaman, 1990, 1991; Seaman et al., 1992, 1997). Results of detailed performance evaluations of the MM5 modeling system in regulatory air quality application studies have been widely reported in the literature (e.g., Emery et al., 1999; Tesche et al., 2000, 2003), and many studies have involved comparisons with other prognostic models such as the Regional Atmospheric Modeling System (RAMS) and the Systems Application International Mesoscale Model. The MM5 enjoys a far richer application history in regulatory modeling studies compared with RAMS or other models. Furthermore, in evaluations of these models in over 60 recent regional scale air quality application studies since 1995, it has generally been found that the MM5 model tends to produce somewhat better photochemical model inputs than alternative models. For these and other reasons set forth in the MM5 modeling protocol developed by the contractor performing the meteorological modeling, Barons Advanced Meteorological Systems, LLC (BAMS) (Olerud and Sims, 2003), MM5 was selected as the meteorological modeling system for this study.

4.2.2. MM5 Configuration

Based on the extensive sensitivity testing carried out by Olerud and Sims (2003), the MM5 (version 3.6, MMP) configuration to be used by BAMS modelers will consist of the following:

- Nested 36/12 kilometer (km) grids, with 34 vertical layers
- Two way nesting, no feedback
- Initialization and boundary conditions from Eta analysis fields
- Pleim-Xiu (PX) soil model
- Asymmetric Convective Mixing (ACM) PBL model
- Kain-Fritsch 2 cumulus parameterization
- Mixed phase (Reisner 1) cloud microphysics
- Rapid Radiative Transfer Model radiation
- Snow effect turned on
- ETA model sea surface temperature
- 24-category United States Geological Survey (USGS) vegetation datasets
- Thermal roughness by the Garratt method
- Standard FDDA analysis nudging on 36 km and 12 km grid nests

4.2.3. MM5 Evaluation

The MM5 modeling results will be evaluated using plots and statistical analyses to determine if the model performance is adequate for the air quality modeling exercise. Some of the plots and statistics to be generated include:

- Spatial plots of model predictions with the appropriate observations overlaid. These will provide a visual to determine how well such meteorological parameters as temperature, mixing ratios, and winds are being captured by the model.

- Graphical statistical plots for surface temperature, mixing ratio, wind speeds, wind direction, and cloud cover. These will include time series of modeled/observed means, bias/error, and index of agreement.

- Daily accumulated precipitation plots of modeled versus observed.

- Tabular statistics for temperature, winds, mixing ratio, and cloud cover for various domains.

- Comparison of satellite versus modeled cloud images.

- Comparison of surface analysis maps to the MM5 pressure/wind maps

- Comparison of profiler observations with modeled winds

4.2.4. Meteorological Data

Meteorological data are being generated using the MM5 prognostic meteorological model by BAMS. BAMS is operating the MM5 at 5-day increments for 2002 on the 36 km and 12 km grid with a 14-day spin up period for the end of December 2001. The meteorological observations to be used for statistics come primarily from University Corporation for Atmospheric Research's (UCAR's) ds472.0 archive. These data are quality controlled and converted to NetCDF format, thus allowing the data to be visualized on the model fields via Package for Analysis and Visualization of Environmental data (PAVE). Due to the unreliability in precipitation values in the UCAR dataset, precipitation statistics are calculated from the 24-h gridded accumulations available from the Climate Prediction Center (CPC). However, these fields undergo grid transformation to match our 36-km and 12-km domains from their original 0.25- degree resolution. The statistics are only calculated over cells that MM5 deems to be land since the CPC analyses are derived primarily from rain gauges.

For aloft analyses, standard sounding observations from the National Center for Environmental Predictions (NCEP) ds353.4 archive are processed. These observations are quality controlled and used to produce model/observation skewT sounding plots for selected sites. Additionally, the observations are integrated into sigma levels that match the MM5 specifications and subsequently can be statistically analyzed for performance at sigma levels 9, 17, and 22 (~500m, ~1600m, ~3400m, respectively). Qualitative profiler plots showing model/observed hourly winds are also created based upon the data stored at the Forecast Systems Lab.

4.3. SMOKE Emissions Modeling System

The SMOKE Emissions Processing System Prototype was originally developed at the Micro-computing Center of North Carolina (Coats, 1995; Houyoux and Vukovich, 1999). As with most "emissions models," SMOKE is principally an *emission processing system* and not a true *emissions modeling system* in which emissions estimates are simulated from "first principles." This means that, with the exception of mobile and biogenic sources, its purpose is to provide an efficient, modern tool for converting emissions inventory data into the formatted emission files required by an air quality simulation model. For mobile sources, SMOKE actually simulates emissions rates based on input mobile-source activity data, emission factors and outputs from transportation travel-demand models.

SMOKE was originally designed to allow emissions data processing methods to utilize emergent high-performance-computing as applied to sparse-matrix algorithms. Indeed, SMOKE is the fastest emissions processing tool currently available to the air quality modeling community. The sparse matrix approach utilized throughout SMOKE permits both rapid and flexible processing of emissions data. The processing is rapid because SMOKE utilizes a series of matrix calculations instead of less efficient algorithms used in previous systems. The processing is flexible because the processing steps of temporal projection, controls, chemical speciation, temporal allocation, and spatial allocation have been separated into independent operations wherever possible. The results from these steps are merged together at a final stage of processing.

SMOKE supports area, mobile, fire and point source emission processing and includes biogenic emissions modeling through a rewrite of the Biogenic Emission Inventory System, version 3 (BEIS3). SMOKE has been available since 1996, and it has been used for emissions processing in a number of regional air quality modeling applications. In 1998 and 1999, SMOKE was redesigned and improved with the support of the USEPA for use with USEPA's Models-3/CMAQ. The primary purposes of the SMOKE redesign were support of: (a) emissions processing with user-selected chemical mechanisms and (b) emissions processing for reactivity assessments.

SMOKE contains a number of major features that make it an attractive component of the modeling system (Seppanen, 2003). The model supports a variety of input formats from other emissions processing systems and models including the Inventory Data Analyzer (IDA), Emissions Modeling System – 2003 (EMS), and the Emissions Preprocessor System 2.x (EPS). It supports both gridded and county total land use scheme for biogenic emissions modeling. Although it is not necessary for our purposes, SMOKE can accommodate emissions files from up to 10 countries and any pollutant can be processed by the system.

Recent computational improvements to SMOKE include:

- Enhanced disk space requirements compared with other emissions processing software

- Run-time memory allocation, eliminating any need to recompile the programs for different inventories, grids, or chemical mechanisms
- Updated Input/Output Applications Programming Interface (I/O API) libraries

A number of science features have been incorporated into the latest version of SMOKE (version 2.0), including:

- Any chemical mechanism can be used to partition pollutants to model species, as long as the appropriate input data are supplied
- Integration with the MOBILE6.2 on-road mobile source emissions model including link based processing
- Support of plume-in-grid processing
- Integration of the BEIS3 emissions factors in SMOKE

Notable features of SMOKE from an applications standpoint include:

- Improved control strategy input formats and designs
- Control strategies can include changes in the reactivity of emitted pollutants, a useful capability, for example, when a solvent is changed in an industrial process
- No third party software is required to run SMOKE, although some input file preparation may require other software
- Integration with Models-3 file formats and settings
- Improved data file formats
- Support of various air quality model emissions input formats (e.g., CMAQ, MAQSIP, UAMIV, UAM-V, REMSAD and CAMx)
- Enhanced quality assurance pre- and post-processing
- Fully integrated with Models-3, which will provide the SMOKE Tool for SMOKE input file preparation
- Enhanced treatment of growth and control factors
- Improved emissions reporting and Quality Assurance (QA) capabilities
- Improved temporal allocation

The Carolina Environmental Program at the University of North Carolina is continuing model development activities with SMOKE. The emissions modeling will employ the SMOKE version 2.0, released on September 30, 2003. The SMOKE executables, scripts and databases may be downloaded through the Community Modeling and Analysis (CMAS) center's Model Clearinghouse.

4.4. CMAQ Modeling System

4.4.1. CMAQ Overview

For more than a decade, USEPA has been developing the Models-3 CMAQ modeling system with the overarching aim of producing a "One-Atmosphere" air quality modeling system capable of addressing ozone, fine particulate matter, visibility and acid deposition within a common platform (Dennis et al., 1996; Byun et al., 1998a; Byun and Ching, 1999; Pleim et al., 2003). The original justification for the Models-3 development emerged from the challenges posed by the 1990 CAAA and USEPA's desire to develop an advanced modeling framework for “holistic” environmental modeling utilizing state-of-science representations of atmospheric processes in a high performance computing environment (Ching et al., 1998). USEPA completed the initial stage of development with Models-3 and released the CMAQ model in mid 1999 as the initial operating science model under the Models-3 framework (Byun et al., 1998b). The most recent rendition is CMAQ version 4.4, which was released in October 2004.

CMAQ consists of a core Chemical Transport Model (CTM) and several pre-processors including the Meteorological-Chemistry Interface Processor (MCIP), initial and boundary conditions processors (ICON and BCON), and a photolysis rates processor (JPROC). USEPA is continuing to improve and develop new modules for the CMAQ model and typically provides a new release each year. In the past, USEPA has also provided patches for CMAQ as errors are discovered and corrected. More recently, USEPA has funded the CMAS center to support the coordination, update and distribution of the Models-3 system.

Another reason for choosing CMAQ as the atmospheric model is the ability to do one-atmospheric modeling. Since NCDAQ will be using the same modeling exercise for both the ozone and $PM_{2.5}$ attainment demonstrations SIPs, as well as the regional haze SIP, having a model that can handle both ozone and particulate matter is essential. A number of features in CMAQ’s theoretical formulation and technical implementation make the model well-suited for annual PM modeling. In CMAQ, the model approach has been adapted to dynamically represent the PM size distribution using three log-normal modes (2 fine and 1 coarse). Transfer of mass between the aerosol and gas phases is assumed to be in equilibrium and all secondary aerosols (sulfate, nitrate, secondary organic aerosols) are assumed to be in the fine modes. The thermodynamics of inorganic aerosol composition are treated using the ISORROPIA module. Aerosol composition is coupled to mass transfer between the aerosol and gas phases. For aqueous phase chemistry, the Regional Acid Deposition Model (RADM) is currently employed. This scheme includes oxidation of sulfur dioxide (SO_2) to sulfate by ozone, hydrogen peroxide, oxygen catalyzed by metals and radicals. The impact of clouds on the PM size distribution is treated empirically. For wet deposition processes, CMAQ uses the RADM/Regional Particulate Model approach. Particle dry deposition is included as well. CMAQ contains three options for treating secondary organic aerosol (SOA), latest being the Secondary Organic Aerosol Model (SORGAM) that was updated in August 2003 to be a reversible semi-volatile scheme whereby VOCs can be converted to condensable gases that can then form SOA and then evaporate back into condensable gases depending on atmospheric conditions.

4.4.2. CMAQ Configuration

NCDAQ and SCDHEC propose to run CMAQ (version 4.4). The model would be set up and exercised on a nested 36/12 km grid domain, employing one-way grid nesting. That is, boundary conditions for the 12 km grid simulation are extracted from the 36 km run using the CMAQ BCON processor. A total of 19 vertical layers would be implemented, extending up to a region top of 100 mb (approximately 15 km above ground level).

The Piecewise Parabolic Method advection solver would be used along with the spatially varying (Smagorinsky) horizontal diffusion approach and K-theory for vertical diffusion. MM5 meteorological output based on the Pleim-Xiu Land-Surface Model (LSM) and the ACM PBL scheme will be used, and the recently updated CMAQ MCIP2.3 would process the MM5 data using the "pass through" option. The Carbon Bond version 4 (CB4) gas-phase, RADM aqueous-phase, and AERO3/ISORROPIA aerosol chemistry schemes will be used. Treatment of reversible secondary organic aerosols would be simulated by the SORGAM implementation in CMAQ (version 4.4).

Testing completed with VISTAS evaluated three photochemical mechanisms: CB4, CB4-2002 and SAPRC99. CB4-2002 produced nearly identical results as CB4 but took much longer to run since it is only implemented in the slower SMVGEAR chemistry solver, compared to CB4 that is also implemented in the faster Euler Backward Iterative chemistry solver. Thus, CB4-2002 was dropped from consideration. Comparisons of CB4 and SAPRC99 found they produced mostly similar but different model performance. However, no one mechanism performed better than any other mechanism across all species, sites, and periods. The testing only evaluated the mechanism's base case performance, not their response to emission reductions. Given that CB4 runs twice as fast as SAPRC99, the CB4 mechanism was chosen for use.

4.4.3. Initial and Boundary Condition Data

The CMAQ default Initial Concentrations (ICs) will be used along with a ~15 day spin up period to eliminate any significant influence of the ICs. The CMAQ Boundary Conditions (BCs) for the initial simulations will be based on seasonal averages of 3-hour 2001 GEOS-CHEM global simulation model output. VISTAS and other Regional Planning Organizations (RPOs) are finding a 2002 GEOS-CHEM simulation that would be used to define days specific high time resolved (e.g., 3-hourly) CMAQ BCs.

4.5. Model Limitations

All mathematical models possess inherent limitations owing to the necessary simplifications and approximations made in formulating the governing equations, implementing them for numerical solution on fast computers, and in supplying them with input datasets and parameters that are themselves approximations of the full state of the atmosphere and emissions processes. The more important limitations of the various modeling systems to be employed are noted in this section.

4.5.1. MM5

Four different configurations of the MM5 LSM and PBL were evaluated. Depending on the meteorological variable (e.g., winds, temperature, moisture) and location (e.g., mountains, coastal, east, west) different LSM_PBL configurations performed better. The PX_ACM LSM_PBL configuration was selected because it was consistently near the top performing configuration in the southeastern US across variables and locations and was never the worst-performing configuration. However, there are numerous limitations in the MM5 with the LSM and PBL treatment being some of the most important. The MM5 PX_ACM frequently predicts very low PBL heights that can appear as "holes" in the spatial distribution of PBL heights that do not appear physically realistic and may affect air quality modeling. Although the MM5 PX_ACM configuration model performance in the southeastern US mostly met performance benchmarks, the performance was much worse in the western US. In addition, there is a stochastic component of real world meteorology that is not captured by MM5. For example, for some ozone episodes stagnation is an important attribute that MM5 fails to simulate well as it tries to organize the flow fields. However, the MM5 model represents approximately 20 years of development by various researchers.

4.5.2. SMOKE

In early testing, a number of undocumented features of the SMOKE 1.5b version necessitated re-runs of the emissions processing software to overcome errors and/or ambiguities in source documentation and QA reporting. It is unclear whether similar conditions will be encountered with the SMOKE 2.0 release. As a full software release, rather than a "beta" version, SMOKE 2.0 is expected to be more robust and more fully-documented than the SMOKE 1.5b release. However, with any newly-released software system, there is the potential for errors and/or ambiguities to affect the emissions modeling schedule. Should problems arise or issues be encountered which would require additional SMOKE runs or potential SMOKE modifications or alternate modeling methods, NCDAQ and SCDHEC will immediately notify stakeholders and make recommendations for resolving the issues. Upon receipt of technical direction from the stakeholders, appropriate corrective action will be taken.

