The State of the
Southern Oxidants Study (SOS)
Policy-Relevant Findings in
Ozone and PM$_{2.5}$ Pollution Research
1994-2000

Edited by:
Ellis B. Cowling and Cari Furiness
SOS Office of the Director, North Carolina State University
Raleigh, North Carolina 27606

On Behalf of the SOS Executive Committee* and
Contributors to this "State of the Southern Oxidants Study-2:"

Eric Apel, National Center for Atmospheric Research Section 2.6
Carlos Cardelino, Georgia Institute of Technology Sections 2.2, 2.7
*William Chameides, Georgia Institute of Technology Section 2.7
*Ellis Cowling, North Carolina State University Sections 1, 2.1, 2.10, 3
Peter Daum, Brookhaven National Laboratory Section 2.4
Robin Dennis, U. S. Environmental Protection Agency Section 2.8
Fred Fehsenfeld, NOAA Aeronomy Laboratory Section 2.3
Cari Furiness, North Carolina State University Sections 2.9, 2.10
Phyllis Garris, North Carolina State University Appendix A
Michael Hardesty, NOAA Environmental Technology Laboratory Section 2.5
Walter Heck, North Carolina State University Section 2.9
William Hunt, North Carolina State University Section 2.1
Robert Imhoff, Tennessee Valley Authority Section 2.8
John Jansen, The Southern Company Section 2.10
*C. S. Kiang, Georgia Institute of Technology Section 2.10
Prasad Kasibhatla, Duke University Section 2.8
Larry Kleinman, Brookhaven National Laboratory Sections 2.4, 2.7
Peter McMurry, University of Minnesota Section 2.10
*Richard McNider, University of Alabama in Huntsville Section 2.8
*James Meagher, NOAA Aeronomy Laboratory Section 2.3
William Neff, NOAA Environmental Technology Laboratory Section 2.5
*Leonard Newman, Brookhaven National Laboratory Section 2.3
David Parrish, NOAA Aeronomy Laboratory Section 2.6
Tom Pierce, U. S. Environmental Protection Agency Section 2.2
Armistead (Ted) Russell, Georgia Institute of Technology Sections 1, 3
Christoph Senff, NOAA Environmental Technology Laboratory Section 2.5
Sandy Sillman, University of Michigan Section 2.7
Gail Tonneson, University of California in Riverside Section 2.7
Allen White, NOAA Environmental Technology Laboratory Section 2.5
Fred Vukovich, SAIC International Section 2.1
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Partial List of Ph.D. Dissertations and M. S. Theses 1988-2000

Appendix B: SOS Cooperating Universities, Organizations, and Principal Investigators ................................................................................................................................. B1
1. OVERVIEW OF SOS

During the past 12 years, the Southern Oxidants Study (SOS) has become an important source of policy-relevant findings in ozone pollution research. Results achieved, mainly during the past five years, include the following.

1. Confirming several of the reasons suggested in the NRC (1991) report about why ozone management efforts in the United States "largely have failed": need for more robust air quality standards, regionality of ozone and particulate matter air pollution, importance of biogenic precursors of ozone and PM$_{2.5}$, inadequate NO$_x$ measurement instruments, need for improved emissions inventories and air quality models, etc.

2. Further quantifying the importance of biogenic and other natural emissions in the formation and accumulation of ozone and PM$_{2.5}$ in the SOS region—including isoprene from trees, ammonia from animal agriculture, and NO$_x$ from both well-fertilized soils and lightning as well as combustion of fossil fuels.

3. Improving understanding of urban/rural exchange of ozone and its chemical precursors.

4. Developing and using superior instruments to better characterize the pollution climate of the SOS region—both chemically and meteorologically—and using this knowledge to improve prognostic air-quality models.

5. Developing and using observation-based methods to evaluate and improve emissions inventories and improve the performance of emissions-based air-quality models.

6. Improving understanding of the vertical, horizontal, daytime, and nocturnal interactions among urban plumes, power plant plumes, and both natural and mobile sources of precursors in determining rural and urban exposures to ozone under a wide variety of meteorological conditions and in regions with distinctive patterns of land use and industrial development.

7. Evaluating a wide variety of measurement instruments and approaches for characterizing PM$_{2.5}$ in both rural and urban areas throughout the SOS region and understanding some epidemiologically relevant features of these exposures.

8. Participation of SOS scientists in the research and assessment activities of NARSTO. Bill Chameides, Chief Scientist for SOS, served as a co-chair of the Science Team that prepared the 2000 NARSTO Assessment (NARSTO Synthesis Team, 2000). Nineteen SOS scientists served as senior authors or co-authors for nine of 24 NARSTO Critical Review Papers. Also, 58 of the 195 other scientific papers cited in the NARSTO Assessment Document were prepared by SOS scientists and engineers and included scientific findings from SOS.

KEY CITATIONS:
See page 6
1.1. HISTORICAL BACKGROUND AND EVOLUTION OF SOS

Before SOS was initiated in 1988, one of the most poorly characterized regions of high tropospheric ozone, PM$_{2.5}$, and regional haze concentrations in North America was the ten-state area of the southeastern United States. This broad territory extends more than 2500 km west from the Atlantic Ocean and about 1000 km north from the Gulf of Mexico. It includes three physiographically distinct geographical areas: 1) the low-lying (0 to about 200 meters above sea level), relatively flat, 100-200 km wide Coastal Plain areas of North and South Carolina, Georgia, Florida, Alabama, Mississippi, Louisiana, and Texas; 2) the hilly Piedmont regions (200-500 meters above sea level) within the states of North and South Carolina, Georgia, Alabama, Mississippi, Louisiana, Texas, Kentucky and Tennessee; and 3) the high-elevation Appalachian Mountain and Cumberland Plateau regions (500-2000 meters above sea level) within the states of North and South Carolina, Georgia, Alabama, Mississippi, Kentucky and Tennessee.

About 26% of the total US population (about 66 million people) live and work within the boundaries of the SOS measurement and modeling domain which covers about 1.2 million km$^2$. The Coastal Plain and Piedmont portions of the SOS study region are sub-tropical in climate, with warm, humid summers, and extended periods of intense sunshine. The highest-elevation plateau and mountain portions of the SOS study domain are nearly boreal in general climate with cool summers and a high frequency of cloud. Rural parts of the SOS region are dominated by intensively managed commercial hardwood and pine forests and both crop and animal agriculture.

Although still lagging economically behind some other parts of the United States and southeastern Canada, the SOS study region has been expanding very rapidly in both human population and manufacturing-based and service-based economic activity, especially during the past 25 years. This combination of rapid urban, suburban, industrial, commercial, transportation, and tourism growth, and further intensification of agricultural and forest operations, has resulted in substantial increases in ozone and PM$_{2.5}$ concentrations and precursor emissions in large parts of the ten-state SOS region.
1.1.1. Meteorology and Climate of the SOS Region

The SOS region has generally weak summertime winds compared with the northeastern and most of the midwestern parts of the US and southeastern Canada. In fact, the maximum frequency of air stagnation days for the North American continent is centered over the Great Smoky Mountain National Park on the border between North Carolina and Tennessee. This combination of weak winds and moderate mixing heights make the SOS region generally less well ventilated than most other parts of North America. As a result of these unique climatological, meteorological, geographical, biological, land-use, population-growth, industrial-development, and chemical-emissions factors, 31 of the 96 (32%) ozone non-attainment counties in the United States are located in the 10-state SOS study domain using the 1-hour standard and 138 of the 453 (30%) counties using the 8-hour standard.

Although peak ozone concentrations in the SOS region are generally somewhat lower (125-175 ppb) than in the northeastern or midwestern United States (150-200) ppb, average summertime ozone concentrations are generally higher—50-80 ppb compared to 40-70 ppb, respectively. Also, the SOS region tends to have higher rural/regional background concentrations of ozone than northeastern and midwestern parts of the US.
1.1.2. Origin of SOS

These unique pollution climate characteristics of the SOS region led Dr. C. S. Kiang of Georgia Tech to postulate in the early 1980s that air quality management approaches developed in other parts of the United States may not be appropriate for the southeastern part of the country. To address this concern, a *Workshop on Atmospheric Photochemical Oxidants: A Southern Perspective* was held on the campus of Georgia Tech in June 1988. At the conclusion of this workshop, recommendations were formulated for a coordinated, long-term cooperative research program focusing on the formation, accumulation, and management of photochemical oxidants in the South (Rodgers and Chameides, 1988).

At about this same time, three other landmark publications altered conventional wisdom about the scientific underpinnings of ozone management in the United States – Chameides et al.’s (1988) paper on “The Role of Biogenic Hydrocarbons in Urban Photochemical Smog: Atlanta as a Case Study,” Russell’s (1988) paper, “Ozone Pollution: The Hard Choices,” and the National Research Council (1991) report, “Rethinking the Ozone Problem in Regional and Urban Air Pollution.” The major conclusions from these publications were that the United States’ ozone management approaches “largely have failed.”