Features are continuing to be developed in the SMOKE emissions model. As it is not as mature as some other emission models (e.g., EMS, EPS, etc.), SMOKE does not include as many features. NCDAQ and SCDHEC will keep abreast of SMOKE development activities to identify new features that will assist in the emissions modeling.

4.5.3. CMAQ

Like all air quality models, a major limitation of CMAQ is the input for emissions, meteorological, and IC/BC data. Key science limitations in the model itself include the nitrate formation chemistry. Testing found the CMAQ nitrate performance suspect with winter overestimations and summer underestimations. Other science limitations in the current version of CMAQ include inadequate treatment of sea salt and the assumption that all secondary PM is in the fine mode. Lack of any two-way grid nesting limits the ability of the model to properly resolve point source plumes or urban photochemistry. Other limitations of CMAQ include its computational requirements, such as the need for excessive disk space.

4.6. Model Input Requirements

Each of the modeling system components has significant database requirements. These data needs fall into two categories: those required for model setup and operation, and those required for model evaluation testing. The main input data base requirements for the meteorological, emissions, and air quality models are identified in the following section.

4.6.1. MM5

The databases required for setting up, exercising, and evaluating the MM5 model for the 2002 season consist of various fixed and variable inputs.

- <u>Topography</u>: High resolution (e.g., 30 sec to 5 min) topographic information derived from the Geophysical Data Center global datasets from the NCAR terrain databases are available for prescribing terrain elevations throughout the 36 km and 12 km grid domain.

- Vegetation Type and Land Use: Vegetation type and land use information on the 36 km grid may be developed using the PSU/NCAR 10 min. (~18.5 km) databases while for the 12 km grids, the USGS data are available.

- Atmospheric Data: Initial and boundary conditions to the MM5 may be developed from operationally analyzed fields derived from the NCEP ETA (40 km resolution) following the procedures outlined by Stauffer and Seaman (1990). These 3-hr synoptic-scale initialization data include the horizontal wind components (u and v), temperature, and relative humidity at the standard pressure levels, plus sea-level pressure and ground temperature. Here, ground temperature represents surface temperature over land and sea-surface temperature over water.

- Water Temperature: Water temperatures required on both 36 km and 12 km grids can be derived from the ETA skin temperature variable. These temperatures are bi-linearly interpolated to each model domain and, where necessary, filtered to smooth out irregularities.

- Clouds and Precipitation: While the non-hydrostatic MM5 treats cloud formation and precipitation directly through explicit, resolved-scale, and parameterized sub-grid scale processes, the model does not require precipitation or cloud input. The potential for precipitation and cloud formation enters through the thermodynamic and cloud processes formulations in the model. The only precipitation-related input required is the initial mixing ratio field that is developed from the National Weather Service (NWS) and NMC datasets previously discussed.

- Multi-Scale FDDA: The standard "multi-scale" data assimilation strategy to be used on the 36 km and 12 km grids will objectively analyze three-dimensional fields produced every 3 hours from the NWS rawinsonde wind, temperature, and mixing ratio data, and similar analyses are generated every three hours from the available NWS surface data.

4.6.2. SMOKE

The databases required to set up and operate SMOKE are as follows:

- Area source emissions in IDA format
- Off-road mobile source emissions in IDA format
- Stationary point source emissions in IDA format
- Utility emissions
    - Continuous Emissions Monitoring (CEM) emissions, day specific for actual 2002
    - 5-year average CEM emissions, day specific for typical 2002
    - Based on Integrated Planning Model (IPM) modeling for future year
- Wildfire emissions
    - Day specific for actual 2002
    - Multi-year average for typical year 2002 and future year
- On-road motor vehicle activity data
- MOBILE6.2 input parameters

Also required for annual modeling are data files specific for:

- Temporal allocation
- Spatial allocation
- Speciation

4.6.3. CMAQ

The CMAQ CTM requires the following inputs:

- Three-dimensional hourly meteorological fields that will be generated by the CMAQ MCIP2.3 processing of the BAMS MM5 output
- Three-dimensional hourly emissions generated by SMOKE
- Initial conditions and boundary conditions (IC/BC)
- Topographic information
- Land use categories
- Photolysis rates generated by the CMAQ JPROC processor

5.0 Grid Specifications and Modeling Domains

This chapter summarizes the model domain definitions including the model domain, resolution, map projections and nesting schemes for high resolution sub-domains.

5.1. Horizontal Modeling Domain

A coarse grid continental US domain with a 36 km horizontal grid resolution will be used as the outer grid domain for MM5 modeling. The CMAQ domain is nested within the MM5 36 km domain. Figure 5-1 shows the MM5 horizontal domain as the outer most, blue grid with the CMAQ 36 km domain nested in the MM5 domain. To achieve finer spatial resolution in the VISTAS states, NCDAQ and SCDHEC will also use a one-way nested high resolution grid with a 12 km grid resolution. Figure 5-2 shows the 36 km CMAQ continental grid and the high resolution, nested 12-km grid in the VISTAS states. Figure 5-3 shows in more detail the 12 km grid for the VISTAS region.

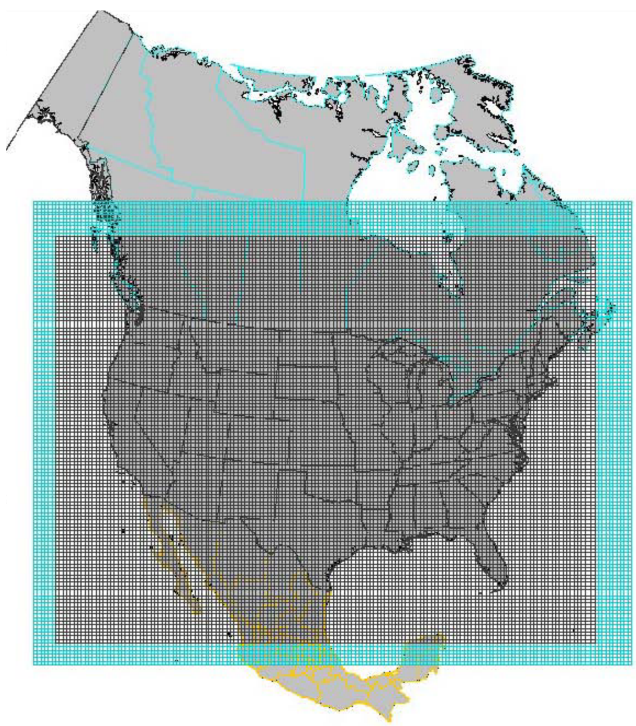

Figure 5-1: The MM5 horizontal domain is the outer most, blue grid, with the CMAQ 36 km domain nested in the MM5 domain.

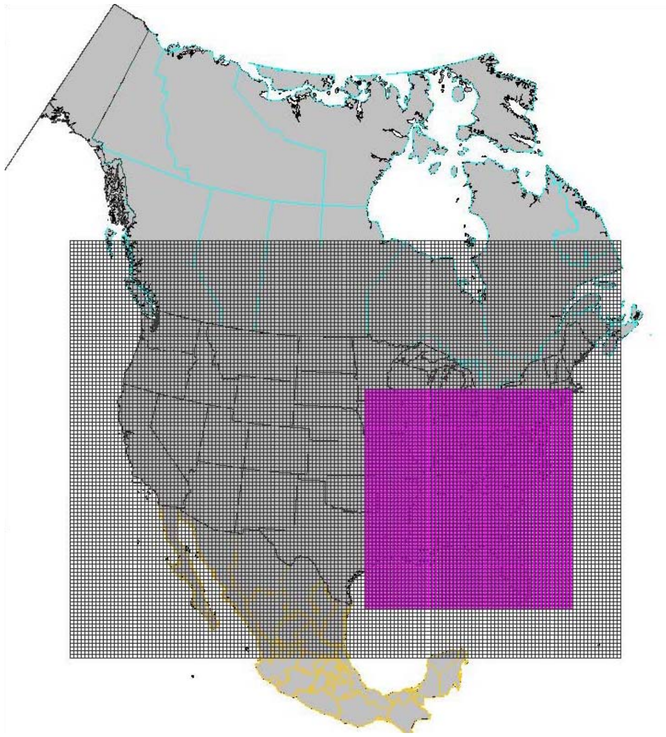

Figure 5-2: The 36 km CMAQ continental grid and the high resolution, nested 12-km grid over the VISTAS states.

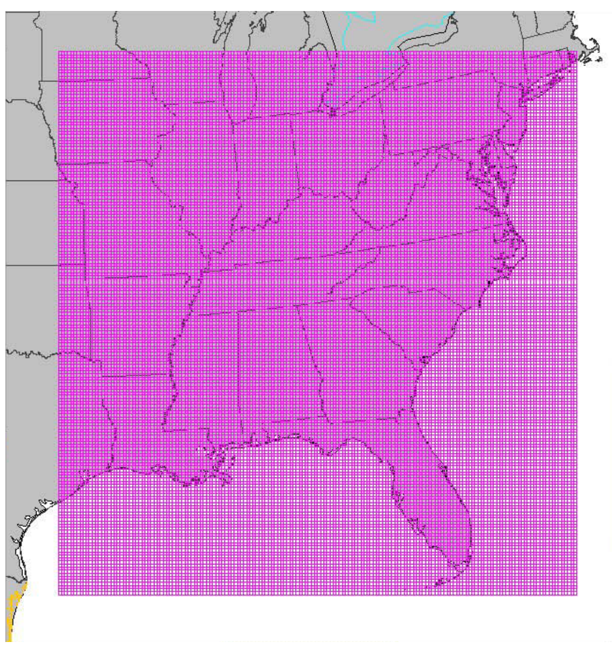

Figure 5-3: A more detailed view of the 12 km grid over the VISTAS region.

Both MM5 and CMAQ employ the RPO unified grid definition for the 36 km continental domain. The RPO unified grid consists of a Lambert-Conformal map projection using the map projections parameters listed in Table 5-1.

Table 5-1: RPO Unified Grid Definition.

PARAMETER	VALUE
projection	Lambert-conformal
1^{st} true latitude (alpha)	33 degrees
2^{nd} true latitude (beta)	45 degrees
x center	- 97 degrees
y center	40 degrees

The MM5 36 km grid includes 164 cells in the east-west dimension by 128 cells in the north-south dimension. The CMAQ 36 km grid includes 148 cells in the east-west dimension and 112 cells in the north-south dimension. Since the MM5 coarse grid is also nested in the Eta grid, there is a possibility of boundary effects near the MM5 boundary that occur as the Eta meteorological variables are being simulated by MM5 and must come into dynamic balance with MM5's algorithms. Thus, a larger MM5 domain was selected to provide a buffer of 8 to 9 grid cells around each boundary of the CMAQ 36 km domain. This is designed to eliminate any errors in the meteorology from boundary effects in the MM5 simulation at the interface of the MM5 and Eta grids. The buffer region used here exceeds the USEPA suggestion of at least 5 grid cell buffer at each boundary.

Table 5-2 lists the number of rows and columns and the definition of the X and Y origin (i.e., the southwest corner) for the 36 km and 12 km grids for both MM5 and CMAQ. Note that the CMAQ grid is rotated 90 degrees relative to the MM5 grid, so rows and columns are reversed. In Table 5-2 "Dot" refers to the grid mesh defined at the vertices of the grid cells while "cross" refers to the grid mesh defined by the grid cell centers. Thus, the dimension of the dot mesh is equal to the cross mesh plus one. Finally, note that the grid definition for the CMAQ MCIP and CMAQ Chemical Transport Model (CCTM) are identical.

Table 5-2: Grid Definitions for MM5 and CMAQ.

MODEL	COLUMNS DOT (CROSS)	ROWS DOT (CROSS)	XORIGIN	YORIGIN
MM5 36km	129 (128)	165 (164)	-2952000	-2304000
CMAQ 36km	149 (148)	113 (112)	-2736000	-2088000
MM5 12km	190 (189)	181 (180)	7200	-1656000
CMAQ 12km	169 (168)	178 (177)	108000	-1620000

5.2. Vertical Modeling Domain

The CMAQ vertical structure is primarily defined by the vertical grid used in the MM5 modeling. The MM5 model employed a terrain following coordinate system defined by pressure, using 34 layers that extend from the surface to the 100 mb. Table 5-3 lists the layer definitions for both MM5 and for CMAQ. A layer averaging scheme is adopted for CMAQ to reduce the computational cost of the CMAQ simulations. The effects of layer averaging were evaluated in conjunction with the VISTAS modeling effort and were found to have a relatively minor effect on the model performance metrics when both the 34-layer and a 19-layer CMAQ models were compared to ambient monitoring data.

Table 5-3: Vertical Layer Definition For MM5 Simulations (Left Most Columns), And Approach For Reducing CMAQ Layers By Collapsing Multiple MM5 Layers (Right Columns).

MM5					**CMAQ 19L**				
Layer	Sigma	Pres. (mb)	Height (m)	Depth (m)	Layer	Sigma	Pres .(mb)	Height (m)	Depth (m)
34	**0.000**	**100**	**14662**	**1841**	**19**	**0.000**	**100**	**14662**	**6536**
33	0.050	145	12822	1466		0.050	145		
32	0.100	190	11356	1228		0.100	190		
31	0.150	235	10127	1062		0.150	235		
30	0.200	280	9066	939		0.200	280		
29	**0.250**	**325**	**8127**	**843**	**18**	**0.250**	**325**	**8127**	**2966**
28	0.300	370	7284	767		0.300	370		
27	0.350	415	6517	704		0.350	415		
26	0.400	460	5812	652		0.400	460		
25	**0.450**	**505**	**5160**	**607**	**17**	**0.450**	**505**	**5160**	**1712**
24	0.500	550	4553	569		0.500	550		
23	0.550	595	3984	536		0.550	595		
22	**0.600**	**640**	**3448**	**506**	**16**	**0.600**	**640**	**3448**	**986**
21	0.650	685	2942	480		0.650	685		
20	**0.700**	**730**	**2462**	**367**	**15**	**0.700**	**730**	**2462**	**633**
19	0.740	766	2095	266		0.740	766		
18	**0.770**	**793**	**1828**	**259**	**14**	**0.770**	**793**	**1828**	**428**
17	0.800	820	1569	169		0.800	820		
16	**0.820**	**838**	**1400**	**166**	**13**	**0.820**	**838**	**1400**	**329**
15	0.840	856	1235	163		0.840	856		
14	**0.860**	**874**	**1071**	**160**	**12**	**0.860**	**874**	**1071**	**160**
13	0.880	892	911	158	**11**	**0.880**	**892**	**911**	**158**
12	**0.900**	**910**	**753**	**78**	**10**	**0.900**	**910**	**753**	**155**
11	0.910	919	675	77		0.910	919		
10	**0.920**	**928**	**598**	**77**	**9**	**0.920**	**928**	**598**	**153**
9	0.930	937	521	76		0.930	937		
8	**0.940**	**946**	**445**	**76**	**8**	**0.940**	**946**	**445**	**76**
7	**0.950**	**955**	**369**	**75**	**7**	**0.950**	**955**	**369**	**75**
6	**0.960**	**964**	**294**	**74**	**6**	**0.960**	**964**	**294**	**74**
5	**0.970**	**973**	**220**	**74**	**5**	**0.970**	**973**	**220**	**74**
4	**0.980**	**982**	**146**	**37**	**4**	**0.980**	**982**	**146**	**37**
3	**0.985**	**986.5**	**109**	**37**	**3**	**0.985**	**986.5**	**109**	**37**
2	**0.990**	**991**	**73**	**36**	**2**	**0.990**	**991**	**73**	**36**
1	**0.995**	**995.5**	**36**	**36**	**1**	**0.995**	**995.5**	**36**	**36**
0	**1.000**	**1000**	**0**	**0**	**0**	**1.000**	**1000**	**0**	**0**

6.0 Development of Emissions Inventories

There are five different emission inventory source classifications; stationary point sources area sources, off-road mobile sources, on-road mobile sources, and biogenic sources. Stationary point sources are those sources that emit greater than a specified tonnage per year and the data is provided at the facility level. Stationary area sources are those sources whose emissions are relatively small but due to the large number of these sources, the collective emissions could be significant (i.e., dry cleaners, service stations, etc.) Off-road mobile sources are equipment that can move but do not use the roadways, i.e., lawn mowers, construction equipment, railroad locomotives, aircrafts, etc. On-road mobile sources are automobiles, trucks, and motorcycles that use the roadway system. Biogenic sources are emissions from natural sources, such as trees, crops, grasses and natural decay of plants.

Emission estimates for stationary point and area sources, as well as for off-road mobile sources are calculated and formatted for processing through the SMOKE emissions processing system, which formats the data into air quality model ready files. On-road mobile source emissions are estimated within the SMOKE system, which uses the USEPA's MOBILE6.2 model, with modeling meteorology and various mobile inputs. The biogenic emissions are also estimated within the SMOKE system, using the USEPA's BEIS model, with modeling meteorology.

In addition to the various source classifications, there are also various types of emission inventories. The first is the actual base year inventory. This inventory is the base year emissions that correspond to the meteorological data, for this modeling effort is 2002. These emissions are used for evaluating the air quality model performance.

The second type of inventory is the typical base year inventory. This inventory is similar to the actual base year, however for sources that may have significant changes from year to year a more typical emission value is used. In this modeling effort, typical emissions were developed for the electric generating units and the wildland fire emissions. The air quality modeling results using these emissions are used in calculating the relative reduction factors used in the attainment demonstration test.

The future year base inventory is an inventory developed for some future year for which attainment of the ozone standard is needed. For this modeling project, the future year inventory will be 2009, the last complete year for which the standard must be attained. It is the future year base inventory that control strategies and sensitivities are applied to determine what controls, to which source classifications, must be made in order to attain and maintain the ozone standard.

In the sections that follow, the inventories used for each source classifications are discussed.

6.1. Point Source Emissions

The point source emissions will be separated into electric generating units (EGU) and non-EGU categories. The reason for splitting the point source inventory is that the EGU sources account for the majority of the point source NO_x emissions and hour specific data is available for these sources through the USEPA's acid rain database. Using this more refined data will help improve the air quality modeling performance. Annual emissions will be used for the non-EGU sources.

All point sources will be spatially allocated in the domain based on the stationary source geographic coordinates. If a point source is missing its latitude/longitude coordinates, the source will be placed in the center of its respective county.

6.1.1. Electric Generating Units

Actual Base Year Inventory

For EGU sources with USEPA reported 2002 CEM data or with 2002 hourly emissions provided by stakeholders, actual hourly data will be used. For the sources where USEPA CEM data are utilized, NO_x, SO_2, and heat input-based hour-specific profiles were developed and applied to NO_x, SO_2, and all other emissions, respectively. The annual emission values that have been provided will be maintained, but will be distributed using hourly to annual profiles. For sources where hour-specific data was provided by stakeholders, this data will be substituted for USEPA CEM-based emissions and distributions.

To temporally allocate the remaining EGU point sources, the NO_x, SO_2, and heat input data will be collected from the 2002 CEM datasets, and used to develop unit-level temporal distributions. The hourly, day of week, and monthly specific temporal profiles will be used in conjunction with the emissions inventory supplied emissions data to calculate hourly EGU emissions by unit.

Typical Base Year Inventory

Since the NO_x emissions from EGU sources are a significant part of the emissions inventory, a typical base year emissions inventory was developed for these sources to avoid anomalies in emissions due to variability in meteorology, economic and outage factors in 2002. This approach is consistent with the USEPA's modeling guidance.

To develop a typical year 2002 emissions inventory for EGU sources, for each unit the average CEM heat input for 2000 through 2004 was divided by the 2002 actual heat input to generate a unit specific normalizing factor. This normalizing factor was then multiplied by the 2002 actual emissions. The heat inputs for the period 2000 through 2004 were used since the modeling current design values use monitoring data from this same 5-year period.

If a unit was shutdown for an entire year during the 2000 through 2004 period, the average of the years the unit was operational was used. If a unit was shutdown in 2002, but not permanently shutdown, the emissions and heat inputs 2001 (or 2000) were used in the normalizing calculations.

Future Base Year Inventory

As part of the VISTAS modeling, VISTAS and the Midwest Regional Planning Organization (MRPO) contracted with ICF Resources, L.L.C., to generate future year emission inventory for the electric generating sector of the contiguous US using the IPM. IPM is a dynamic linear optimization model that can be used to examine air pollution control policies for various pollutants throughout the contiguous US for the entire electric power system. The dynamic nature of IPM enables the projection of the behavior of the power system over a specified future period. The optimization logic determines the least-cost means of meeting electric generation and capacity requirements while complying with specified constraints including air pollution regulations, transmission bottlenecks, and plant-specific operational constraints. The versatility of IPM allows users to specify which constraints to exercise and populate IPM with their own datasets.

Since the modeling is based on the USEPA's prior analyses for which detailed public documentation is available, a summary of only the incremental changes that were proposed by VISTAS and MRPO as part of this analysis are presented here.

The VISTAS analysis is based on the USEPA modeling applications using IPM (V.2.1.6). As per the analytical needs of VISTAS and MRPO, the following changes were made to the underlying assumptions in the USEPA Base Case (V2.1.6):

i) The underlying database in the VISTAS analysis is USEPA's National Electric Energy Data System Database, with changes based upon the comments and technical directions from VISTAS and MRPO's stakeholders. The changes focused on existing installations of NO_x, SO_2 and particulate matter controls, NO_x emission rates, SO_2 emission limits, capacity of existing units, heat rate and unit identifications of selected units in the VISTAS and MRPO regions.

ii) The analysis covers the period between 2007 and 2030. To make the model size and run time tractable, IPM is run for a number of selected years within the study horizon known as run years. Each run year represents several calendar years in the study horizon, and all calendar years within the study horizon are mapped to their representative run years. Although results are only reported for the run years, IPM takes into account all years in the study horizon while developing the projections.

iii) The Duke Power and Progress Energy control technology investment strategies for complying with North Carolina's Clean Smokestacks Rule were explicitly hardwired in the analysis.

iv) The USEPA's Clean Air Interstate Rule (CAIR) rule implemented as part of this analysis is broadly consistent with the USEPA 40 CFR Parts 51 et. al., Supplemental Proposal for the Rule to Reduce Interstate Transport of Fine Particulate Matter and Ozone, proposed on June 10, 2004. Alabama, Arkansas, Delaware, District of Columbia, Florida, Georgia, Illinois, Indiana, Iowa, Kansas, Kentucky, Louisiana, Maryland, Massachusetts, Michigan, Minnesota, Mississippi, Missouri, New Jersey, New York, North Carolina, Ohio, Pennsylvania, South Carolina, Tennessee, Texas, Virginia, West Virginia, Wisconsin are the states affected by the CAIR SO_2 and the CAIR annual NO_x policies starting 2010. Connecticut is affected by an ozone season NO_x policy. The CAIR plants affected by the annual NO_x policy are capped at 1.6 million tons starting 2010 and 1.33 million tons starting 2015. The power plants affected by the CAIR SO_2 policy have to surrender two Title IV SO_2 allowances for every ton of SO_2 emitted starting 2010 and three Title IV SO_2 allowances for every ton of SO_2 emitted starting 2015.

6.1.2. Non-Electric Generating Units

2002 Base Year Inventory

For the non-EGU sources, the same inventory will be used for both the actual and typical base year emissions inventories. The non-EGU category will use annual emissions, which will be temporally allocated to month, day, and hour using source category code (SCC) based allocation factors. These factors will be based on the cross-reference and profile data supplied with the SMOKE 2.0 version.

The non-EGU sources annual emissions will be the 2002 VISTAS inventory based on the 2002 Consolidated Emissions Reporting Rule (CERR) submitted data for all states in the modeling domain unless a state or RPO provides updated data.

Future Year Base Inventory

The general approach for assembling future year data is to use recently updated growth and control data consistent with USEPA's CAIR analyses, supplement these data with available stakeholder input, and provide the results for stakeholder review to ensure credibility. To assemble growth/control data needed for the final 2009 inventories, the VISTAS contractor will perform the following activities:

- Use the final 2002 VISTAS inventory as the starting point for the future base year inventory.
- Obtain, review, and apply the most current growth factors developed by USEPA, based on forecasts from an updated Regional Economic Models, Inc. model (version 5.5) and the latest *Annual Energy Outlook* published by the Department of Energy.
- Obtain, review, and apply any State-specific or sector-specific growth factors submitted by stakeholders.
- Obtain information regarding sources that have shut down after 2002 and work with the states to determine if these sources should be removed from the future year inventory.
- Obtain, review, and apply control assumptions that are expected to be in place by 2009.

Controls Applied to the Non-EGU Inventory

1-hour Ozone SIP

Information about control programs for the 1-hour ozone nonattainment areas came from the report by E.H. Pechan and Associates entitled *VOC and NO_x Control Measures Adopted by States and Nonattainment Areas for 1999 NEI Base Case Emissions Projection Calculations*. The report identified and compiled a listing of the VOC and NO_x control measure programs expected to be implemented after 1999, as well as an estimate of their influence on projected emissions. Five nonattainment areas in the VISTAS region were included: Atlanta, Birmingham, metro Washington DC (including several counties in Virginia), Louisville, and northern Kentucky.

Emission reductions requirements from NO_x Reasonably Available Control Technology (RACT) in 1-hour Ozone SIP areas were implemented prior to 1999. These reductions should already be accounted for in the VISTAS 2002 inventory since the 2002 inventory was based on 2002 actual emissions submitted by the States.

NO_x SIP Call

For non-EGU sources, Phase I of the NO_x SIP call applies to large industrial boilers and turbines, and cement kilns. States in the VISTAS region affected by the NO_x SIP call have developed rules for the control of NO_x emissions that have been approved by the USEPA. The VISTAS contractor has reviewed the available state rules and guidance documents to determine the affected sources and ozone season allowances.

For the sources within North Carolina, NCDAQ has decided to use the 2007 emission allowances for the 2009 future year inventory. The allowances are given in terms of tons per ozone season (the five month period from May to September). To calculate annual emissions, the capped allowances were multiplied by a factor of 12/5.

The Phase II rule applies to large internal combustion engines, which are primarily used in pipeline transmission service at compressor stations. NCDAQ has established emissions caps for three facilities affected by the Phase II NO_x SIP call rule and will apply these caps to the future year inventory.

For the other states in the VISTAS region, affected units were identified using the same methodology as was used by USEPA in the proposed Phase II rule (i.e., a large internal combustion engine is one that emitted, on average, more than 1 ton per day during 2002). The final rule reflects a control level of 82 percent for natural gas-fired internal combustion engines and 90 percent for diesel or dual fuel categories. Therefore, these control levels were applied to the identified sources.

Maximum Achievable Control Technology Regulations

The USEPA anticipates reductions in PM and SO_2 as a result of the Industrial Boiler/Process Heater maximum achievable control technology (MACT) standard. The methods used to account for these reductions are the same as those used for the Interstate Air Quality Transport Rule. Since the attainment demonstration is utilizing one atmosphere modeling, the reductions for these pollutants were accounted for.

MACT requirements were also applied, as documented in the USEPA report entitled *Control Packet Development and Data Sources,* dated July 14, 2004. The point source MACTs and associated emission reductions were designed from Federal Register notices and discussions with USEPA's Emission Standards Division staff. Emission reductions will be applied only for MACT standards with an initial compliance date of 2002 or greater, since effects from MACT with earlier compliance dates should already be accounted for in the 2002 base year inventory.

The future year base inventory does not include the NO_x co-benefit effects of the Gas Turbines or stationary Reciprocating Internal Combustion Engines MACT regulations, which USEPA estimates to be small compared to the overall inventory.

Petroleum Refinery Initiative

Three refineries in the VISTAS region are affected by two October 2003 Clean Air Act settlements under the USEPA Petroleum Refinery Initiative. The refineries are: (1) the Chevron refinery in Pascagoula, Mississippi; (2) the Ergon refinery in Vicksburg, Mississippi; and (3) the Ergon refinery in Newell, West Virginia. Although these sources are not within North Carolina or South Carolina, the expected emission reductions will be accounted for in the 2009 modeling.

NO_x RACT in 8-hour Ozone SIP

NCDAQ will make every effort to include NO_x RACT controls for 8-hour ozone nonattainment areas in the VISTAS region. However, since cost is a factor of consideration in a RACT determination, it may not be known at the time of the final modeling which sources will be subject to actual controls.

SCDHEC will make every effort to include NO_x RACT controls for 8-hour ozone nonattainment areas in the VISTAS region. Specifically, the plan is to submit expected 2009 and 2018 emissions for Bowater RACT accounting for RACT controls (if applicable).

Clean Air Interstate Rule

As stated in the preamble to the CAIR rule, the rule would not require or assume additional emission reductions from non-EGU boilers and turbines.

6.2. Stationary Area Source Emissions

Stationary area sources include sources whose emissions are relatively small but due to the large number of these sources, the collective emissions could be significant (i.e., combustion of fuels for heating, structure fires, service stations, etc.). Emissions are estimated by multiplying an emission factor by some known indicator of collective activity, such as fuel usage, number of household or population. Thus, a variety of activity level data is collected, including, US Census economic data, forestry and agriculture agency data, and other data sources. Stationary area source emissions are estimated on the county level.

Actual Base Year Inventory

A portion of the area source 2002 base year inventory for North Carolina was developed by NCDAQ and provided to the VISTAS contractor. The remaining portion of the area source inventory was calculated by the VISTAS contractor. The sources estimated by the contractor included emissions from animal husbandry, wildland fires, and particulate matter from paved and unpaved roads. For the other states within the modeling domain, the state supplied data or the CERR data was used.

Area source categories estimated by NCDAQ were identified from a list in the USEPA guidance document EPA-450/4-91-016, *Procedures for the Preparation of Emission Inventories of Carbon Monoxide and Precursors of Ozone*, and from the Emission Inventory Improvement Program (EIIP) technical reports.

In general, emission factor estimation approaches were used to calculate area source emissions. Emission factors may be grouped as per capita emission factors; commodity consumption-related emission factors; and level-of-activity based emission factors. The emission factors were obtained from the *Procedures for the Preparation of Emission Inventories of Carbon Monoxide and Precursors of Ozone*, from the EIIP technical reports, or the USEPA's *AP-42, Compilation of Air Pollutant Emission Factors, Fifth Edition*.