Stimulated and encouraged by these highly critical perspectives, nearly 200 of the nation's most able air-quality scientists and engineers and a few from abroad joined the SOS research program from more than a dozen universities and 35 industrial, state, federal, and public interest groups. They were convinced that “rethinking” the ozone problem was indeed essential, that a “new paradigm for air-quality research” was needed, and that the southern US should be used as a “natural laboratory” in which to “test essentially every assumption that has undergirded ozone management approaches since 1970.” Thus, the SOS Science Team is systematically pursuing the 18 policy-relevant issues shown in Figure 1.1, especially as they pertain to ozone, but also to PM$_{2.5}$ public health and regional haze problems.

During 1995-1997, and especially after the transition from an ozone only to an “ozone and PM$_{2.5}$” program in 1998 and the addition of the Southern Company/EPRI’s SEARCH and ARIES programs and the TEXAQS 2000 Study, the number of scientists, engineers, and graduate and postdoctoral students increased to almost 500 persons in more than 80 institutions and organizations.
### SOS Systematically Pursues Scientific Issues

**RELATED TO OZONE and PM$_{2.5}$ POLICY ASSUMPTIONS**

#### Issues Related to Assumptions about Regulatory Strategies
1. Advantages and limitations of alternative forms of the primary (public health based) and secondary (public welfare based) National Ambient Air Quality Standards
2. Veracity of the twin concepts of State Implementation Plans and Attainment Counties and Non-Attainment Counties
3. Veracity of the concept of "attainment demonstrations" based on mathematical modeling of a limited number of "exceedance events" under extreme weather conditions
4. Needs for regionally focused as well as locally focused management strategies and tactics
5. Needs to distinguish among "NO$_x$-sensitive," "VOC-sensitive," and "transitional" regimes

#### Issues Related to Assumptions about the Adequacy of Emissions Inventories and Models
6. Importance of both natural and human sources of ozone and PM$_{2.5}$ precursors
7. Need for improvement of mathematical models for estimation of NO$_x$, VOC, CO, CH$_4$, SO$_2$ and NH$_3$ emissions from biogenic and other natural sources and from point, area, and mobile human sources

#### Issues Related to Assumptions about Traditional and Innovative Ways of Thinking about Ozone and PM$_{2.5}$
8. Need for careful thinking about long-term climatological trends and season-long exposures as well as short-term meteorological episodes and weekday and weekend day exposures
9. Need for stochastic as well as deterministic chemical and meteorological thinking

#### Issues Related to Assumptions about Air Quality Models
10. Complementarity of observation-based as well as emissions-based air-quality models
11. Needs for improvement of regional-scale and urban-scale air-quality models
12. Needs for both long-term (seasonal) as well as short-term (episodic) air-quality models

#### Issues Related to Assumptions about Implementation of Ozone Abatement and Mitigation Programs
13. Adequacy of commercially available instrumentation for monitoring of ozone, NO$_x$, speciation of NO$_y$, NH$_3$, and speciation of VOC (especially volatile aldehydes, alcohols, acids, esters, and hydrocarbons with more than 10 carbon atoms)
14. Adequacy of guidance for development of emissions inventories
15. Effectiveness of regulatory practices that distinguish "reactive" from "negligibly reactive" VOCs and then exclude "negligibly reactive" VOCs from ozone and PM$_{2.5}$ precursor inventory requirements
16. Adequacy of guidance for development of State Implementation Plans
17. Reliability of predictions for public health advisories for ozone, PM$_{2.5}$, and regional haze
18. Adequacy of planning for public education and both public and commercial acceptance and expected costs of alternative management strategies and mitigation options

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Figure 1.1. SOS scientists and engineers have pursued a variety of policy-relevant scientific issues—by systematically questioning essentially every assumption that undergirds ozone-and particulate matter management approaches used in the US since the early 1970s.
With these 18 policy assumptions in mind, it soon became apparent that attempts to decrease ozone and PM$_{2.5}$ pollution and their effects on public health, ecosystems, and regional haze in various parts of the US are confounded by a number of critical factors including:

1. Almost complete ignorance among public health scientists about what specific features of PM$_{2.5}$ and their physiological mechanisms of action determine their effects on the respiratory and cardiovascular systems of humans.

2. Non-linearities and complexities in the photochemical reactions that lead to formation and accumulation of ozone and PM$_{2.5}$ can render ineffective many management strategies that are VOC-based, NO$_x$-based, SO$_2$-based, or NH$_3$-based unless these non-linearities and complexities, and their variations from location to location, are well understood.

3. Long-range transport of ozone and PM$_{2.5}$ and their respective precursor chemicals can overwhelm local efforts to decrease emissions of ozone and PM$_{2.5}$ precursors.

4. The strong influence of seasonal and both day-time and night-time meteorological processes on the severity and frequency of pollution episodes can confound trend analyses and mask both local and regional pollution-management efforts and/or their apparent success or lack of effectiveness.

5. Large uncertainties associated with emissions inventories and lack of ambient exposure data documenting the actual impact that management efforts and regulations have on these emissions and the public health, regional haze, or other air-quality related values that are to be protected.

6. Lack of reliable methods and dependable instrumentation for routine measurements of: a) speciation of VOC and NO$_x$, b) concentrations of NO$_x$ and NH$_3$, and c) such meteorological factors as mixing height and wind speed and direction at various altitudes.

7. Lack of seasonal air-quality models and exposure standards that will support or encourage management approaches designed to "avoid a bad summer" rather than "a bad few-day episode."

8. Lack of comprehensive chemical, meteorological, and climatological data sets with which to test both numerical and conceptual models of urban and regional scale ozone, PM$_{2.5}$, and regional haze formation and accumulation processes.

**KEY CITATIONS:**


1.1.3. Development of the SOS Research Paradigm

With these and other critical uncertainties in mind, the SOS Science Team developed and has continued to evolve a "new paradigm for air-quality research." It follows many of the NRC (1991) recommendations for a long-term “coherent and focused study of tropospheric ozone and related aspects of air quality.”

Since its conception during the 1988 Workshop, SOS has developed and evolved as a long-term, cooperative, regionally focused, air quality research and assessment program. SOS is implemented through a unique voluntary alliance of research universities, federal research and regulatory agencies, private sector research organizations, and regional and state air-quality management organizations. The program is guided by a philosophy that all stakeholders in the rural and urban tropospheric ozone and PM$_{2.5}$ issues are welcome to participate and contribute to the maximum extent of their interest and ability.

This unique, university-led, collaborative alliance of nearly 500 individual investigators (see Appendix B) has enjoyed more than a decade of sustained financial and in-kind support from various parts of EPA, NOAA, DOE, TVA, EPRI, and the Southern Company. Periodic financial and in-kind contributions also have been provided by the 10 states of the SOS region – Alabama, Florida, Georgia, Kentucky, Louisiana, Mississippi, North Carolina, South Carolina, Tennessee, and Texas – and by EPA Regions 4 and 6. In addition, matching funds have been provided by more than three dozen research universities. As outlined more thoroughly in Section 1.7, federal, state, industrial, and university investments in SOS research totaled about $6 million per year from 1990-1995. Since 1995, total investments in SOS and SOS-affiliated research have increased from a minimum of about $11 million to a maximum of about $15 million per year.

The SOS paradigm is based on the following major principles and associated research approaches.

1. Ozone, regional haze, and PM$_{2.5}$ involve many of the same photochemical formation and accumulation processes and many of the same chemical precursors – NO$_x$, VOC, CO, and CH$_4$ in the case of ozone and NO$_x$, VOC, CO, CH$_4$, SO$_2$, and NH$_3$ in the case of PM$_{2.5}$ and regional haze. Thus pollutant management approaches that consider these similarities and overlaps are likely to be more efficient and cost-effective in decreasing ozone and PM$_{2.5}$ exposures.

2. Ozone, regional haze, and PM$_{2.5}$ all are secondary pollutants which are so fundamentally regional in sources of precursors and scope that regional scale measurements of all three
pollutants and their several precursors are essential to understand both their formation and
cost-effective management.

3. Biogenic and other natural sources of isoprene and oxygenated VOCs, NOx from well-
fertilized crop lands and lightning, and NH3 from livestock operations are so abundant in the
SOS regions, and so reactive or important, that they must be quantified.

4. Observation-based strategies, tactics, and models are essential to efficient and cost-effective
management of ozone, PM2.5, and regional haze. This is true fundamentally because it is the
chemical precursors actually present and the meteorological processes actually occurring in the atmosphere that lead to formation and accumulation of these pollutants. For this reason,
decisions about management approaches should be based on direct measurements in the atmosphere. Managers can no longer depend on estimates of the precursors believed to be present on the basis of inadequate emissions inventories, or use of "typical summer day"
representations of the chemistry and/or meteorology during any given pollutant episode or seasonal period of exposure.