The emissions from area sources were estimated by multiplying an emission factor by the appropriate indicator of collective activity for each source category within the inventory area. An indicator is any parameter associated with the activity level of a source that can be correlated with the air pollutant emissions from that source, such as fuel usage, number of households, or population. The values of these indicators are gathered from various sources (government reports, census, trade groups, employment data, direct surveys, etc.) as appropriate.

For the animal husbandry and fertilizer application emissions, the Carnegie Mellon University ammonia model was used. For paved and unpaved roads particulate matter emissions, emissions developed by the USEPA as part of their 2002 National Emissions Inventory development effort was used.

Wind blown dust and sea salt emissions were not included in the inventory. These source categories are sources of particulate matter and therefore, do not effect the 8-hour ozone attainment modeling demonstration.

For wildland fires, i.e., wildfires and prescribed burns, monthly estimates of fire emissions, which include burn acreage and biomass loading information will be used. Depending on the completeness and quality of the data, attempts will be made to calculate spatial and temporal distributions of the fire emissions, rather than relying on standard distribution profiles. Data will be obtained through consultation with stakeholders that participate in the VISTAS Fire Special Interest Work Group. The fire data will be split into two groups, small fires estimated on a county level and treated as an area source; and large fires that will be treated as a point source.

Typical Base Year Inventory

The actual base year inventory will serve as the typical base year inventory for all area source categories except for wildland fires. For this source category, development of a typical year fire inventory provided the capability of using a comparable dataset for both the base year and future years. Thus, fire emissions would remain the same for air quality modeling in both the base and any future years. The VISTAS Fire Special Interest Work Group was consulted and decided to use State level ratios of acres over a longer term record (three or more years) developed for each fire type relative to 2002. The 2002 acreage was then scaled up or down based on these ratios to develop a typical year inventory.

Future Year Base Inventory

The VISTAS contractor generated the future base year emissions inventory used in the attainment demonstration modeling. The general approach used to calculate the future base year emissions for stationary area sources was as follows:

- Use the final 2002 VISTAS base year inventory as the starting point for the future base year inventory.
- Obtain any State specific growth factors and/or future controls from the States to use in developing the projections.
- Back calculate uncontrolled emissions for the 2002 base year inventory based on existing controls reported for the 2002 base year inventory.
- Controls (including control efficiency, rule effectiveness and rule penetration) provided by the States or originally developed for use in estimating projected emissions for the USEPA's Heavy Duty Diesel rulemaking emission projections and used in the CAIR projections were then used to calculate controlled emissions. State submitted controls had precedence over the USEPA developed controls.
- Growth factors supplied from the States or the USEPA's CAIR emission projections were then applied to project the controlled emissions to the appropriate year. In some cases, the USEPA's Economic Growth and Analysis System Version 5 growth factors were used if no growth factor was available from either the States or the CAIR growth factor files.

6.3. Non-Road Mobile Source Emissions

Non-road mobile sources are equipment that can move but do not use the roadways, such as construction equipment, aircraft, railroad locomotives, lawn and garden equipment, etc. For the non-road mobile source inventory, the list of sources to inventory came from the USEPA's NONROAD2005 model and the USEPA guidance document, *Procedures for Emission Inventory Preparation Volume IV: Mobile Sources*. For the majority of the non-road mobile sources, the emissions can be estimated using the USEPA's NONROAD model. For the three source categories not included in the NONROAD model, i.e., aircraft engines, railroad locomotives and commercial marine, more traditional methods of estimating the emissions were used.

2002 Base Year Inventory

For the non-road mobile sources, the same inventory will be used for both the actual and typical base year emissions inventories. All non-road mobile source emissions, except for aircraft engines, commercial marine vessels and railroad locomotives, were estimated using the USEPA NONROAD2005 model. This model predicts the emissions for non-road equipment based upon the year inputted into the model.

For railroad locomotive emissions, emission factors were supplied by the *Procedures for Emission Inventory Preparation Volume IV: Mobile Sources* document, which were then multiplied by a variety of different activity levels (i.e., gallons of fuel per county for railroad locomotive engines). Refinements could be made using information from *Development of*

Railroad Emission Inventory Methodologies (SR2004-06-02) from the Southeastern States Air Resource Managers, Inc.

Aircraft emissions at airports were calculated by VISTAS contractors using landing and take off data from Federal data sources. These will be reviewed and refined as appropriate for the Charlotte, Greensboro, and Raleigh-Durham airports. Emissions are calculated using the Federal Aviation Administration's (FAA's) Emissions and Dispersion Modeling System version 4.2, when there is sufficient detail to employ it.

Commercial marine emissions are estimated by procedures described in *Commercial Marine Activity for Deep Sea Ports in the United States (EPA420-R-99-020).*

Future Base Year Inventory

For the source categories estimated using the USEPA NONROAD model, the model was used to create a future base year inventory. The NONROAD model takes into consideration rules that are in effect that could impact the emissions from these source categories. For the four largest airports in North Carolina, the FAA's Terminal Area Forecast will be used to project growth in aircraft emissions.

For the commercial marine, railroad locomotives and the remaining airport emissions, the VISTAS contractor will project the future base year emissions using the following guidelines:

- Use the final 2002 VISTAS inventory as the starting point for the future base year inventory.
- Detailed inventory data (both before and after controls) for 1996 and 2010 will be obtained from the USEPA's Clean Air Interstate Rule Technical Support Document. Straight-line interpolations between 1996 and 2010 will be used to create a combined growth and control factor. This is done at the State-County-SCC-Pollutant level of detail.
- Obtain, review and apply any State-specific growth factors submitted.
- Apply adjustments to account for additional emission reductions do the low sulfur non-road diesel fuels.

6.4. On-Road Mobile Source Emissions

Highway mobile sources are considered those vehicles that travel on the roadways and comprise over 30 percent of the NO_x emissions in North Carolina, and 42 percent of the NO_x emissions in South Carolina. Emissions from motor vehicles occur throughout the day while the vehicle is in motion, at idle, parked, and during refueling. Each of these emissions sources needs to be estimated in order to properly reflect the total emissions from this source category. In its simplest terms emissions from highway mobile sources are calculated by multiplying an activity level, in this case daily vehicle miles traveled (VMT) as provided by the North Carolina Department of Transportation (NCDOT), by an emission factor.

The USEPA developed the MOBILE model to estimate emission factors based on information on the way vehicles are driven in a particular area. The newest version of the MOBILE model, MOBILE6.2, will be used to develop the on-road mobile source emissions estimates for carbon monoxide (CO), NO_x, PM, and VOC emissions. Key inputs for the MOBILE model include information on the age of vehicles on the roads, the average speed of those vehicles, what types of road those vehicles are traveling on, and any control programs (e.g., emissions inspection programs). Inputs are combined with gridded, day-specific temperature data to calculate the gridded, temporalized emission estimates. Of note, whereas the on-network emissions estimates are spatially allocated based on link location and subsequently summed to the grid cell level, the off-network emissions estimates are spatially allocated based on a combination of the Federal Highway Administration version 2.0 highway networks and population. For the North Carolina 36/12 km modeling, no link-based data will be used. The MOBILE6 emissions factors are based on day-specific temperatures predicted by the meteorological model. For the South Carolina 36/12 km modeling, no link-based data will be used.

6.4.1. Speed Assumptions

Emissions from motor vehicles vary with the manner in which the vehicle is operated. Vehicles traveling at 65 miles per hour (mph) emit a very different mix of pollutants than the car that is idling at a stoplight. NCDAQ will collect hourly speeds per functional class for this modeling effort. Information from Travel Demand Models will be used where available. SCDHEC will use MOBILE 6.2 default speed assumptions for this modeling effort.

6.4.2. Vehicle Age Distribution

The North Carolina vehicle age distribution comes from NCDOT annual registration data. Both statewide and area specific registration data is provided. The only areas with “area specific” registration data include the Charlotte/Gastonia, Raleigh/Durham and Greensboro/ Winston-Salem areas. The latest available age distribution at the time of the modeling will be used. SCDHEC will use MOBILE 6.2 default vehicle age distribution for this modeling effort.

6.4.3. Vehicle Mix Assumptions

The North Carolina statewide vehicle mix will be developed by NCDAQ using the latest available, at the time of the modeling, Highway Performance Maintenance System count data. The raw data is converted into MOBILE6.2 format following the method outlined in the August 2004 guidance document *EPA420-R-04-013, Technical Guidance on the Use of MOBILE6.2 for Emissions Inventory Preparation*. For the Metrolina nonattainment area, area-specific vehicle count data will be used to generate the vehicle mix for all road types except for urban and rural interstates. Local data is not available for the interstates; therefore, the State-wide mix data will be used.

Version 2 of the SMOKE model uses the MOBILE5 eight vehicle classification format for the vehicle mix. Therefore, the current vehicle mix format used by NCDAQ had to be converted from the sixteen MOBILE6 vehicle classification format to correlate to the MOBILE5 eight vehicle classification system. This was done using the guidance provided by the USEPA.

SCDHEC will use the MOBILE 6.2 default vehicle mix assumptions for this modeling effort.

6.4.4. Temperature Assumptions

MOBILE6 in the SMOKE emissions model uses the gridded (modeled) meteorology data to calculate temperature. Spatial and temporal temperature averaging will be implemented to minimize the SMOKE (mobile) run times.

6.4.5. Vehicle Inspection and Maintenance Program Assumptions

In the early 1990's, North Carolina adopted emissions inspection requirements for vehicles in nine urban counties. This program tests emissions at idle for 1975 and newer gasoline powered light and heavy duty vehicles. The program is a basic, decentralized tailpipe test for Hydrocarbons and CO only.

In 2002, North Carolina implemented a new vehicle emissions inspection program referred to as onboard diagnostics (OBDII). This program covers all light-duty gasoline powered vehicles that are model year 1996 and newer. The program was implemented in the original nine tailpipe test counties and expanded to a total of forty-eight counties by January 1, 2006. In addition, the idle test will be phased-out in 2006 in the original nine counties. In order to accurately reflect these OBDII tests, two separate programs must be incorporated into the 2002 input files. The implementation dates of each program are also included in the input files.

South Carolina does not have any inspection and maintenance programs.

6.4.6. RVP Assumptions

Reid Vapor Pressure (RVP) reflects a gasoline's volatility. North Carolina has adopted the Phase II RVP of 7.8 psi during June-September as a control measure for the following counties: Davidson, Durham, Forsyth, Gaston, Guilford, Mecklenburg, Wake, Granville, and Davie. Lower RVP leads to lower volatile organic compound emissions from gasoline handling and lowers vapor losses from motor vehicles. The remaining areas have a RVP of 9.0 psi during June-September. For remaining months, RVPs are as follows:

- October RVP = 13.5 psi statewide
- November RVP = 13.5 psi statewide
- December RVP = 15 psi statewide
- January RVP = 15 psi statewide
- February RVP = 13.5 psi statewide
- March RVP = 13.5 psi statewide
- April RVP = 13.5 psi statewide
- May RVP = 9.0 psi statewide

South Carolina has an RVP of 9.0 psi for all counties during May-September, as indicated in USEPA's Guide on Federal and State Summer RVP Standards for Conventional Gasoline Only (EPA420-B-05-012 November 2005). For remaining months, RVPs follow the ASTM D4814 Standard Specification for Automotive Spark-Ignition Engine Fuel. They are as follows:

- October RVP = 13.5 psi statewide
- November RVP = 13.5 psi statewide
- December RVP = 13.5 psi statewide
- January RVP = 13.5 psi statewide
- February RVP = 13.5 psi statewide
- March RVP = 13.5 psi statewide
- April RVP = 13.5 psi statewide

6.4.7. VMT Assumptions

Mobile source emissions are calculated by multiplying emission factors by daily VMT. In this modeling exercise, NCDAQ will use VMT from Travel Demand Models where available. For all other areas the VMT data will be provided by the NCDOT. SCDHEC will use VMT provided by the South Carolina Department of Transportation (SCDOT).

6.5. Biogenic Source Emissions

A revised version of a commonly used biogenic emissions model, the Biogenic Emissions Inventory System, has recently been developed and tested by USEPA over two separate modeling domains/episodes. This version of the model (BEIS-3, v0.9) contains several changes over BEIS-2, including the following:

- Vegetation input data -- are now based on a 1-km Biogenic Emissions Landuse Database (BELD3) vegetation data base,
- Emission factors – many updates including some recent North American Research Strategy for Tropospheric Ozone (NARSTO) modifications,
- Environmental algorithm -- includes a sunlit/shaded leaf solar radiation model.

A series of sensitivity modeling simulations has been completed and concluded that the more recent BEIS-3 methodology will impact base case model ozone predictions in most parts of the US. The preliminary tests have also shown that the newer biogenic emissions do not appear to have a large effect on: 1) the control signal response, 2) relative reduction factors resulting from a projected emissions change, or 3) overall regional model performance in the eastern US.

For this particular application of BEIS-3, version 0.9 as currently incorporated in the SMOKE processor will be used. This means that: 1) soil nitric oxide (NO) emissions shall be prepared without the input of specific soil moisture and precipitation data and 2) methanol emissions will not be modeled explicitly. Otherwise, the modeling should be identical to a BEIS-3 (v1.0) application.

The BELD-3 landuse data on a Lambert conformal grid at 1-km resolution have already been developed, are available, and will be used to estimate biogenic emissions in this study. The BEIS model also requires as input hourly, gridded temperature and solar radiation data to estimate biogenic emissions, and these data will be derived from the MM5 predictions.

6.6. Development of Modeling Inventories

The SMOKE emissions model will be used to create the air quality model ready files. The chemical speciation method used is the CB4 mechanism. The gridding surrogates are based off the 2000 census data and are the most up to date available. The temporal profiles used to disaggregate the annual emissions to the appropriate month, day and hour are the latest available profiles provided with the SMOKE model with the exception of the EGU profiles, which will be developed based on CEM data.

For each model-ready emissions inventory, separate air quality model-ready files will be created for the EGU point sources, non-EGU point sources, area sources, dust, low-level fires, elevated fires, non-road mobile sources, on-road mobile sources, and biogenic emissions.

7.0 Quality Assurance Plan

This section discusses the Quality Assurance (QA) procedures that will be used in the SIP modeling. The QA procedures listed here describe the combined efforts to be employed by VISTAS, NCDAQ, and SCDHEC. The VISTAS contractors will perform QA on modeling inputs and outputs for the modeling region as a whole. NCDAQ and SCDHEC will perform QA on their respective emission inventories, as well as look at near state data for reasonableness. Additionally, the State agencies will review the modeling outputs for reasonableness.

7.1. Quality Assurance Objectives

In December 2002, the USEPA published extensive guidance on developing a Quality Assurance Project Plan (QAPP) for modeling studies (EPA, 2002). The objective of a QAPP is to ensure that a modeling study is scientifically sound, robust, and defensible. The new USEPA guidance suggests that a QAPP should include the following elements:

- A systematic planning process including identification of assessments and related performance criteria
- Peer reviewed theory and equations
- A carefully designed life-cycle development process that minimizes errors
- Clear documentation of assumptions, theory, and parameterization that is detailed enough so others can fully understand the model output
- Input data and parameters that are accurate and appropriate for the problem
- Output data that can be used to help inform decision-making
- Documentation of any changes from the original quality assurance plan

Moreover, the USEPA guidance specifies that different levels of QAPP may be required depending on the intended application of the model, with a modeling study designed for regulatory purposes requiring the highest level of quality assurance.