5. Rural/urban and urban plume/point source plume interactions must be elucidated.

6. Seasonal models, seasonal ambient air-quality standards, and direct measurement of public
health, ecological impacts, and visibility impairment outcomes may help increase the
efficiency and cost-effectiveness of air-quality management approaches.

7. Independent analytical approaches that support robust scientific conclusions and explicit
analysis of air quality management implications of these scientific findings must be carefully
formulated and communicated to users. For these purposes, as discussed in Section 1.6.3,
many SOS scientists use Guidelines for Formulation of Statements of Scientific Findings to be Used for Policy Purposes developed by the NAPAP Oversight Review Board (NAPAP, 1991).

KEY CITATIONS:
1.1.4. Transition of SOS from an "Oxidants Only" to an "Oxidants and PM$_{2.5}$" Research and Assessment Program

During 1997, EPA promulgated two new National Ambient Air Quality Standards. The Ozone standard was changed from a 1-hour standard of 120 ppb to an 8-hour standard of 80 ppb. Also, a new standard for PM$_{2.5}$ was added to the existing annual and 24-hour PM$_{10}$ standards. During the spring of 1998, in part in response to EPA's promulgation of these two new standards (both of which were later remanded by court decisions for reconsideration by EPA), SOS began its transition from a policy-relevant research and assessment program concerned primarily with ozone and other oxidants into a similar program concerned with fine particulate matter and ozone other oxidants. In making this transition, SOS retained its traditional focus on each of the nine distinctive features shown in bold type in the second paragraph of Section 1.1.3. SOS was especially careful to ensure that the program would in fact continue to be "policy relevant" without becoming "policy driven."

In making this transition, SOS also was careful to retain its traditional focus on:

1. Regional and local sources of biogenic and anthropogenic precursor chemicals,
2. Observation-based methods for evaluation of emissions inventories,
3. Rigorous field testing of chemical and meteorological measurement methods,
4. Rural/urban exchange of both ozone and PM$_{2.5}$ and their several precursor chemicals,
5. Using a combination of aircraft-based and ground-based chemical and meteorological measurement platforms to explore urban and power plant plumes in all of their temporal and spatial dimensions in both rural and urban areas within the 10-state SOS region,
6. Complementary use of both observation-based and emissions-based air-quality models,
7. Retaining both a scientific and moral commitment to thorough analysis, interpretation, and publication of policy-relevant scientific findings, and, whenever possible,
8. Following up scientific publications with carefully crafted translations, packaging, and delivery of scientific findings [and policy implications of these findings] with information, graphic displays, and briefing forums that are specifically designed to be of practical value to air-quality managers in industry, in municipal, state, and federal government organizations, and in public-interest and commercial-trade organizations.
1.1.5. **Organization of the SOS Science Team**

The nearly 500 scientists, engineers, graduate students, and postdocs who participate in SOS are drawn from more than 80 organizations and institutions across the United States. As shown in Table 1.1, these include 40 research universities in this country and abroad, 26 federal research or regulatory organizations, 6 private and industrial organizations, 10 state environment and natural resource organizations, and various county and municipal organizations – especially in the states of Georgia, Tennessee, and Texas where SOS focused its rural and urban research and assessment efforts.

Since SOS involves so many different investigators and institutions, coordination of research activities is essential. Early on, SOS’s sponsors established a coordination entity – the SOS Office of the Director (SOS-OD). This headquarters office was led by C. S. Kiang of Georgia Tech from 1988-93 and Ellis Cowling of North Carolina State University from 93-through the present. As shown in Figure 1.2, during 1995-2000, the SOS Science Team involved five specific **Taskgroups** and a seven-member **Executive Committee**:

1. **The SOS Taskgroup on Measurements, Technology, and Standards (SOS-MTS)**, led by Eric Apel of the National Center for Atmospheric Research, ensures the reliability of measurement techniques and instrumentation before they are used in the field.

2. **The SOS Taskgroup on Chemical and Meteorological Measurements (SOS-CMM)**, led by C. S. Kiang and Rodney Weber of Georgia Tech and James Meagher of NOAA, plans and coordinates all ground-based, aircraft-based, and balloon-based chemical rural and urban meteorological measurement and monitoring activities.

3. **The SOS Taskgroup on Emissions and Effects (SOS-EE)**, led by Walter Heck and Cari Furiness of NC State University, maintains a limited focus, especially on ecological effects and related research needs and develops “research grade emissions inventories” that include biogenic emissions of reactive VOCs such as isoprene, NO emissions by soil microorganisms, NO produced by lightning, and improvement of existing models for estimation of emissions from point, area, and mobile sources.

4. **The SOS Task Group on Models and Model Evaluation (SOS-MME)**, led by Richard McNider of the University of Alabama in Huntsville evaluates and improves emissions-based air-quality models and emissions models. SOS-MME and also pioneered development of an observation-based model (OBM) and a Season-long Regional Air Quality Model (SMRAQ).

5. **The SOS Taskgroup on Analysis and Assessment of Alternative Strategies (SOS-A³S)**, led by William Chamedies of Georgia Tech and Ellis Cowling of NC State, focuses on exactly what its name implies.
Table 1.1. Organizations that participate in SOS.

<table>
<thead>
<tr>
<th>Research Universities</th>
<th>Government and Private Sector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baylor University</td>
<td>Aerodyne Research, Inc.</td>
</tr>
<tr>
<td>Boston College</td>
<td>Aerosol Dynamics, Inc.</td>
</tr>
<tr>
<td>Brigham Young University</td>
<td>Atmosphere Research and Analysis, Inc.</td>
</tr>
<tr>
<td>Clarkson University</td>
<td>Environ Corporation</td>
</tr>
<tr>
<td>Colorado State University</td>
<td>Environment Canada</td>
</tr>
<tr>
<td>Duke University</td>
<td>EPRI</td>
</tr>
<tr>
<td>Emory University</td>
<td>Mantech Environmental Technology</td>
</tr>
<tr>
<td>Georgia Institute of Technology</td>
<td>NARSTO</td>
</tr>
<tr>
<td>Harvard University</td>
<td>NASA Marshall Space Flight Center</td>
</tr>
<tr>
<td>Mercer University</td>
<td>NASA Goddard Space Flight Center</td>
</tr>
<tr>
<td>North Carolina State University</td>
<td>NASA Jet Propulsion Laboratory</td>
</tr>
<tr>
<td>Ohio University</td>
<td>National Center for Atmospheric Research</td>
</tr>
<tr>
<td>Oregon Graduate Institute</td>
<td>National Research Council of Canada</td>
</tr>
<tr>
<td>Pennsylvania State University</td>
<td>National Inst. for Environmental Studies</td>
</tr>
<tr>
<td>Purdue University</td>
<td>National Inst. of Standards and Technology</td>
</tr>
<tr>
<td>Rice University</td>
<td>NOAA Aeronomy Laboratory</td>
</tr>
<tr>
<td>South Dakota School Mines &amp; Technology</td>
<td>NOAA Environmental Technology Lab.</td>
</tr>
<tr>
<td>Texas A &amp; M University</td>
<td>NOAA Air Resources Laboratory</td>
</tr>
<tr>
<td>Univ. of Agric. Sciences, Vienna, Austria</td>
<td>NOAA Forecast Systems Laboratory</td>
</tr>
<tr>
<td>University of Alabama in Huntsville</td>
<td>Netherlands Energy Research Center</td>
</tr>
<tr>
<td>University of California at Berkeley</td>
<td>Research Triangle Institute</td>
</tr>
<tr>
<td>University of California at Los Angeles</td>
<td>Southern Company</td>
</tr>
<tr>
<td>University of California at Riverside</td>
<td>State of North Carolina</td>
</tr>
<tr>
<td>University of California at San Diego</td>
<td>State of Georgia</td>
</tr>
<tr>
<td>University of Colorado</td>
<td>Tennessee Valley Authority</td>
</tr>
<tr>
<td>University of Delaware</td>
<td>Texas Hazardous Waste Center</td>
</tr>
<tr>
<td>University of Denver</td>
<td>Texas Nat. Res. Conservation Commission</td>
</tr>
<tr>
<td>Univ. of Heidelberg, Heidelberg, Germany</td>
<td>URS Corporation</td>
</tr>
<tr>
<td>University of Houston-Clear Lake</td>
<td>U.S. Department of Commerce</td>
</tr>
<tr>
<td>University of Innsbruck, Innsbruck, Austria</td>
<td>USDOE Pacific Northwest National Lab.</td>
</tr>
<tr>
<td>University of Maryland</td>
<td>USDOE Brookhaven National Laboratory</td>
</tr>
<tr>
<td>University of Miami</td>
<td>USDOE Fed. Energy Technology Center</td>
</tr>
<tr>
<td>University of Michigan</td>
<td>USDOE Lawrence Berkeley National Lab.</td>
</tr>
<tr>
<td>University of Minnesota</td>
<td>USEPA National Exposure Research Lab.</td>
</tr>
<tr>
<td>University of Tennessee</td>
<td>USDOE Oak Ridge National Laboratory</td>
</tr>
<tr>
<td>University of Texas at Austin</td>
<td>USEPA Nat. Health &amp; Env. Research Lab.</td>
</tr>
<tr>
<td>Washington State University</td>
<td>USEPA National Center for Env. Research</td>
</tr>
<tr>
<td>Western Michigan University</td>
<td>USEPA Nat. Center for Env. Assessment</td>
</tr>
<tr>
<td>York Univ. North York, Ontario, Canada</td>
<td>USEPA Off. Air Quality Plan. &amp; Standards</td>
</tr>
<tr>
<td></td>
<td>USEPA Region 4, Atlanta, Georgia</td>
</tr>
<tr>
<td></td>
<td>USEPA Region 6, Dallas, Texas</td>
</tr>
</tbody>
</table>
Figure 1.2. Organizational Chart for the Southern Oxidants Study (SOS) and the Southern Center for Integrated Study of Secondary Air Pollutants (SCISSAP).
The **SOS Executive Committee** includes SOS Chief Scientist William Chameides, and Senior Advisor C. S. Kiang, both of Georgia Tech; Fred Fehsenfeld and James Meagher of NOAA’s Aeronomy Laboratory; Leonard Newman of Brookhaven National Laboratory; Richard McNider of the University of Alabama in Huntsville; and Ellis Cowling of NC State University in his role as Director of SOS. The major purposes of the Executive Committee are to:

a) coordinate research approaches among SOS investigators,

b) ensure efficient use of human, financial, and instrumentation resources – especially the "core funds" provided by EPA through its Cooperative and Interagency Agreements,

c) encourage coordination between SOS and SOS-affiliated research and assessment activities, and

d) facilitate the contributions of SOS to NARSTO (formerly North American Research Strategy for Tropospheric Ozone).
1.2. SOS RURAL FIELD MEASUREMENT NETWORKS

To understand the long-distance transport not only of ozone, PM$_{2.5}$, and their respective precursor chemicals, and the regional background for physical and chemical exchange of ozone and its precursors between rural and urban areas, SOS deployed a three-tiered series of long-term rural and regional-scale monitoring networks within which its short-term urban intensive field measurement campaigns were embedded. These three regional networks – collectively called the Southeastern Regional Oxidant Networks (SERON) – were designed to achieve high spatial and temporal resolution as well as state-of-the-science characterization of atmospheric chemistry including air concentrations of O$_3$, NO, speciated NO$_y$, speciated VOC, PAN, CO, and a wide variety of meteorological parameters. As shown by the map in Figure 1.3, the SOS-SERON networks include the following.

- The Spatial Ozone Network (SOS-SON) of about 40 continuously monitoring ground-level rural ozone sites in 8 states.
- The Southeastern Consortium Intermediate Oxidant Network (SOS-SCION) for monitoring O$_3$, NO, NO$_y$, and speciated hydrocarbon concentrations at a smaller number of rural sites.
- The Southeastern Network for Intensive Oxidant Research (SOS-SENIOR) for characterizing detailed chemical and meteorological processes occurring at various rural sites using state-of-the-science instrumentation.

Figure 1.3. Schematic of SERON networks.
During 1996-2000, each of these rural-focused networks was transformed as described below. Funding limitations in SOS beginning in 1996 and some increases in ozone monitoring investments by the states and some industries in the SOS region led to gradual replacement of the formally recognized 40-station SOS-SON Network with a less formally recognized set of about 30 sites within the AIRS data base maintained by EPA and later to the Tennessee Valley PM$_{2.5}$ Partnership Network (see Section 1.4).

Following EPA’s promulgation of a National Ambient Air Quality Standard for PM$_{2.5}$ in 1997 and SOS’ success in winning an EPA Competitive Grant titled The Southeastern Center for Integrated Study of Secondary Air Pollutants (SOS-SCISSAP), beginning in 1998, the original 8-11 site SOS-SCION Network was transformed from an "ozone-focused network" into an "ozone- and PM$_{2.5}$-focused network" for measurement of ozone and PM$_{2.5}$, and their respective precursors. The research approach followed in this transformation of the SOS-SCION Network (paired sets of adjacent rural- and urban-focused PM$_{2.5}$ research characterization sites) was funded separately by the Southern Company and EPRI through EPRI's Tailored Collaboration Group matching-funds mechanism. Thus, the former SOS-SCION Network was changed significantly and is now known as the Southeastern Aerosol Research and Characterization (SEARCH) study.

After its initial and highly successful intensive characterization of regional background ozone and precursor concentrations at ground level in 1990-1994, the SOS-SENIOR Network was replaced in 1995 and subsequent years by equally intensive rural ozone and precursor measurements using highly instrumented aircraft.

SEARCH is one of a series of six "SOS-affiliated" or "SOS-derived" research activities which are funded separately but maintained in close cooperation with SOS (see Section 1.4, items 1-6). These studies involve many of the same SOS investigators who found professional and personal satisfaction through SOS – by learning to "reason together carefully" in debating research priorities and then deciding what goals and objectives to pursue, and then voluntarily agreeing to "work together harmoniously" to fulfill those mutually agreed goals and objectives with whatever financial and in-kind support they can persuade their own institutions and other cooperating organizations to provide.
1.3. **SOS URBAN FIELD MEASUREMENT CAMPAIGNS**

Embedded within the three tiered SOS-SERON Networks, SOS mounted five major summertime-only, urban-focused, intensive field measurement and modeling campaigns – the first two were focused on ozone and its precursors, the last three on ozone, PM$_{2.5}$, and their respective precursors. Table 1.2 displays the distinctive features of each of the urban areas chosen as sites for the SOS field campaigns. Items 1 – 5 below describe each specific SOS urban study.

Table 1.2. Characteristics/Distinctive Features of Four Major Urban Non-Attainment Areas Studied by SOS.

<table>
<thead>
<tr>
<th>Characteristic or Feature</th>
<th>Atlanta, GA</th>
<th>Nashville, TN</th>
<th>Dallas-Fort Worth, TX</th>
<th>Houston-Galveston, TX</th>
</tr>
</thead>
<tbody>
<tr>
<td>Population</td>
<td>2.9 million</td>
<td>1.0 million</td>
<td>4.0 million</td>
<td>4.0 million</td>
</tr>
<tr>
<td>Area of Non-Attainment Counties</td>
<td>3991 mi$^2$</td>
<td>2790 mi$^2$</td>
<td>4266 mi$^2$</td>
<td>7767 mi$^2$</td>
</tr>
<tr>
<td>Inland vs. Coastal</td>
<td>Inland city</td>
<td>Inland city</td>
<td>Inland city</td>
<td>Coastal city</td>
</tr>
<tr>
<td>Elevation</td>
<td>330 meters</td>
<td>600 meters</td>
<td>800 meters</td>
<td>0-80 meters</td>
</tr>
<tr>
<td>Physiographic Region</td>
<td>Piedmont</td>
<td>Piedmont</td>
<td>Piedmont</td>
<td>Coastal Plain</td>
</tr>
<tr>
<td>Land Use Nearby</td>
<td>60% mixed forest 40% cropland</td>
<td>70% hardwood forest 30% cropland</td>
<td>70% scrub oak 30% rangeland</td>
<td>60% scrub oak 40% crop/range</td>
</tr>
<tr>
<td>Latitude</td>
<td>33° 83 min N</td>
<td>36° 18 min N</td>
<td>32° 75 min N</td>
<td>29° 75 min N</td>
</tr>
<tr>
<td>Longitude</td>
<td>84° 36 min W</td>
<td>86° 76 min W</td>
<td>96° 77 min W</td>
<td>95° 33 min W</td>
</tr>
<tr>
<td>Emissions in Non-Attainment Counties (tons):</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NO$_x$-power plants</td>
<td>58,000</td>
<td>14,000</td>
<td>21,000</td>
<td>79,000</td>
</tr>
<tr>
<td>NO$_x$-fuel combustion</td>
<td>11,000</td>
<td>12,000</td>
<td>9,000</td>
<td>126,000</td>
</tr>
<tr>
<td>NO$_x$-other industrial</td>
<td>22,000</td>
<td>11,000</td>
<td>21,000</td>
<td>29,000</td>
</tr>
<tr>
<td>NO$_x$-motor vehicles</td>
<td>142,000</td>
<td>41,000</td>
<td>132,000</td>
<td>116,000</td>
</tr>
<tr>
<td>NO$_x$-off-highway</td>
<td>54,000</td>
<td>21,000</td>
<td>83,000</td>
<td>205,000</td>
</tr>
<tr>
<td>Total NO$_x$</td>
<td>291,000</td>
<td>100,000</td>
<td>270,000</td>
<td>557,000</td>
</tr>
<tr>
<td>VOC-industrial sources</td>
<td>102,000</td>
<td>58,000</td>
<td>73,000</td>
<td>158,000</td>
</tr>
<tr>
<td>VOC-mobile+off-highway</td>
<td>152,000</td>
<td>39,000</td>
<td>138,000</td>
<td>123,000</td>
</tr>
<tr>
<td>VOC-biogenic sources</td>
<td>163,000</td>
<td>47,000</td>
<td>92,000</td>
<td>247,000</td>
</tr>
<tr>
<td>Total VOC</td>
<td>421,000</td>
<td>144,000</td>
<td>307,000</td>
<td>530,000</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>1,611,000</td>
<td>415,000</td>
<td>1,272,000</td>
<td>1,249,000</td>
</tr>
<tr>
<td>Ozone Designation</td>
<td>Serious</td>
<td>Marginal</td>
<td>Serious</td>
<td>Severe</td>
</tr>
<tr>
<td>Ozone, 2nd max, 1-hr</td>
<td>157 ppbv</td>
<td>120 ppbv</td>
<td>118 ppbv</td>
<td>203 ppbv</td>
</tr>
<tr>
<td>Ozone, 4th max, 8-hr</td>
<td>126 ppbv</td>
<td>91 ppbv</td>
<td>94 ppbv</td>
<td>121 ppbv</td>
</tr>
<tr>
<td>PM$_{10}$, 24-hr</td>
<td>3.1 μm m$^{-3}$</td>
<td>5.6 μm m$^{-3}$</td>
<td>4.4 μm m$^{-3}$</td>
<td>5.2 μm m$^{-3}$</td>
</tr>
</tbody>
</table>