The QAPP also provides a valuable resource for project management. It can be used to document data sources and assumptions used in the modeling study, and it can be used to guide project personnel through the data processing and model application process to ensure that choices are consistent with the project objectives.

The guidance document also addresses model development, coding and selection of models, and model performance requirements. VISTAS and NCDAQ/SCDHEC modeling are using an existing USEPA sponsored model hence our QAPP will focus primarily on documenting data sources and QA of data processing performed by the model team. QA objectives for specific aspects of the project are discussed below, and these will be incorporated into a QAPP that conforms to the USEPA guidance document for modeling studies.

7.2. Emissions Model Inputs and Outputs

Emissions QA and Quality Control (QC) are the most critical steps in performing air quality modeling studies. Emissions processing can be time consuming and involves complex manipulation of many different types of large datasets. If errors are made and rigorous QA measures are not in place, these errors may remain undetected, resulting in delays and wasted time and resources.

7.2.1. VISTAS QA Effort

As part of the VISTAS QA effort, an "Emissions Gatekeeper" function will be implemented. The role of this Gatekeeper is to perform quality assurance activities on the following emissions inventory data:

- Emissions inventory data obtained from the VISTAS emissions inventory contractors

- The emission inventory to be used for modeling outside of the states in the VISTAS region.

Specifically, the Emissions Gatekeeper will review the content and format of the provided emission inventories, ensuring an appropriate appraisal of the emissions data and estimates for the VISTAS States. Other tasks will include any additional translation from mass emissions files into the emissions modeling input file structure necessary for modeling. The VISTAS Study Team will supplement these activities with QA checks on the intermediate and model output files using internal and public domain visualization and diagnostic packages.

This multistep emissions QA/QC approach includes the initial emissions QA/QC by the Emissions Gatekeeper described above, as well as QA/QC by the Emissions Modeler during the processing of emissions, and then additional QA/QC by the air quality modeler of the processed model ready emission files. This multistep process, with three separate groups involved in the QA/QC of the emissions, is much more likely to catch any errors prior to the air quality model simulations.

7.2.2. Emissions Modeling QA/QC

Modeling QA involves performing data quality checks, assuring simulation accuracy, and recognizing and identifying problems as they happen; it is the process of looking for glaring faults in the model input and output data (I/O) and determining whether the input data are producing the desired results. Scrutiny of the I/O using standard statistical analyses can reveal problems in the data and/or the model setup. Using a standard approach for analyzing emissions model I/O establishes reference points to use when scrutinizing the data. Seeking these indicators of correct model performance allows QA personnel to determine the accuracy of the simulations and whether faults in the data or model configuration exist.

QA documentation will include records of model configuration, details about data files, simulation records, and final report generation. After finishing each QA step, the modeler will record the result and his/her initials on a QA checklist.

Data formats will be confirmed using the SMOKE manual to check text files and using PAVE to check binary netCDF files, such as the meteorology inputs. Sanity checks look for glaring errors in the file contents and ensure that the data make sense in the context of how they will be used and relative to similar or reference datasets.

Lead modelers will oversee the entire modeling process, perform the majority of the SMOKE modeling, and receive and archive input and output data. Secondary modelers will perform some of the SMOKE modeling, organize the SMOKE QA reports into emissions summaries for data QA and reporting, and will generate custom QA summaries and reports for troubleshooting any problems encountered during the modeling process.

Outside reviewers will be solicited from outside the emissions modeling team on a volunteer basis to conduct periodic reviews/audits of the data and modeling process. Outside reviewers will consist of peers, co-workers not working directly on the inventory in question, state inventory contacts and stakeholders.

7.2.3. SMOKE Log Files

Each of the programs that make up SMOKE produces a log at run time. Stored in a single directory for each unique simulation, the logs contain information about the configuration of SMOKE, the names and locations of the input and output files used in the simulation, and any warnings, notes, or errors (collectively called "flags") that occurred during model execution. Generated as text files, the logs are named according to the program that created them and the emissions source modeled by the simulation, and the names include identifiers that distinguish the simulation from all others. The logs are usually the first source of information consulted in determining whether a simulation completed as expected or for troubleshooting suspected problems.

7.2.4. SMOKE QA Reports

Two types of QA reports are generated by SMOKE. One set is created by the program *Smkmerge* and the other by the program *Smkreport*. While both programs allow users to configure the content of the reports, *Smkreport* is a more powerful reporting program that was designed specifically as a QA tool. Controlled by configuration files, *Smkreport* can create text reports at every step in the emissions generation process. In addition to creating reports from information drawn from the intermediate SMOKE data matrices (e.g., the temporal matrix), *Smkreport* can summarize the amount of emissions assigned to different temporal, spatial, and chemical profiles; normalize emissions by population; and report the amount of emissions allocated to each vertical layer per model-hour. *Smkreport* also allows the targeted reporting of emissions at specific sources, plants, grid cells, or subdomains.

The program *Smkmerge* creates either state- or county-level reports at each of the major steps in the emissions generation process (spatial allocation, temporal allocation, chemical allocation or speciation, and merging). Although *Smkmerge* cannot create as many different report types as *Smkreport*, *Smkmerge* does have the ability to report biogenic emissions totals, whereas *Smkreport* can create reports only for anthropogenic emissions sources.

7.2.5. Visualization Tools

Visualization is an important part of the QA/QC procedure. Viewing bar charts and pie charts of the data verifies that more populous urban counties have greater emissions then the rural counties. Additionally, the PAVE visualization tool is used to graphically view the data to make sure that the data appears reasonable both spatially and temporally.

Visualization tools will be used to assist in the QA process for the emissions data both before and after being processed through the SMOKE emissions model. The air quality data will also employ visualization tools to view the modeling results to ensure that the modeling results look reasonable.

7.2.6. Document Tracking

In order to keep track of the details of modeling, certain notes and files will be maintained. Notes will be kept of files produced on desktop computers as to origin and purpose. These notes may be maintained in a logbook or by using the file properties summary tag available for files in the Windows operating system. Files in the workstation will be similarly tracked. It may be useful to maintain a log within directories for this purpose.

7.3. Meteorological Model Outputs

As part of the VISTAS QA effort, a "Meteorological Gatekeeper" will be tasked with providing an independent review and quality assurance of the meteorological modeling and related datasets developed by the VISTAS meteorological modeling contractor (BAMS) and used subsequently by the emissions and air quality modeling teams. This Gatekeeper QA review ensures that any potential problems with the datasets (should they exist) are identified and corrected in a timely manner. In the case of meteorology, the Gatekeeper's independent QA analysis of the MM5 meteorological datasets serves to provide direct assistance to the emissions and air quality modeling team as it undertakes to ratify the SMOKE model outputs and to diagnose CMAQ model performance and sensitivity analyses.

In addition to having personal responsibility for the quality and chain of custody of the meteorological datasets supplied by other VISTAS contractors, the Meteorological Gatekeeper will be responsible for ensuring and maintaining the integrity of the data files uploaded to the project website. This website, hosted by UCR (University California – Riverside), serves as the repository of data for the ENVIRON/UCR/Alpine modeling centers and for the VISTAS Technical Analysis Workgroup participants. In performing the Gatekeeper quality assurance activity, one of the first steps is to conduct an independent operational evaluation on the MM5 model results at 36 km and 12 km grid scale. This evaluation covers surface and aloft wind direction, temperature, mixing ratio, precipitation, and PBL depths on a continental scale (36 km) and subregional scale (12 km) basis.

The Gatekeeper will also perform supplemental, ad hoc analysis of pertinent MM5 fields (e.g., PBL depths) where that might be useful to the emissions and air quality modeling teams. Another task of the Gatekeeper will be to exercise MCIP version 2.3 to read the MM5 outputs from BAMS and produce binary input files for the CCTM to provide the complete set of parameters necessary in the emissions processing and air quality modeling.

In summary, the quality assurance plan for the meteorological data will include the following elements:

- Upon receiving the MM5 and MCIP 2.3 output files from BAMS, NCDAQ and SCDHEC will verify the integrity of the file transfer (i.e., no missing and/or corrupted files).
- Since the CMAQ modeling domain is a subset of the MM5 domain, NCDAQ and SCDHEC will verify that the modeling domain and vertical layer structures in the MCIP files are identical to the CMAQ modeling domain.
- Several days of the MM5 output will be selected and the meteorological modeling team will reprocess the MM5 files with MCIP v2.3 using the predetermined MCIP options. The MCIP files will then be compared with those provided by BAMS to verify that identical results from the MCIP processing were obtained.
- Horizontal and vertical plots of temperature, pressure, precipitation, modeled flow patterns, PBL heights, etc. will be created to assess whether the MCIP output fields are reasonable.
- The VISTAS 2002 MM5 simulation will be evaluated using the same surface observations, subdomains and procedures as used to evaluate the Western Regional Air Partnership 2002 MM5 simulation as an independent QA and evaluation of the database.
- Plots constructed by the VISTAS Gatekeeper will be made available on the VISTAS website for viewing and download (http://pah.cert.ucr.edu/vistas/vistas2/index.shtml).

7.4. Air Quality Model Inputs and Outputs

Key aspects of QA for the CMAQ input and output data include the following:

- Verification that correct configuration and science options are used in compiling and running each model of the CMAQ modeling system, where these include the MCIP, JPROC, ICON, BCON and the CCTM.
- Verification that correct input datasets are used when running each model.
- Evaluation of CCTM results to verify that model output is reasonable and consistent with general expectations.
- Processing of ambient monitoring data for use in the model performance evaluation.
- Evaluation of the CCTM results against concurrent observations.
- Backup and archiving of critical model input data.

The most critical element in the QA plan for CMAQ simulations is the QA/QC of the meteorological and emissions input files. The major QA issue specifically associated with the air quality model simulations is verification that the correct science options were specified in the model itself and that the correct input files were used when running the model. For the CMAQ model, a system of naming conventions was employed which uses environment variables in the compile and run scripts that guarantee that correct inputs and science options are used. A redundant naming system is also used so that the name of key science options or inputs is included in the name of CMAQ executable program, in the name of the CMAQ output files, and in the name of the directory in which the files are located. This is accomplished by using the environment variables in the scripts to specify the names and locations of key input files. For example, if a model simulation is performed using the CB4 mechanism, all compile and run scripts contain the variable definition "$MECH = CB4," and this variable is hard coded into the script for the executable name, the output file name, and the output directory name. This procedure produces long file/directory names but it effectively prevents mistakes or makes mistakes readily apparent if they do occur.

A second key QA procedure is to never "recycle" run scripts (i.e., the original runs scripts and directory structure that were used in performing a model simulation). For example, if a simulation is performed with the SAPRC mechanism, instead of editing the original scripts to specify "$MECH = SAPRC," a parallel directory structure with a new set of scripts to perform the SAPRC simulations will be created. This provides a permanent archive of the scripts that were used in performing model simulations. In addition, output from the model simulation will be directed to a log file that provides a record of input file names, warning messages, etc., that will be archived.

Post-processing QA of the CMAQ output files similar to that described for the emissions processing will be performed. Animated graphics interchange format (GIF) files using PAVE will be generated to search for unexpected patterns in the CMAQ output files. In the case of model sensitivity studies, the animated GIFs will be prepared as difference plots for the sensitivity case minus the base case. Often, errors in the emissions inputs can be discovered by viewing the animated GIFs. Finally, 24-hour average plots for each day of the CMAQ simulations will be produced. This provides a summary that can be useful for more quickly comparing various model simulations.

8.0 Model Performance Evaluation

USEPA guidance (EPA, 2005, pg. 85; EPA, 2001, pg 227) suggests that model performance be evaluated based on two components:

- How well the model is able to replicate observed concentrations of ozone and precursors, and

- How accurately the model characterizes the sensitivity of changes in component concentrations to changes in emissions.

Each component suggests a different type of evaluation procedure, with the first being "operational evaluation," and the second being "diagnostic evaluation." Since the attainment test is a relative test, it is not as necessary to exactly duplicate ozone concentrations. As a result, there is now more emphasis placed on the diagnostic model evaluation.

This section outlines the method used to evaluate model performance. Working with the knowledge that many states involved with the VISTAS regional haze work would want to apply some of the work to their individual SIPs for 8 hour ozone and $PM_{2.5}$, plans were put in place to perform exhaustive analysis of all atmospheric constituents, including ozone. NCDAQ and SCDHEC intend to build off the modeling efforts with VISTAS; therefore, the model performance evaluation will be an extension of VISTAS efforts.

8.1. Model Evaluation Tools (Operational Evaluation)

8.1.1. Statistical Performance Metrics

In compliance with USEPA's September 2006 guidance document *Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of the Air Quality Goals for Ozone, $PM_{2.5}$ and Regional Haze*, VISTAS will compile a suite of metrics for use in evaluating model performance. The standard set of statistical performance measures suggested by USEPA for evaluating ozone models includes: normalized bias, normalized gross (unsigned) error, fractional bias, fractional gross error, and fractional bias in standard deviations. Several other measures will be included in the final report to fulfill the requirements in the 8-hour ozone guidance (addition of average peak prediction accuracy), and to better accommodate other modeling groups with their comparison of modeling efforts. A list of metrics for calculation on a routine basis using the UCR analysis package is listed in Table 8-1. The metrics calculated in conjunction with VISTAS will include the examination of various atmospheric constituents, including ozone.

Typically, the statistical metrics are calculated at each monitoring site across the full computational domain for all simulation days. During the VISTAS CMAQ evaluation, the gas-phase and aerosol statistical measures shown in Table 8-1 will be computed for the full 36 km and 12 km domains, as well as for the individual RPOs and on other subdomains as appropriate. Temporally, the statistical measures will be computed for the appropriate averaging times: 1 hr for ozone, and gas-phase precursors such as NO, nitrogen dioxide (NO_2), CO, SO_2, 8-hour for ozone, and 24-hour for sulfate, nitrate, $PM_{2.5}$, and other aerosol species. These results will then be averaged over annual, monthly, and seasonal periods for display, further analysis, and reporting. Should it become necessary as part of model performance diagnosis, the statistics will be aggregated in other ways, e.g., (a) day vs. night, (b) weekday vs. weekend, (c) precipitation vs. non-precipitation days, (d) month of the year, and (e) the 20% haziest/cleanest days, in order to help elucidate model performance problems. For the purposes of the 8-hour ozone SIP for the Metrolina nonattainment area, only the statistics for 1-hour and 8-hour ozone will be reported. The statistics for the pollutants and precursors will be reviewed internally for reasonableness.