Counties within these four ozone non-attainment areas include:
- Nashville -- Davidson, Rutherford, Sumner, Williamson, Wilson.
- Dallas-Fort Worth -- Collin, Dallas, Denton, Tarrant.
- Houston-Galveston -- Brazoria, Chambers, Fort Bend, Galveston, Harris, Liberty, Montgomery, Waller.
1) SOS Field Intensives in the Atlanta, Georgia Metropolitan Area. These ozone-focused studies consisted of short-term exploratory studies during the summers of 1990 and 1991 followed by a major six-week-long field measurement campaign from July 15 to August 31, 1992. This study involved about 77 ground-based chemical and meteorological measurements sites and a series of tower-based and tethered-balloon-based measurements of ozone, its precursors, and meteorology. Since scientific findings from this first SOS Urban Intensive in Atlanta were thoroughly discussed in the first State of SOS Document (Chameides and Cowling, 1995), they will not be discussed further in this document.

2) SOS Nashville/Middle Tennessee Ozone Study. This ozone-focused field study was carried out in the 11-state region surrounding Nashville/Middle Tennessee. It began with a 3-week exploratory study during the summer of 1994 and culminated in a six-week-long major field measurement campaign from June 19 to July 28, 1995. Leadership for the study was provided by Jim Meagher of TVA who coordinated measurements at 116 ground-based and tall-building and tower-based chemical and meteorological measurement sites and a series of six airborne chemical measurement platforms including both fixed-wing NOAA, NASA, and DOE aircraft and a TVA helicopter. This study included a three-tiered hierarchy of progressively more sophisticated surface air quality measurements including: a) 108 "Level I" surface ozone monitors; b) six "Level II" sites providing continuous high sensitivity measurements of ozone, SO₂, NO, NO₃, and CO, canister sampling for speciated VOC measurements, wind speed and direction, temperature, relative humidity, and solar radiation; and c) two "Level III" sites that provided detailed research-grade photochemistry and meteorology measurements using rawinsonde and ozonesonde releases and a radar profiler/radar acoustic sounding system. Research grade, day-specific, emissions inventories were produced for the six-week intensive period. They included biogenic, point source, and mobile sources based on daily activity logs, traffic counters, vehicle mix, tunnel studies, and a subregional domain inventory.

The most significant feature of the Nashville/Middle Tennessee Ozone Study was a coordinated series of 40+ aircraft studies which had the following five general objectives and guiding "mentors":

1. Measurements of ozone formation in the Nashville urban plume under free-flow and stagnation conditions – Peter Daum and Larry Kleinman of Brookhaven National Laboratory.
2. Measurements of ozone formation and destruction in power plant plumes – Noor Gillani of TVA.

3. Detailed subregional characterization of atmospheric chemistry and meteorology to evaluate urban-rural exchange and provide observational data sets for model evaluations – Robin Dennis of EPA.

4. Regional characterization flights to provide context and contrast for air quality measurements in Nashville. They extended north to the Great Lakes, south to the Gulf of Mexico, west to Missouri and Arkansas, and east to the Appalachian Mountains – Michael Trainer of NOAA.

5. Side-by-side intercomparisons of aircraft measurements for the in situ sampling aircraft and overflights for the remote sensing aircraft – Gerd Hübler and James Meagher of NOAA.

3) **SOS Nashville '99 Field Study.** This follow-up to the SOS Nashville/Middle Tennessee Ozone Study in 1994-95 consisted of a four-week-long field measurement campaign during July 1999 with a similar array of ground-based measurement sites and four aircraft-mounted chemical measurement platforms. The Nashville '99 field measurement campaign was designed to answer the following scientific questions:

   a) By what specific aerosol measurement methods can SOS achieve maximally beneficial characterization of aerosols in both urban and rural areas of the SOS region?

   b) What are the linkages (similarities and differences) between the chemical, biological, and meteorological processes that govern formation and accumulation of ozone and fine particulate matter?

   c) What is the relative efficiency of production of ozone and fine particulate matter in urban plumes compared to that in power-plant plumes?

   d) In what ways are the rates and efficiencies of ozone and fine particulate matter production and accumulation different in large urban areas compared to small urban areas -- especially in cases where an air mass spends an extended period traversing a very large urban area?

   e) How do nighttime meteorological and chemical processes influence the rates, efficiencies, and areal extent of ozone and fine particulate matter formation and accumulation?

   f) What meteorological and chemical factors determine the regionality and/or locality of ozone and fine particulate matter accumulation events? In particular:

      i) How do the processes that govern ozone accumulation in isolated urban areas surrounded by high-isoprene-emitting forests differ from those in urban areas in which urban plumes overlap from one urban or non-forested area to another?

      ii) How important are urban heat-island phenomena in determining the regionality and or locality of ozone and fine particulate matter formation and accumulation processes?
4) **SOS Initial Supersite in Atlanta, Georgia.** This study was one of two "Initial Supersites" established at the request of EPA's PM-Supersite program in EPA's Office of Air Quality Planning and Standards. The other "Initial Supersite" was in Fresno-Bakerfield, California. Both "Initial" sites were part of EPA's effort to increase the nation's capacity to monitor PM$_{2.5}$ in a reliable way in various parts of the country. Under the leadership of SOS' Chief Scientist, Bill Chameides, SOS brought together in Atlanta during August 1999, the most comprehensive array of particulate-matter measurement instruments ever assembled in the US. The measurement site was located in a mixed commercial and industrial area about 8 km west of the center of Atlanta where routine PM$_{2.5}$ characterization measurements had been made as a part of the SEARCH and ARIES programs for more than a year. This major instrument-intercomparison and PM$_{2.5}$-characterization study included a wide variety of instruments for determining the mass, particle size distribution, chemical composition of individual particles, and chemical composition of hourly-collected filter samples collected on all days of the week, and simultaneous gas and particle measurements.

5) **Texas Air-Quality Study (TEXAQS 2000).** Peter Daum and Larry Kleinman of Brookhaven National Laboratory provided leadership for this major field measurement campaign in the eastern half of Texas. The study was headquartered in Houston, TX where EPA established one of its operational PM Supersites under the leadership of David Allen of the University of Texas at Austin and Matt Fraser of Rice University. The six-week intensive field measurement campaign began on August 1 and extended to September 15, 2000. It involved nearly 100 ground-based chemical and meteorological measurement sites, and six airborne measurement platforms including aircraft from NOAA, NASA, DOE, and Baylor University. Two "Super-Chemistry" sites were set up to measure a wide array of trace gas and aerosol species – one at LaPorte Airport in the heart of the petrochemical industry surrounding the Houston Ship Channel, and the other at the top of a 30-story building on the west side of downtown Houston. More than 250 scientists were involved with the field measurements. Most will remain involved in the analysis, interpretation, and publication phases of this study.

TEXAQS 2000 was designed to compare and contrast ozone and aerosol formation processes in and around two huge sprawling petrochemical-dominated metropolitan areas in the eastern half of Texas – Dallas-Fort Worth, an inland, somewhat more northerly metropolitan area with large emissions of VOC and NO$_x$, and Houston-Galveston, a more southerly and coastal urban-
industrial complex with its heavily industrialized Ship Channel and land-sea breeze-reversal processes which often give a "double dose" of VOC, NO\textsubscript{x}, SO\textsubscript{2}, and Cl pollutants (see Table 1.2). Although these metropolitan areas are similar in size and population, the emissions mix and processing conditions are very different, affording an opportunity to study the effect of differences in industrial and biogenic emissions on ozone/aerosol formation. Also, ambient VOC/ NO\textsubscript{x} ratios for parts of Houston are much larger than those in any other US city.

Five major research themes are being pursued through the TEXAQS 2000 Study:

- **Atmospheric dynamics and transport** – especially with reference to 1) land/sea breeze influences on transport and dispersion of ozone and PM\textsubscript{2.5}, 2) height and intensity of mixing within the planetary boundary layer (PBL), and 3) processes of entrainment and detrainment from the PBL.

- **Ozone formation and distribution** – by 1) quantifying the relative contributions and reactivities of anthropogenic and biogenic VOCs, and 2) determining instantaneous rates and efficiencies of ozone formation as a function of time, location, and precursor concentrations.

- **Particle formation and distribution** – by measuring 1) large-scale spatial distributions of PM\textsubscript{2.5} and PM\textsubscript{10}, 2) evolution of aerosols downwind from point sources and urban areas, 3) identifying conditions under which new particles are formed, and 4) determining if aerosols are a sink for NO\textsubscript{y}.

- **Emission inventories** – by making a wide variety of ambient measurements and calculations designed to identify and quantify sources of error in estimates of anthropogenic and biogenic emissions including unscheduled and as yet undocumented releases of VOCs in the Houston Ship Channel.

- **Modeling improvements** – by developing 1) "ground truth" tests of the skill of models to simulate both horizontal transport and vertical dispersion processes, 2) comprehensive data bases against which model performance can be evaluated, and 3) data and information by which to judge the adequacy of the meteorological and chemical representations used in these models.
1.4. SOS AND SOS-AFFILIATED OZONE AND PM$_{2.5}$ CHARACTERIZATION STUDIES

This series of six additional ozone and PM$_{2.5}$ studies was initiated as SOS began its transition from an "ozone only" to an "ozone and particulate matter" research and assessment program. As indicated earlier, this transition was made in part in response to EPA's increased emphasis on the regional haze and public health impacts of PM$_{2.5}$, and in part as a result of the restructuring of EPRI, TVA, and other parts of the electric utility sector. Each study has its own general and specific purposes, leadership arrangements, and its own distinctive mechanisms of funding. But they all have derived from and been major contributing parts of SOS's general purpose – characterizing ozone and PM$_{2.5}$ exposures in various parts of the SOS region and better understanding the chemical and meteorological processes of their formation, accumulation, and their public health and visibility impairment effects.

1. Tennessee Valley PM$_{2.5}$ Partnership Monitoring Network. This cooperative study began in May 1997 and will continue indefinitely under the leadership of Bill Parkhurst in TVA's Environmental Research Laboratory. This network is an outgrowth of TVA's general interest and concern, and that of its various state, National Park Service, and EPRI partners, to understand the sources and process within the Tennessee Valley that affect regional haze, acid rain, public health, economic development, compliance with state and federal ozone and PM air-quality regulations, and prevention of significant deterioration in TVA's operating area. Financial and in-kind support for this Network are provided by the TVA Fossil Power Group, various state and municipal agencies within the Tennessee Valley, the National Park Service, and EPRI. As shown in Figure 1.4, the 12 monitoring sites in the Tennessee Valley Partnership Network include: 2 regional remote sites, 1 regional background site, 3 suburban sites, and 6 urban sites (the latter with various degrees of residential, commercial, and industrial development) in various parts of Tennessee, western Kentucky, and northern Mississippi and Alabama. Measurements at all 12 sites include: PM$_{2.5}$ mass using Federal Reference Method samplers. Measurements also include ozone at five sites, PM$_{2.5}$ chemical speciation (including trace metals and both organic and elemental carbon) at four sites, and visual range at one site.
2. **SOS-Southern Center for Integrated Study of Secondary Air Pollutants (SOS-SCISSAP).** This research initiative began under the leadership of SOS Chief Scientist, William Chameides in October 1998 and will continue through September 2001. This SOS project is funded through an EPA Competitive Grant to Georgia Tech. Its objectives are to answer the following scientific questions:

1. What are the concentrations and composition of PM$_{2.5}$ in urban and rural locales in the southern United States? To what extent do temporal and spatial variations in these parameters correlate with those of ozone and its precursor compounds?

2. What are the major precursor compounds and sources for PM$_{2.5}$ in urban and rural locales in the South? To what extent do these compounds and sources correspond to and/or correlate with the sources of natural and anthropogenic ozone precursors (i.e., VOC, NO$_x$, CO, and CH$_4$)?

3. How are the formation rates and concentrations of ozone and PM$_{2.5}$ as well as the PM$_{2.5}$ chemical composition affected by the relative emissions and concentrations of NO$_x$, SO$_x$, NH$_3$, CO, CH$_4$ and VOC species? What are the chemical mechanisms responsible for these relationships?
The principal sites for PM\textsubscript{2.5} sample collection and analysis in SOS-SCISSAP are located in Atlanta, GA and Hendersonville and Dickson, TN. Measurements made at these sites include a custom designed three-channel Particle Composition Monitor and associated ion chromatograph and gas-chromatograph/mass spectrometer instruments that together permit determinations of total particle mass as well as the following chemical constituents: NH\textsubscript{3}, HNO\textsubscript{3}, HONO, SO\textsubscript{2}, Na\textsuperscript{+}, Ca\textsuperscript{++}, NH\textsubscript{4}\textsuperscript{+}, Cl\textsuperscript{-}, NO\textsubscript{2}\textsuperscript{-}, NO\textsubscript{3}\textsuperscript{-}, SO\textsubscript{4}\textsuperscript{2-}, total elemental carbon, total organic carbon including formic, acetic, and oxalic acids, other speciated organic compounds, and trace metals.

3. Southeastern Aerosol Research and Characterization (SEARCH) study. [Excerpted from SEARCH Fact Sheet, \url{http://www.atmospheric-research.com}]. In July 1997 EPA revised the national ambient air quality standards for ground-level ozone and particulate matter. EPA’s action created a new standard for fine particulate matter (PM\textsubscript{2.5}) and set its levels at 15 micrograms per cubic meter (ug/m\textsuperscript{3}) for an annual average (averaged over 3 years) and 65 ug/m\textsuperscript{3} for a daily average (3-year average of the 98\textsuperscript{th} percentile daily concentration). Analysis of the very limited existing data suggests that the new PM\textsubscript{2.5} standard will be more difficult to achieve than the older PM\textsubscript{10} standard and will dramatically increase the number of PM nonattainment areas.

Unlike other criteria pollutants such as ozone, fine particles typically comprise mixtures of hundreds of compounds. Therefore, in order to identify sources of PM\textsubscript{2.5} and to attribute health effects to specific components, we must measure PM\textsubscript{2.5} composition as well as its mass.

Consistent with its July 1997 Presidential directive, EPA will not require control of PM\textsubscript{2.5} precursors until after it has conducted further scientific review of the PM\textsubscript{2.5} standards and it has officially designated nonattainment areas. Such designation is expected in the 2004 to 2005 time frame. State implementation plans (SIPs) must be submitted within three years of the EPA attainment designation.

Given this ambitious schedule, EPA is leading the states in a massive monitoring program to characterize the chemical and physical nature and geographical distribution of PM\textsubscript{2.5}. A nationwide network consisting of more than 1100 PM\textsubscript{2.5} monitoring sites is currently in place. A small subset of these (the “speciation network”) will be devoted to compositional measurements. The "speciation" network is being implemented in phases during 2000 and 2001. EPA has also initiated a series of so-called "SuperSites" across the nation dedicated to gathering detailed
information and performing sophisticated aerosol measurements in support of methods
development, health studies, and atmospheric process research. An Integrated SuperSite
Experiment (ISSE) is planned for July 2001. EPRI has been advising EPA on the design and
implementation of this program, and a dialogue has been established to coordinate public and
private sector efforts.

From the outset, it has been clear that public-private collaboration could greatly accelerate
our understanding of the PM$_{2.5}$ issue. Therefore, Southern Company and EPRI have taken the
initiative to deploy instrumentation designed to measure PM$_{2.5}$ mass and composition over a
broad geographical region of the Southeast on a rapid time track. Building on the existing
SCION component of the Southern Oxidants Study, Southern Company and EPRI have
established a highly instrumented eight-station network in the states of AL, FL, GA and MS.
Figure 1.5 shows a map of the network. Several of the sites in Figure 1.5 are operated in
collaboration with State or local air monitoring networks. In addition, the Jefferson Street site is
the focal point of a major epidemiological study in the City of Atlanta, ARIES (described below)
and was the site of EPA's first SuperSite experiment in August 1999.