Table 8-1: Statistical Metrics

Statistical Measure	Shorthand Notation	Mathematical Expression	Notes
Accuracy of Paired Peak	A_p	$\frac{P - O_{peak}}{O_{peak}}$	
Coefficient of Determination	r^2	$\frac{\left[\sum_{i=1}^{N}\left(P_i - \overline{P}\right)\left(O_i - \overline{O}\right)\right]^2}{\sum_{i=1}^{N}(P_i - \overline{P})^2 \sum_{i=1}^{N}(O_i - \overline{O})^2}$	P_i= prediction at time and location i; O_i = observation at time and location i; $\overline{P}$ = arithmetic average of P_i, i = 1, 2, . . ., N; $\overline{O}$ = arithmetic average of O_i, i = 1, 2, . . ., N;
Normalized Mean Error	NME	$\frac{\sum_{i=1}^{N}\left\lvert P_i - O_i\right\rvert}{\sum_{i=1}^{N} O_i}$	Reported as %
Root Mean Square Error	RMSE	$\left[\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2\right]^{\frac{1}{2}}$	Reported as %
Fractional Gross Error	F_E	$\frac{2}{N}\sum_{i=1}^{N}\left\lvert\frac{P_i - O_i}{P_i + O_i}\right\rvert$	Reported as %
Mean Absolute Gross Error	MAGE	$\frac{1}{N}\sum_{i=1}^{N}\left\lvert P_i - O_i\right\rvert$	
Mean Normalized Gross Error	MNGE	$\frac{1}{N}\sum_{i=1}^{N}\frac{\left\lvert P_i - O_i\right\rvert}{O_i}$	Reported as %
Mean Biased	MB	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$	Reported as concentration
Mean Normalized Bias	MNB	$\frac{1}{N}\sum_{i=1}^{N}\frac{(P_i - O_i)}{O_i}$	Reported as %
Mean Fractionalized Bias (Fractional Bias)	MFB	$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$	Reported as %

Table 8-1: Statistical Metrics (Continued)

Statistical Measure	Shorthand Notation	Mathematical Expression	Notes
Normalized Mean Bias	NMB	$\dfrac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N} O_i}$	Reported as %
Bias Factor	BF	$\dfrac{1}{N}\sum_{i=1}^{N}\left(\dfrac{P_i}{O_i}\right)$	Reported as BF:1 or 1:BF or in fractional notation (BF/1 or 1/BF)

8.1.2. Graphical Representations

The core operational air quality model evaluation will utilize numerous graphical displays to facilitate quantitative and qualitative comparisons between CMAQ predictions and measurements. Together with the statistical metrics listed in Table 8-1, the graphical procedures are intended to help: (a) identify obviously flawed model simulations, (b) guide the implementation of any performance improvements in the 2002 model input files in a logical, defensible manner, and (c) to help elucidate the similarities and differences between the alternative CMAQ simulations. These graphical tools are intended to depict the model's ability to predict the observed gaseous species, such as ozone, and fine particulate species concentrations. The core graphical displays to be considered for use in model performance evaluation include the following:

- Spatial mean concentration time series plots
- Time series plots at monitoring locations
- Ground-level gas-phase and particulate concentration maps (i.e., tile plots)
- Concentration scatter plots stratified by station, by time, and by network
- Bias and error stratified by concentration
- Bias and error stratified by time
- Histogram plots of the statistical metrics, stratified by day, by pollutant, by subregion (e.g., 12 km vs. 36 km, by RPO), and by monitoring network
- Quantile - Quantile (Q-Q) plots
- Animations of predicted hourly ozone concentration

These graphical displays will be generated, where appropriate, for the full annual cycle as well as for monthly and seasonal periods.

8.2. Model Performance Testing (Diagnostic Evaluation)

Rarely does a modeling team find that the first simulation satisfactorily meets all (or even most) model performance expectations. Based on experience, initial simulations that "look very good" usually do so as the result of compensating errors. The norm is to engage in a logical, documented process of model performance improvement wherein a variety of diagnostic probing tools and sensitivity testing methods are used to identify, analyze, and then attempt to remove the causes of inadequate model performance. This is invariably the most technically-challenging and time consuming phase of a modeling study. The annual CMAQ model base case simulations are expected to present some performance challenges that may necessitate focused diagnostic and sensitivity testing in order for them to be resolved. It is hoped that these diagnostic and/or sensitivity tests can be adequately carried out within the resources and schedule. Where practical, diagnostic or sensitivity analyses, if needed, could be performed on selected episodes within the annual cycle, thereby avoiding the time-consuming task of running CMAQ for the full 2002 period. Below, the types of diagnostic and sensitivity testing methods that might be employed in diagnosing inadequate model performance and devising appropriate methods for improving the model response are identified.

8.2.1. Traditional Sensitivity Testing

Model sensitivity experiments are useful in three distinct phases, or "levels", of an air quality modeling study and all will be used as appropriate. These levels are:

- **Level I**: Model algorithm evaluation and configuration testing
- **Level II**: Model performance testing, uncertainty analysis and compensatory error diagnosis
- **Level III:** Investigation of model output response (e.g., ozone, aerosol, deposition) to changes in precursors as part of emissions control scenario analyses.

The Level I and Level II cover the aspect of operational evaluation, while Level III covers diagnostic evaluation.

The Level I sensitivity tests with CMAQ have already been completed in the initial VISTAS configuration and diagnostic analyses. However, given that open community nature of CMAQ and the frequent science updates to the model and supporting data bases, it is possible that some additional configuration sensitivity testing will be necessary.

Potential Level II sensitivity analyses might be helpful in accomplishing the following tasks:

- To reveal internal inconsistencies in the model
- To provide a basis for compensatory error analysis
- To reveal the parameters (or inputs) that dominate (or do not dominate) the model's operation
- To reveal propagation of errors through the model
- To provide guidance for model refinement and data collection programs

The merits of performing Level II sensitivity testing will depend upon whether performance problems are encountered. In addition, the number of tests possible, should performance difficulties arise, will be limited by the available schedule and resources. From past experience with CMAQ and other models, it is possible to identify examples of sensitivity runs that could be useful in model performance improvement exercises with the annual 2002 CMAQ simulation. These include:

- Modified biogenic emissions estimates
- Modified on-road motor vehicle emissions
- Modified air quality model vertical grid structure
- Modified boundary conditions
- Modified fire emissions
- Modified EGU emissions
- Modified ammonia emission estimates
- Modified aerosol/Nitric Pentoxide/Nitric acid (HNO_3) chemistry
- Modified ammonia and HNO_3 deposition velocities

Note that in a few cases [e.g., vertical grid structure, ammonium (NH_4) emissions estimates], some sensitivity experimentation has already been carried out by VISTAS. To the extent that this information can help guide the future diagnostics analyses, this earlier work will be used.

Level III sensitivity analyses have two main purposes. First, they facilitate the emissions control scenario identification and evaluation processes. Currently, four complimentary sensitivity "tools" can be used in regional photochemical models depending upon the platform being used. These methods include: (a) traditional or "brute force" testing, (b) Decoupled Direct Method, (c) Ozone Source Apportionment Technology and PM Source Apportionment Technology, and (d) Process Analysis. Each method has its strong points and they will be employed where needed. The second purpose of Level III sensitivity analyses is to help quantify the estimated reliability of the air quality model in simulating the atmosphere's response to significant emissions changes.

Examples of Level III monthly or annual sensitivity runs for Phase II might include:

- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to SO_2 emissions
- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to elevated point source NO_x emissions
- Ozone, sulfate, nitrate, ammonium and other aerosol sensitivities to ground level NO_x emissions
- Sulfate, nitrate, ammonium and other aerosol sensitivities to ammonia

The need to perform sensitivity experimentation (Levels I, II, or III) will depend on the outcome of operational performance evaluations. If such a need arises, the ability to actually carry out selected sensitivity and/or diagnostic experiments will hinge on the availability resources and sufficient time to carry out the analyses. Clearly, selection of the specific analysis method will depend upon the nature of the technical question(s) being addressed at the time.

8.3. Air Quality and Ozone Column Data

Data from ambient monitoring networks for both gas and aerosol species are used in the model performance evaluation. Table 8-2 summarizes ambient monitoring networks used to collect data for Air Quality model performance evaluation. Data have been compiled for all networks listed except the Photochemical Assessment Monitoring Stations (PAMS) and PM Super-sites.

Additional data used in the air quality modeling include the Total Ozone Mapping Spectrometer (TOMS). TOMS data provides ozone column data, is available for 24-hour average, and is obtained from http://toms.gsfc.nasa.gov/eptoms/ep.html. The TOMS data is used in the CMAQ radiation model to calculate photolysis rates.

Table 8-2: Overview of Ambient Data Monitoring Networks.

Monitoring Network	**Chemical Species Measured**	**Sampling Period**	**Data Availability/Source**
The Interagency Monitoring of Protected Visual Environments (**IMPROVE**)	Speciated $PM_{2.5}$ and PM_{10} (see species mappings)	1 in 3 days; 24 hr average	http://vista.cira.colostate.edu/improve/Data/IMPROVE/improve_data.htm
Clean Air Status and Trends Network (**CASTNET**)	Speciated $PM_{2.5}$, Ozone (see species mappings)	Approximately 1-week average	http://www.epa.gov/castnet/data.html
National Atmospheric Deposition Program (**NADP**)	Wet deposition (hydrogen (acidity as pH), sulfate, nitrate, ammonium, chloride, and base cations (such as calcium, magnesium, potassium and sodium)), Mercury	1-week average	http://nadp.sws.uiuc.edu/
Air Quality System (**AQS**) Aka Aerometric Information Retrieval System (**AIRS**)	CO, NO_2, O_3, SO_2, $PM_{2.5}$, PM_{10}, Pb	Typically hourly average	http://www.epa.gov/air/data/
Speciation Trends Network (STN)	Speciated PM	24-hour average	http://www.epa.gov/ttn/amtic/amticpm.html
Southeastern Aerosol Research and Characterization (**SEARCH**)	24-hr $PM_{2.5}$ (FRM Mass, OC, BC, SO_4, NO_3, NH_4, Elem.); 24-hr PM coarse (SO_4, NO_3, NH_4, elements); Hourly $PM_{2.5}$ (Mass, SO_4, NO_3, NH_4, EC, TC); and Hourly gases (O_3, NO, NO_2, NO_y, HNO_3, SO_2, CO)	Hourly or 24hour average, depending on parameter.	Electric Power Research Institute (EPRI), Southern Company, and other companies. http://www.atmospheric-research.com
USEPA Particulate Matter Supersites	Speciated $PM_{2.5}$		http://www.epa.gov/ttn/amtic/supersites.html
Photochemical Assessment Monitoring Stations (**PAMS**)	Varies for each of 4 station types.		http://www.epa.gov/ttn/amtic/pamsmain.html
National Park Service Gaseous Pollutant Monitoring Network	Acid deposition (Dry; SO_4, NO_3, HNO_3, NH_4, SO_2), O_3, meteorological data	Hourly	http://www2.nature.nps.gov/ard/gas/netdata1.htm

9.0 Control Strategy

It is important to remember that photochemical models are tools; they do not make decisions. The results from photochemical models are one of several pieces of information that decision-makers must consider when adopting control strategies. To ensure that the modeling analyses provide information that meets the needs of the decision makers, it is imperative that the air quality modelers and decision makers agree upon the type and amount of information that is needed to meet the study objectives. This section outlines the process behind developing and evaluating emission control strategies to be employed for the 8-hour ozone SIP.

9.1. Control Strategy Design

9.1.1. Emission Sensitivity Test

To begin the process of control strategy design a series of simulations using across-the-board reductions of VOC, NO_x, or VOC and NO_x combined can be run. The purpose of these simulations is to evaluate the relative effectiveness of VOC and NO_x controls.

Errors in emission estimates can lead to errors in control decisions. Important sources in future year inventories can be simulated at the lower and upper bounds of their estimated accuracy. In doing this, NCDAQ and SCDHEC can find out if changes, within the known accuracy of the emission estimates, can lead to different decisions for control strategies. Once the future year inventories are assembled, the sources with the highest uncertainty can be identified. These sources could include biogenic emissions, motor vehicle exhaust, and gasoline evaporation. VOC speciation profiles can also be included in these sensitivity tests.

9.1.2. Isopleth Construction

From the emissions sensitivity tests, isopleths relating uniform reductions of VOC and NO_x emissions to peak ozone can be constructed. These isopleths can give some insight into emission reduction goals, but are not designed to evaluate specific control strategies. They do not simulate real controls that change temporal and spatial distributions as well as the organic mix of species. With these limitations in mind, the isopleths can help design the control measures that may reduce levels close to ambient standards. If resources are available, a series of simulations covering a range of actual control measures will be run. From these simulations, peak ozone isopleths can be generated for the entire area as well as for individual sites. These isopleths can be used to design appropriate and defensible control strategies. In addition, isopleths of population exposure can be prepared and used to assess proposed control measures in an integrated manner.

9.1.3. Ranking Control Strategies

Control strategies should be implemented in an ordered fashion that reduces both peak ozone concentrations and population exposure. Emission controls that affect both VOC and NO_x should be sorted separately from VOC or NO_x only controls. Estimates of control levels that are expected in future years should be made. An attempt to reduce population exposure to a minimum each year while reducing peak ozone, can be made by looking at all potentially available controls and at subsets which focus on VOC only, NO_x only, and combinations of VOC and NO_x control.

9.2. Control Strategy Evaluation

Selection of candidate control strategies will take into consideration the results of the combination of analyses described in the previous sections. Once candidate control strategies are identified, the strategies may be simulated. If needed, an analysis will be performed to investigate the predicted impact of each strategy on air quality and population exposure. The results of these analyses will be summarized both in tabular and graphical form to allow systematic comparison and contrast of all strategies.

To assist decision makers in fully understanding the impact of proposed control strategies, the following products may be prepared as a part of the control strategy evaluation:

1. Peak Ozone Tables
2. Peak Ozone Spatial Plots
3. Difference Plots
4. Population Exposure Tables and Histograms
5. Change in predicted future design values

Each of these products will compare future year base simulations with one or more control simulations. An attempt should be made to minimize population exposure as controls are introduced. To assist in this effort, population exposure and peak ozone statistics can be organized by future year and control strategy. Upon completion of this evaluation, a final control strategy will be selected for detailed evaluation.

9.3. Identification of Control Strategy Scenarios

A designated subcommittee will select the control strategy scenarios to be modeled for demonstrating attainment. The control strategy selection process will follow the current USEPA guidance, and will incorporate our present understanding of ozone formation on an urban and regional scale.

Mandated controls will be modeled first (inspection and maintenance programs, NO_x SIP Call, North Carolina's Clean Smokestacks Act legislation, federal engine standards, federal fuel standards, etc.). If attainment of the ozone NAAQS is not shown, additional alternative control strategies identified by the preceding steps, will be modeled until attainment is reached.

A "frozen" future year dataset will be available for use in testing alternative control strategies. This will consist of a set of model input and output files for each episode. Anyone with access to the model (e.g., power companies and universities) can use these files as long as they do not change future base case emission inventories, meteorology, growth factors, or mandated controls. Alternative controls can be modeled in addition to controls strategies modeled by the states.

10.0 Demonstration of Attainment

This section summarizes the procedures that will be used to demonstrate attainment of the 8-hour ozone NAAQS. An attainment demonstration consists of (a) analyses which estimate whether selected emissions reductions will result in ambient concentrations that meet the NAAQS, and (b) an identified set of measures that will result in the required emissions reductions. Determining necessary emission reductions may be done by relying exclusively on results obtained with air quality models. These include the outcomes of the modeled attainment test plus a screening test to estimate whether a proposed emission reduction suffices to meet the NAAQS.