Objectives of SEARCH are:

1. To work interactively with the States and to assist them in:
   a) meeting their PM$_{2.5}$ monitoring obligations and
   b) gathering a data set appropriate for evaluating and applying (as in SIP development) air
      quality models.

2. To provide an ambient data set with minimal sample adulteration and of sufficient breadth, in
terms of measured variables, geographical diversity and extent, frequency of measurement,
and duration of the measurement campaign such that:
   a) a PM and oxidant climatology for the region will be established,
   b) coarse and fine PM concentrations will be distinguished,
   c) chemical constituents of PM and their physical states will be characterized and
correlations among precursor and product materials in the atmosphere will be determined,
allowing hypotheses regarding pollutant sources to be tested,
   d) insights into aerosol formation mechanisms can be gained,
   e) differences between airborne materials in coastal vs. inland, and rural vs. urban areas will
be documented, and
   f) biases in measurement methods, such as use of a single Teflon filter in the Federal
Reference Method for PM$_{2.5}$, will be characterized.
3. To deploy reliable continuous methods in order to observe and understand processes governing PM$_{2.5}$ and co-pollutant emissions, formation, transport and deposition.

The SEARCH PM collection and characterization methods include:

a) 24-hour Federal Reference Method (FRM) monitors for PM$_{2.5}$,

b) 24-hour Particle Composition Monitors and dichotomous samplers for PM$_{2.5}$, PM$_{10}$, and chemical speciation,

c) 1-minute to 1-hour continuous particle monitors including a Tapered-Element Oscillating Microbalance (TEOM) for PM$_{2.5}$ mass and Ruprecht & Patashnick Model 5400 Particulate Carbon Analyzer for elemental and organic carbon,

d) 1-minute trace gas measurements including ozone, NO, NO$_2$, NO$_y$, HNO$_3$, SO$_2$, and CO,

e) Meteorology including wind speed and direction, temperature, relative humidity, barometric pressure, solar radiation, and precipitation, and

f) Visibility at some sites.

Figure 1.5. Monitoring sites in SEARCH network.
4. Aerosol Research Inhalation Epidemiological Study (ARIES). [Excerpted from ARIES Fact Sheet, http://www.atmospheric-research.com]. Findings from some epidemiology studies have shown discernible associations between daily levels of particulate matter and adverse health effects. Interpretation of these associations has been difficult and controversial because particulate matter can be an index for a range of other substances in air as well as for weather and seasonal patterns.

On the basis of the epidemiology evidence, the United States Environmental Protection Agency (EPA) promulgated new National Ambient Air Quality Standards (NAAQS) for particulate matter 2.5 micrometers in diameter (PM$_{2.5}$) and smaller. These standards address long term (annual average) and short-term (24-hour average) concentrations of PM$_{2.5}$. Although information on PM$_{2.5}$ is limited, it appears likely that many areas of the US will approach or exceed the annual-average threshold for compliance with the annual PM$_{2.5}$ NAAQS. The health-based particulate matter standards will be reconsidered by EPA in the year 2002, based upon a review of new health information.

The mandated timeline for the review process meant that EPA decisions might continue to be hindered by the dearth of high-quality data on PM$_{2.5}$ mass and composition. This signaled the need for a collaborative effort between the public and private sector to facilitate and expedite data acquisition. In January 1998, Southern Company and EPRI formed a consortium of sponsors and eminent researchers to undertake a state-of-the-art air quality, health, and epidemiology study which promises to provide integral scientific input into the regulatory and standard-setting process in the years 2000 and 2001.

Measurements from the Southeastern Aerosol Research and Characterization study (SEARCH) and the convergence of a variety of complementary studies provided the baseline infrastructure for launching such a comprehensive study in Atlanta. After intensive planning and peer-review, investigators initiated ARIES air quality monitoring and health data collection in July 1998. These activities continued on a daily basis through August 2000 and have continued beyond that date for most of the air quality measurements and some health data.

The objective of ARIES is to investigate (via epidemiology and exposure studies) associations between air quality and human health and produce results in time for consideration of the health basis of the NAAQS and for subsequent development of State Implementation
Plans (SIPs). Fine PM may be an indicator (but not necessarily a cause) of adverse effects associated with inhalation — other pollutants, which co-vary with PM, may be the underlying cause. What sets ARIES apart from prior studies is that its focus is not on PM alone but on an unprecedented range of potential agents in the air, including VOCs, aeroallergens, and specific PM components. This comprehensive sampling approach enables a more robust and explicit investigation of the relationship between human health and airborne pollutants.

The study is fundamental by design, so that the results in terms of associations between air quality and health will be generic and not limited to Atlanta, a metropolitan area with a mix of air pollution sources. It is expected that the study will generate hypotheses to be tested through mechanistic studies and will provide data to test the relevance of results from toxicology studies. In short, ARIES will provide the underpinning of health-related studies for years to come.

ARIES is a multi-faceted study in which the disciplines of atmospheric research, epidemiology, exposure assessment, health assessment, and modeling were considered as parts of the whole from the inception of study design. A comprehensive daily monitoring program will provide epidemiologists with a characterization of aerosol (gas and particle) physical, chemical, and biological (aeroallergenic) properties that has not been available to them before. There are four components of ARIES:

- **Air Quality Characterization**: PM$_{2.5}$ mass and composition, as well as related gas-phase and particle-phase pollutants, are measured every day with at least 24-hour time resolution. The air quality field measurements include SO$_2$, CO, NO, NO$_2$, NO$_y$, O$_3$, HNO$_3$, NH$_3$, and VOCs in the gas phase; major ions, including acidity, elemental/organic carbon (EC/OC), elements, water-soluble transition metals, and solvent-extractable carbon in the particle phase; pollen and mold; and particle number and size distribution from nanometers to micrometers in diameter. The representativeness of the ARIES air quality measurement site is also being assessed through specialized studies of spatial variability within Atlanta.

- **Air Pollution Mortality**: daily mortality data are being collected and analyzed in a multi-pollutant ecological time-series study.

- **Air Pollution Morbidity**: daily data on emergency room (ER) visits are collected from nearly all hospitals in the Atlanta area. The focus is on ER visits for coronary and respiratory symptoms. A parallel study is also being conducted to understand the influence of daily air quality on unscheduled physician visits at a large health-maintenance organization. Finally, the health study will evaluate the physiologic responses of a group of patients with more severe cardiac conditions (those with implanted defibrillators).

- **Exposure & Health Assessment**: a personal/indoor/outdoor exposure assessment study will help the epidemiologists assess how well ambient measurements can represent personal exposures for groups of individuals with recent heart attacks and with chronic obstructive
pulmonary disease. This information may also have applications in validation of personal exposure models. The health study will also examine any association between exposure and cardiac response (heart rate variability, electrocardiogram morphology, and symptoms) for these participants.

The first phase of field monitoring for ARIES began in July 1998 and ended in August 2000. ARIES is therefore one of the few studies that will be in a position to provide valuable new monitoring and health data in time for EPA’s review of the PM standard. EPA selected Atlanta as its first designated ‘Supersite’ and conducted an intensive one-month experiment at the ARIES site in August 1999. The cooperative structure of ARIES allows for and fosters collaboration with EPA in integrating these private and public sector experiments.
5. Assessment of Spatial Aerosol Composition in Atlanta (ASACA). This urban-focused PM$_{2.5}$ characterization study is designed to provide further understanding of spatial variability in PM mass and chemical composition in the Atlanta metropolitan area. It was designed to augment and strengthen the data available from both the SEARCH regional and ARIES epidemiological studies from the standpoint of spatial variability. The ASACA program is led by Ted Russell of Georgia Tech with very effective implementation by Andre Butler, who completed the first-year analyses from the four ASACA sites (see Figure 1.6.) for his Ph.D. dissertation in May 2000. The sample collection and analysis methods used in ASACA were very similar to those used in SOS-SCISSAP. Thus detailed records are available for all months of the year for PM$_{2.5}$ mass, sulfate, ammonium, and both elemental and organic carbon. Funding for ASACA is provided by the Georgia Power Company.

Figure 1.6. Measurement sites in ASACA study.
6. Fall Line Air Quality Study (FAQS). This detailed study of three "near-non-attainment" cities in Georgia was initiated in 1999 under the leadership of Michael Chang of Georgia Tech for a 3-year period extending from 1999 through 2002. Chang completed his doctoral dissertation with SOS support in 1994-96. As shown in Figure 1.7, the three cities in question – Augusta, Macon, and Columbus – are arrayed from east to west across the state of Georgia along the so-called Fall Line which divides the Coastal Plain from the Piedmont regions of the state. Funding for this study is provided by a special appropriation from the state legislature. Ozone and PM$_{2.5}$ monitoring sites were established both within the urban core and in nearby rural areas adjacent to each city. The principal scientific objective of the FAQS study is to determine the comparative influence of regional and local sources of ozone and PM$_{2.5}$ precursors in each city. The principal air-quality management objective of FAQS is to determine what practical steps each of these near-non-attainment cities could take to retain their present ozone non-attainment status.