10.1. Ozone Model Attainment Test

The modeled attainment test is the practice of using an air quality model to simulate current and future air quality. For the 8-hour ozone NAAQS, the model estimates are used in a "relative" rather than "absolute" sense. That is, the ratios of the model's future to current predictions at each ozone monitor are used to determine attainment. These site-specific ratios are called relative reduction factors. Future ozone design values are estimated at existing monitors by multiplying the monitor-specific modeling current design value by the modeled relative reduction factor "near" each monitor. If the resulting predicted site-specific future design values are greater than 87 ppb, the modeled attainment test is failed. If the predicted future design values are between 82 and 87 ppb, then additional weight of evidence is needed to corroborate a positive attainment demonstration. If the predicted future design values are below 82 ppb, the area is determined to clearly attain the standard. Equation 10.1 describes the modeled attainment test, applied near monitoring site "x."

$$(DVF) = (RRF)\,(DVB) \qquad \textit{Equation 10.1}$$

(DVB) = the modeling baseline design value monitored at site "x," in units of ppb. Currently the USEPA recommends calculating the DVB by averaging the three design value periods to include the baseline inventory year. In other words, the DVB is based on a 5-year weighted average centered on the baseline inventory year.

(RRF) = the ratio of the future 8-hr daily maximum concentration predicted near a monitor (averaged over each day of the episode) to the current 8-hr daily maximum concentration predicted near the monitor (averaged over each day of the episode).

(DVF) = the estimated future design value for the time attainment is required, ppb.

It is important to consider an array of cells "near" a monitor rather that focusing on the individual cell containing the monitor. This diminishes the likelihood of quirks in the test's results resulting from geometry of the superimposed grid system. Table 10-1 provides the USEPA recommendations for defining "nearby" cells for grid systems having cells of various sizes.

Table 10-1: USEPA Recommendations for Defining nearby Cells

Size of Cell, (km)	Size of the Array of Nearby Cells, (unit less)
<5	7 x 7
>5-8	5 x 5
>8-15	3 x 3
>15	1 x 1

10.2. Screening Test

Per the USEPA Guidance, the states will perform an analysis of unmonitored areas to determine if attainment of the ozone standard is expected in these areas. The unmonitored area analysis, or screening test, will be achieved through the use of the USEPA's Model Attainment Test Software (MATS). This tool will allow for spatial interpolation of baseline monitoring data, which will provide modeling current DVBs for an entire area and not just at monitoring sites. This field is then paired with the modeling results in MATS to produce DVFs for an entire geographic area. This final gradient adjusted spatial field can then be examined for any unmonitored areas that area predicted not to meet the ozone NAAQS. Any violation suggested by this analysis then will then be carefully evaluated.

10.3. Corroborative Analysis

After the completion of the attainment test, the USEPA 8-hour Ozone Guidance suggests additional measures should be taken to further support or refute the attainment test results. This corroboratory evidence is referred to as supplemental analysis when used to further support an attainment demonstration. A weight of evidence determination can be used to conclude that attainment is likely, especially when the predicted future design values are between 82 and 87 ppb. Analysis can include a wide variety of tests and analyses, including the application and results of air quality models, observed air quality trends and estimated emissions trends, and the outcome of observational models.

Should the area, clearly demonstrate attainment (DVF < 82 ppb), then basic supplemental analysis will be performed to further support the test's findings. If either the attainment or screening tests are greater than 87 ppb, it is doubtful that the more qualitative arguments made in a weight of evidence determination can be sufficiently convincing to conclude that the NAAQS for ozone will be attained.

For DVFs between 82 to 87 ppb, a weight of evidence determination will be preformed to supplement the conclusion that the area is expected to attain the NAAQS. The end product of a weight of evidence determination is a document which describes analyses performed, data used, key assumptions and outcomes of each analysis, and why the State believes that the evidence, viewed as a whole, supports a conclusion that the area will attain the NAAQS for ozone.

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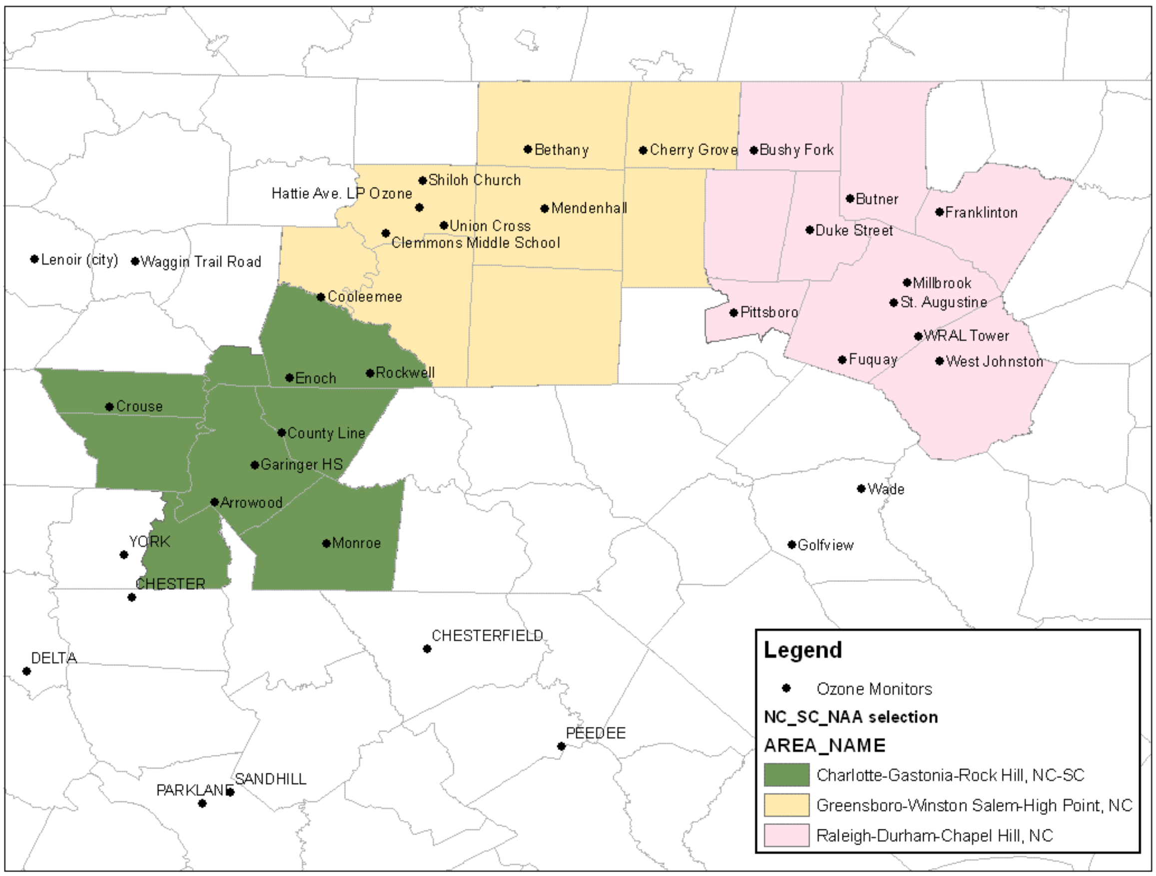
Appendix A: Summer 2002 Episode Summaries

Ozone Monitors in North Carolina Piedmont Area

Below is a map that labels all of the ozone monitors in the North Carolina Piedmont area, including York County, South Carolina. Since the majority of the ozone exceedances occur in the three major urban areas, these are the monitors of greatest concern. The three urban areas include the Metrolina area (Charlotte/Gastonia/Rock Hill nonattainment area), the Triangle area (Raleigh/Durham/Chapel Hill nonattainment area) and the Triad area (Greensboro/Winston-Salem/High Point nonattainment area).



May Episode

The first ozone episode of the year occurred on May 24th and 25th. 8-hour ozone exceedances were largely concentrated around North Carolina, with some scattered exceedances up the east coast to New Jersey. An area of Canadian high pressure moved southward into the eastern United States, bringing cooler than normal temperatures from May 20th through the 22nd. By May 23rd, the surface high pressure was positioned over the southeast, and remained in that location through May 25th. At upper levels, a ridge axis became collocated over the surface high on May 24th through the 25th, which helped to increase stagnation over the southeast. On the 24th conditions were ideal for ozone formation. High temperatures shot upward into the middle to upper 80s on the 24th, the air mass was dry with dewpoints in the 50s, and winds were calm or very light. Every monitor in the Triangle exceeded 0.085 ppm, with the maximum of 0.095 ppm at the St. Augustine monitor in downtown Raleigh. Winds were light southerly in the Metrolina area, leading to 8-hour ozone exceedances in the northern metropolitan area, with a maximum of 0.098 ppm at the Rockwell monitor. A similar pattern occurred in the Triad, with the highest 8-hour ozone values at the Cherry Grove monitor at 0.091 ppm.

The high-pressure area began to move toward the coast on May 25th, while a backdoor cold front pushed into the northernmost areas of the state. The winds turned more southerly across much of North Carolina. The higher winds, combined with higher levels of moisture, led to less ozone formation. Additionally, another area of high pressure pushed south into New England and forced a backdoor cold front into the northernmost areas of the state. There were no 8-hour ozone exceedances in the Triad, while in the Triangle ozone exceedances were confined to downtown and areas to the south. The highest and most widespread 8-hour ozone exceedances were in the Metrolina area, where some recirculation occurred.

June Episodes

Two major ozone episodes occurred in June, the first was from June 3rd through the 5th and the second was from June 10th through the 14th. The first episode was a regional event, characterized by moderately high 1-hour and 8-hour ozone averages across the southeast US. The onset of the first event was a bit unusual. An area of high pressure moved into New England on June 2nd. The position of the high caused some cold air damming against the Appalachian Mountains, and forced a weak cold front southeastward through North Carolina, bringing low humidity air (dewpoints near 55°F) into the state. The high then transitioned offshore on June 4th, switching the flow to the southwest, which caused dewpoints to rise toward 70°F. The highest ozone values during this period were generally on June 4th, with ozone concentrations of 0.106 ppm in Metrolina, as some of the air that was transported to the southwest was redirected toward the northeast due to the wind shift. $PM_{2.5}$ peaked above 30 $\mu g/m^3$ in the Metrolina area on June 4th, and was above 20 $\mu g/m^3$ in the rest of the state. High pressure remained offshore on June 6th, while a cold front was moving through the Midwest. Highest 8-hour ozone was confined to the western Piedmont, where the Metrolina area ozone was 0.097 ppm and the Triad was 0.096 ppm, while the Triangle ozone was lower at 0.087 ppm. $PM_{2.5}$ was in the range of 16 to 23 $\mu g/m^3$. High temperatures throughout the episode were in the 90s. The first episode came to an end on June 6th, as the cold front pushed through North Carolina and off the east coast.

High pressure built into the Great Lakes region from Canada behind the cold front, causing ozone values to rise above 0.085 ppm on June 9th in that region, while ozone in North Carolina began to rebound as the winds began to slacken. The high pressure continued southward and positioned itself over the Southeast on June 10th, triggering stagnation underneath the area of high pressure and causing high ozone up and down the eastern seaboard. Ozone values in North Carolina were highest in the northern half of the state, with ozone at 0.111 ppm in the Triad, and 0.107 ppm in the Triangle. The peak of the episode for the Triad and Metrolina areas occurred on June 11th as the high pressure was beginning to transition offshore. Ozone peaked at 0.118 ppm in Metrolina, at 0.115 in the Triad, and 0.105 ppm in the Triangle.

By the June 12th and June 13th, the area of high pressure was in a classic "Bermuda High" position. With the high in this position, a southwest flow of around 5-10 mph developed, which helped provide some mixing. In this regime, the highest ozone in North Carolina was in the Metrolina area, where 8-hour ozone reached 0.103 ppm on June 12th and 0.106 on June 13th. Ozone levels above 0.085 ppm were restricted to the Triangle on June 14th as a cold front moved through, bringing an end to the second episode of June. High temperatures during the episode ranged from 88-100°F, and dewpoints ranged from the 58-66°F.

The episode of June 18th was caused by an area of high pressure that moved relatively quickly eastward through the Mid-Atlantic States and off the east coast. A weak frontal boundary was located along the North Carolina/South Carolina border. This boundary drifted northward though the day and dissipated. Temperatures were a relatively mild 84-87°F, with dewpoints near 60°F. Of the three major metro areas within North Carolina, only the Triad had monitors barely reach the 8-hour ozone standard of 0.085 ppm, with all other monitors in North Carolina below the standard. In succeeding days, the high pressure moved off the mid-Atlantic and transported cleaner maritime air into the state.

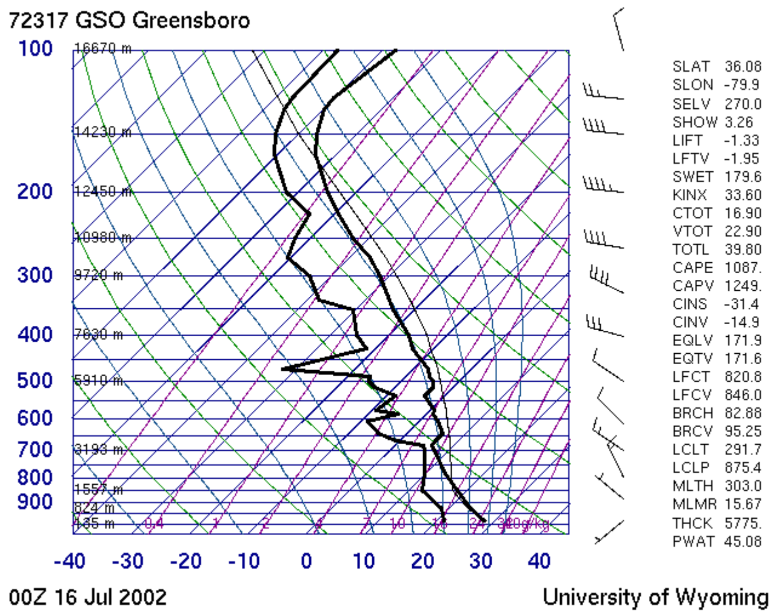
July Episodes

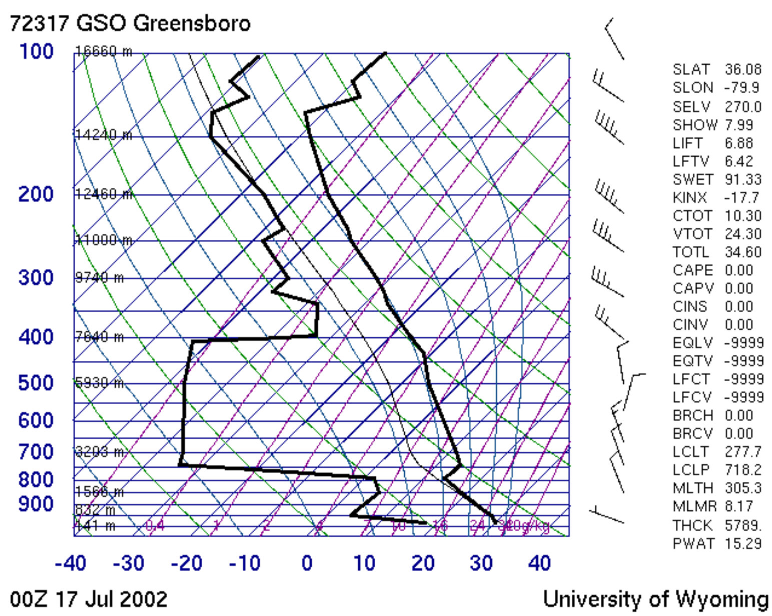
July had three major air quality episodes, and a lesser episode at the beginning of the month. The month began with a few scattered exceedances, all below 0.090 ppm, during the period from July 1st through the 4th. The synoptic trigger for this episode was a stacked high pressure centered over Tennessee and Kentucky. Ozone above 0.085 ppm appeared first over the northeastern US, and then translated southward. High temperatures in the southeast were in the lower to middle 90s, and dewpoints were in the upper 60s to lower 70s. In North Carolina, a general light north/northwest flow caused the formation of a lee trough. Some recirculation was evident as the lee trough shifted east to west.

The first major episode began on July 5th as Bermuda high-pressure system that expanded westward, while at middle and upper levels, a high-pressure ridge developed over the Ohio Valley, while a weak upper trough was positioned along the east coast. The two upper features produced a weak north to northwesterly airflow. An upper level shortwave dropped into the northeast US on July 5th, forcing a cold front southward through the mid-Atlantic. High temperatures peaked near 100°F during this time. The front stalled over the Carolinas late on the 5th and lingered through the 7th, triggering some scattered showers and thunderstorms as well as some cloud cover, causing a slight decline in ozone levels.

The frontal boundary weakened and the Bermuda high pressure reasserted its influence over the eastern seaboard by late afternoon of July 8th. At the same time, the mid and upper level ridge was located over the western two-thirds of the United States, leaving the Carolinas in a light northwesterly upper flow. High temperatures pushed into the 90s, with dewpoints in the upper 50s to mid 60s. Ozone levels peaked on July 8th and July 9th, with values above 0.105 ppm in Metrolina, and between 0.090 and 0.101 ppm in the Triad. A cold front brought an end to the second major episode of the month on July 10th, where only the Triangle and the Triad were above 0.085 ppm.

The third episode of July was shorter in duration, but more intense. In the middle and upper atmosphere, a low-pressure system cut off from the main steering flow and remained qausi-stationary over Kansas and Missouri from July 15th through July 18th. To the east of the upper level low, an upper level ridge axis setup from Alabama northward to Kentucky. The position of the ridge caused a northwesterly downslope flow through the Carolinas. The downsloping caused a considerable amount of warming and drying (see GSO sounding from 00 UTC 16 July and 00 UTC 17 July below). High temperatures were in the mid 90s, with dewpoints ranging from 65-72°F. Ozone values rose from mostly less than 0.065 ppm on July 15th to values between 0.095 and 0.106 ppm on July 16th, with highest values in the Triangle.





The northwest flow continued on July 17th and July 18th, but decreased slightly, allowing for more stagnation and ozone formation. The northwest flow caused the formation of a lee trough on July 17th and July 18th, helping to focus pollutants. Fayetteville experienced their worst ozone day of the year, rising to 0.108 ppm on July 17th, while ozone in Metrolina was 0.116 ppm and the Triangle was 0.107 ppm. Ozone levels in most areas subsided a bit on July 18th, into the 0.090-0.100 ppm range, likely due to some high cirrus that overspread the area. The Metrolina area was an exception, where 8-hour ozone levels rose to 0.119 ppm, the highest values of the ozone season. During this episode, $PM_{2.5}$ values at many locations reached their highest values of the summer, with values approaching and in some locations exceeding 50 $\mu g/m^3$.

July 29th was very minor episode as a Bermuda high set up offshore. Only the Metrolina area had exceedances. High temperatures were in the upper 90s, with dewpoints running quite high in the low to mid 70s. The July 31st episode was caused by a cold front that dropped southward, to just north of North Carolina, stalled and weakened. High temperatures were in the middle 90s with dewpoints near 70°F. Only the Pittsboro monitor in the Triangle area exceeded the 8-hour ozone standard.

August Episodes

On August 1st through 2nd, a moderate episode occurred as a weak continental high pressure moved into the Central Appalachian Mountains, just north of the North Carolina border. High temperatures were in the mid 90s with dewpoints 65-70°F. Ozone levels peaked August 2nd, ranging from 0.090 to 0.096 ppm in the three major metro areas. The episode ended with the passage of a cold front on August 3rd.

Isolated exceedances occurred on August 5th and 6th in the Triad and Metrolina areas with the approach of a cold front. A tropical storm lurking offshore may have triggered some subsidence to enhance a capping inversion. High temperatures during this second moderate episode were in the low to mid 90s, and dewpoints were 65-70°F.

Ozone levels subsided across the eastern US as a series cold front pushed south from Canada and cleaned out the atmosphere. High pressure moved south behind the front and settled over the Ohio Valley from Canada by August 7th. Ozone levels first began to build in eastern Tennessee, northern Georgia, and western North Carolina on August 8th. By August 9th, the area of high pressure had sunk south and was centered over the Carolinas, causing stagnation over the state and leading to 8-hour ozone above 0.090 ppm from the Triad to the Metrolina and Hickory areas. High temperatures were in the upper 80s, with dewpoints near 55 °F. From August 10th through the 13th, the high pressure transitioned offshore to a typical Bermuda high configuration, while a ridge remained over the Carolinas at upper levels. High temperatures rose through the period, peaking in the upper 90s. Dewpoints gradually rose from the mid 50s into the low 60s. Ozone levels continued to rise until the peak of the episode on August 12th, when 8-hour ozone rose to 0.117 ppm in Metrolina, 0.115 ppm in the Triad, and 0.112 in the Triangle. 8-hour ozone levels remained above 0.100 ppm at many locations on August 13th. A cold front brought an end to the episode on August 14th. This episode also contained the highest levels of ozone on a weekend (on August 10th and 11th). $PM_{2.5}$ did not get as high as in other episodes, rising to around 25-30 $\mu g/m^3$ on August 11th through the 13th.

The final air quality episode in August occurred from August 21st through the 23rd. This episode was largely confined to North Carolina, with some elevated ozone in southeast Virginia and northern South Carolina. A weak trough pushed a cold front south through the state late on August 20th. As the trough departed, a Canadian high pressure built down the eastern seaboard on August 21st. The high pressure became vertically stacked ridge built over southeast and remained overhead on August 22nd and especially on August 23rd. High temperatures averaged 95-100°F with dewpoints 68-73°F. Ozone levels were moderately high on August 21st and 22nd, peaking at 0.091 ppm in the Hickory and Metrolina areas on August 21st and on the 22nd reached 0.091 and 0.090 ppm in Metrolina and the Triad, respectively. On August 23rd, a downslope northwest flow developed, pushing a lee trough eastward to the vicinity of the Triangle. Precursors pooling at the lee trough helped to push ozone at every monitor around the Triangle above the 8-hour ozone standard. The West Johnston monitor was the highest, with a 1-hour ozone exceedance of 0.127 ppm, and an 8-hour ozone exceedance of 0.112 ppm. Many 1-hour and 8-hour ozone exceedances also occurred around Metrolina, with the Monroe monitor, southeast of Charlotte, having a 1-hour ozone exceedance of 0.125 ppm, and an 8-hour ozone exceedance of 0.109 ppm. The Triad also had widespread 8-hour ozone exceedances. The episode drew to a close on August 24th as a frontal boundary neared the state and triggered scattered convection. $PM_{2.5}$ was elevated from August 21st to the 24th, ranging from 25 to 35 $\mu g/m^3$ in most areas. The Triad experienced the highest $PM_{2.5}$, topping out at 39.6 $\mu g/m^3$ on August 23rd and 42.7 $\mu g/m^3$ on August 24th.

September

From September 4th through September 11th a widespread episode occurred over the Midwest and Northeast, with North Carolina largely on the periphery of the polluted air mass. The first exceedances in North Carolina occurred on September 4th. During this time a cold front and associated prefrontal trough were approaching North Carolina, while a tropical storm was making landfall in northern Florida. The highest ozone was located between the front and the prefrontal trough, and the subsidence to the north of the tropical storm may have aided in capping the atmosphere. Temperatures were in the low 90s, and dewpoints were in the mid 60s, as ozone near Metrolina reached 0.093 ppm and ozone in the Triad peaked at 0.089 ppm.

Ozone peaked near the same levels on September 5th and 6th as an area of high pressure built southward into the northern Mid-Atlantic States. High temperatures were in the mid 80s, and dewpoints were near 60°F. The weakening tropical storm may have also contributed to a strong capping inversion during this event. September 7th to the 9th saw the high-pressure shift north, with poor air quality shifting north with it. The final ozone exceedance of 2002 occurred on September 11th with an approaching cold front and a departing tropical system north and east of Cape Hatteras. Temperatures held to near 90°F in North Carolina, and dewpoints were in the upper 50s.

Appendix B: Acronyms Used

ACM	Asymmetric Convective Mixing
AERO3/ISORROPIA	Aerosol Chemistry Scheme for CMAQ
AIRS	Aerometric Information Retrieval System
AQS	Air Quality System
BAMS	Barons Advanced Meteorological, LLC
BCON	Boundary Condition Processor
BCs	Boundary Conditions
BEIS3	Biogenic Emission Inventory System, version 3
BELD3	Biogenic Emissions Landuse Database
CAA	Clean Air Act
CAAA	Clean Air Act Amendments
CAIR	Clean Air Interstate Rule
CAMx	Comprehensive Air Quality Model with Extensions
CASNET	Clean Air Status and Trends Network
CB4	Carbon Bond Version 4
CB4-2002	Carbon Bond Version 4 - 2002 update
CCTM	CMAQ Chemical Transport Model
CEM	Continuous Emissions Monitoring
CERR	Consolidated Emissions Reporting Rule
CLT	Charlotte-Douglas International Airport
CMAQ	Community Multiscale Air Quality
CMAS	Community Modeling and Analysis
CO	Carbon monoxide
CPC	Climate Prediction Center
CTM	Chemical Transport Model
DVB	Current Design Value
DVF	Future Design Value
EAC	Early Action Compact
EGU	Electric Generating Unit
EIIP	Emissions Inventory Improvement Program
EMS	Emissions Modeling System
EPA	Environmental Protection Agency, see also USEPA
EPS	Emissions Preprocessing System
ETA	NCEP meteorological model named for the vertical coordinate system used in the model.
FAA	Federal Aviation Administration
FAY	Fayetteville
FDDA	Four Dimensional Data Assimilation
FRM	Federal Reference Method
GIFs	Graphics Interchange Format
GSO	Greensboro
HKY	Hickory
HNO_3	Nitric Acid
I/O	input/output
I/O API	Input/Output Applications Programming Interface
IC/BC	Initial Condition/Boundary Condition

ICON	Initial Condition Processor
ICs	Initial Conditions
IDA	Inventory Data Analyzer
IMPROVE	Integrated Monitoring of Protected Visual Environments
IPM	Integrated Planning Model
ISORROPIA	Inorganic Aerosol Thermodynamics/Partitioning: Model that calculates the composition and phase state of an ammonia-sulfate-nitrate-chloride-sodium-water inorganic aerosol in thermodynamic equilibrium with gas phase precursors.
JPROC	Photolysis Rate Processor
km	kilometer
LSM	Land Surface Model
MACT	Maximum Achievable Control Technology
MATS	USEPA's Model Attainment Test Software
mb	millibar, Measure of atmospheric pressure
MCIP	Meteorological-Chemistry Interface Processor
MCIP2.3	Meteorological-Chemistry Interface Processor (ver. 2.3)
MM5	Mesoscale Meteorological Model, 5 refers to the version number
MM5 PX_ACM	MM5 use of the Pleim-Xiu Soil Model and Asymmetric Convective Mixing PBL model
MOBILE6.2	USEPA vehicle emission factor model, which is a software tool for predicting gram per mile emissions of hydrocarbons, carbon monoxide, oxides of nitrogen, carbon dioxide, particulate matter, and toxics from cars, trucks, and motorcycles under various conditions.
mph	miles per hour
MPP	Massively Parallel Processors
MRPO	Midwest Regional Planning Organization
MSA	Metropolitan Statistical Area
NAAQS	National Ambient Air Quality Standard
NADP	National Atmospheric Deposition Program
NARSTO	North American Research Strategy for Tropospheric Ozone
NCAR	National Center for Atmospheric Research
NCDAQ	North Carolina Division of Air Quality
NCDOT	North Carolina Department of Transportation
NCEP	National Center for Environmental Predictions
NEI	National Emissions Inventory
NH_4	Ammonium
NMC	National Meteorological Center
NO	Nitric Oxide
NO_2	Nitrogen Dioxide
NO_x	Oxides of Nitrogen

NO_x SIP Call	Finding of Significant Contribution and Rulemaking for Certain States in the Ozone Transport Assessment Group Region for Purposes of Reducing Regional Transport of Ozone. Rule designed to mitigate significant transport of NO_x, one of the precursors of ozone.
NO_y	Total Available Nitrogen
NWS	National Weather Service
O_3	Ozone
OBDII	Onboard diagnostics
PAMS	Photochemical Assessment Monitoring Stations
PAVE	Package for Analysis and Visualization of Environmental data
PBL	Planetary Boundary Layer
PM	Particulate Matter
$PM_{2.5}$	Particulate Matter with a diameter less than 2.5 µm
ppb	parts per billion
ppm	parts per million
PSU	Pennsylvania State University
PSU/NCAR	Pennsylvania State University/National Center for Atmospheric Research
PX	Pleim-Xiu
PX_ACM LSM_PBL	MM5 configuration of Pleim-Xiu Land Surface Model, Asymmetric Convective Mixing PBL model
QA	Quality Assurance
QAPP	Quality Assurance Project Plan
QC	Quality Control
Q-Q plots	Quantile-Quantile plots
RACT	Reasonably Available Control Technology
RADM	Regional Acid Deposition Model
RAMS	Regional Atmospheric Modeling System
RDU	Raleigh-Durham International Airport
REMSAD	Regional Modeling System for Aerosols and Deposition
RPO	Regional Planning Organization
RRF	Relative Reduction Factor
RVP	Reid Vapor Pressure
SAPRC99	Photochemical Mechanism in CMAQ
SCBAQ	South Carolina Bureau of Air Quality
SCC	Source Classification Code
SCDHEC	South Carolina Department of Health and Environmental Control
SEARCH	Southeastern Aerosol Research and Characterization
SIP	State Implementation Plan
SMOKE	Sparse Matrix Operator Kernel Emissions
SMVGEAR	Sparse Matrix Vectorized Gear solver
SO_2	Sulfur Dioxide
SOA	Secondary Organic Aerosol
SORGAM	Secondary Organic Aerosol Model
STN	Speciation Trends Network

T	Temperature
TOMS	Total Ozone Mapping Spectrometer
u, v, w	Three Dimensional Wind Components in spherical coordinates : u = E/W; v = N/S; w = vertical
UAMIV	Urban Airshed Model - Version 4
UAM-V	Urban Airshed Model - Version 5
UCAR	University Corporation for Atmospheric Research
UCR	University of California at Riverside and Davis
US	United States
USEPA	United States Environmental Protection Agency
USGS	United States Geological Service
UTC	Universal Time or Greenwich Mean Time
VISTAS	Visibility Improvement State and Tribal Association of the Southeast
VMT	Vehicle Miles Traveled
VOCs	Volatile Organic Compounds
WRF	Weather Research Forecast
Z	Zulu Time, or UTC (Universal Time), or Greenwich Mean Time