![Image of measurement sites in Fall Line Air Quality Study](image-url)

Figure 1.7. Measurement sites in Fall Line Air Quality Study.
1.5. SOS PARTICIPATING INSTITUTIONS, ORGANIZATIONS, INVESTIGATORS, AND MAJOR STAKEHOLDERS

Appendix B lists the institutions, organizations, and the scientists, engineers, graduate students, and postdocs that provide the intellectual leadership and accomplish the detailed research tasks of the SOS research and assessment program. Also included are the names of representatives of some of the more important stakeholder groups with which SOS scientists have interacted during 1994-2000.
1.6. SOS DATA ARCHIVES, WEBSITE ON THE INTERNET, AND PUBLICATIONS POLICIES AND TRADITIONS

1.6.1. SOS Data Archives

Data from the Nashville/Middle Tennessee Ozone Study are archived in a database maintained by Ken Shere and Shawn Roselle at EPA's National Exposure Research Laboratory in Research Triangle Park, NC. Beginning in 1999, the SOS Science Team made the decision that data from all SOS studies and as many as possible of SOS-affiliated research efforts would be archived in the NARSTO Data Archive and Quality Assurance System maintained by Les Hook, Sigurd Christensen, and Meng-Dawn Cheng of the Oak Ridge National Laboratory (ORNL).

1.6.2. SOS Web Site on the Internet

During 1999-2000, Cari Furiness in the SOS Office of the Director made considerable progress in updating the SOS web site on the Internet. The SOS web site – [http://www2.ncsu.edu/ncsu/CIL/southern_oxidants/](http://www2.ncsu.edu/ncsu/CIL/southern_oxidants/) currently contains general SOS information, including newsletters and workshop announcements and

1. Electronic linkages to the SOS data archives maintained by Ken Schere and Shawn Roselle at EPA/NERL and by the NARSTO Data Archive and Quality Assurance System maintained by Les Hook, Sigurd Christensen, and Meng-Dawn Cheng of the Oak Ridge National Laboratory (ORNL);

2. Links to the Archive of SOS Publications within the NCSU Air Quality Library;

3. Information on the objectives, current status, and electronic linkages to SOS-affiliated research including:
   - SOS' Southern Center for Integrated Assessment of Secondary Air Pollutants (SCISSAP),
   - EPRI's regionally focused Southeastern Aerosol Research and Characterization (SEARCH) study,
   - EPRI's epidemiologically-focused Aerosol Research Inhalation Epidemiological Study (ARIES),
   - EPRI's urban-focused Assessment of Spatial Aerosol Composition in Atlanta (ASACA).

Our intention in the future is to increase the value and completeness of information on the SOS website so that prospective users of SOS data, information, and perspectives can meet many
of their needs through the SOS webpages. These information resources should eventually include:

1. Information on the objectives, current status, and electronic linkages to current products of other SOS-affiliated research studies such as:
   - The Tennessee Valley PM$_{2.5}$ Partnership Network, and
   - The Fall Line Air Quality Study (FAQS), and

2. Descriptions of "SOS Perspectives" on such issues as:
   - Means by which to achieve high-quality field measurement programs,
   - Means by which to improve emissions inventories for biogenic and anthropogenic sources of precursors for both PM$_{2.5}$ and ozone,
   - Awareness of the extent of regionality of the PM$_{2.5}$ and ozone management problems, and
   - Awareness of the strengths and limitations of emissions-based and observation-based air quality models for PM$_{2.5}$ and ozone.

3. Better electronic access to SOS data and publications.

1.6.3. SOS Publications Policy

In January 1992, the following policy on sharing, reviewing, and distribution of information from the Southern Oxidants Study was adopted by the SOS Coordinating Council. In addition, SOS scientists are encouraged to use the following Guidelines for the Formulation of Scientific Findings to be used for Policy Purposes in creating statements that synthesize their research results.
THE SOUTHERN OXIDANTS STUDY POLICY ON SHARING, REVIEW AND DISTRIBUTION OF INFORMATION

SOS information is intended for the use and beneficial application by the participants, policy makers, and the general public to further advance the state of scientific and technical knowledge regarding the formation of ambient ozone [and particulate matter].

The policy set forth herein is designed to recognize all existing agreements between sponsor and investigator; foster free exchange of information among participants; avoid debilitating controversy within SOS; and provide all participants with opportunities to review and comment on relevant materials.

Information is defined as data, papers for publication, promotional materials, press releases, intellectual property, and all internal and external program reports and public outreach program communications.

Data

These would initially exist at two levels. Level I data are typically initial observations and data products that have not been officially checked and validated, but may be useful in providing preliminary consolidated data sets for interpretative and diagnostic analysis by participants. These data are generally not approved for public release. Level II data contain the official data and operational archives of SOS.

Distribution

Level I Data: may be distributed only within participant and co-investigator groups in response to a request or as part of an initial automatic distribution approved by a project oversight committee or the Coordinating Council. All data shall be made available to participants no later than 12 months after their collection. Recipients of these data are expected to proactively participate in the quality control of the data. They may make free use of these data in their work. However, prior to reporting any findings of fact, or opinion, based upon these data, the recipient must submit such reports to the data supplier for review and comment.

Level II Data: data contained in the SOS official data and operational archives have been approved for public release by the Coordinating Council. All data shall be finalized and approved as Level II data within 18 months of collection and submitted to the appropriate SOS archive. These data may be released upon request. Distribution will normally be effected through the SOS Management Center or appropriate Data Management Center.

Papers for Publication

The principal author of said papers shall have the responsibility for seeking comments of affected program participants with respect to proposed publication. Other participants shall be informed of the availability of proposed paper by the SOS Management Center and may comment directly to the author, if desired. Comments will be solicited concurrently with submission for publication.
Promotional Materials and Press Releases

Each participant is free to promote individual research efforts. However, when the work of another organization is entrained within that research, or when attribution is ascribed, or the name of another entity evoked; comment and approval must be solicited from these later entities prior to release or publication of the information.

Intellectual Property

The rights to intellectual property shall be governed by existing patent, copyright, contract and federal law and in accordance with any memoranda of agreement of understanding in force.

Internal and External Reports

Internal reports will be distributed only among participants. A copy will be kept on file at the SOS Management Center and made available upon request to program participants. External reports are those that summarize, integrate, and/or interpret SOS results and are meant for public distribution. Such reports will first be reviewed and approved for release by the appropriate Program or Executive Committee and the Coordinating Council.

Regulatory Agencies

Regulatory agencies operating air monitoring sites which provide data to SOS are not limited as to when hourly averaged criteria pollutant data can be released to the public or reported as required by regulation.

Approval

This policy statement has been thoroughly reviewed by the Coordinating Council and program participants. It is hereby accepted and approved as the Southern Oxidants Study official Policy on Sharing, Review, and Distribution of Information.

[Signed]

Robert H. Collom, Jr.
Chairman, Coordinating Council
January 1, 1992
GUIDELINES FOR THE FORMULATION OF SCIENTIFIC FINDINGS
TO BE USED FOR POLICY PURPOSES

The following guidelines in the form of checklist questions were developed by the NAPAP Oversight Review Board to assist scientists in formulating presentations of research results to be used in policy decision processes.

1) **IS THE STATEMENT SOUND?** Have the central issues been clearly identified? Does each statement contain the distilled essence of present scientific and technical understanding of the phenomenon or process to which it applies? Is the statement consistent with all relevant evidence-evidence developed either through NAPAP or SOS research or through analysis of research conducted outside of NAPAP or SOS? Is the statement contradicted by any important evidence developed through research inside or outside of NAPAP or SOS? Have apparent contradictions or interpretations of available evidence been considered in formulating the statement of principal findings?

2) **IS THE STATEMENT DIRECTIONAL AND, WHERE APPROPRIATE, QUANTITATIVE?** Does the statement correctly quantify both the direction and magnitude of trends and relationships in the phenomenon or process to which the statement is relevant? When possible, is a range of uncertainty given for each quantitative result? Have various sources of uncertainty been identified and quantified, for example, does the statement include or acknowledge errors in actual measurements, standard errors of estimate, possible biases in the availability of data, extrapolation of results beyond the mathematical, geographical, or temporal relevancy of available information, etc. In short, are there numbers in the statement? Are the numbers correct? Are the numbers relevant to the general meaning of the statement?

3) **IS THE DEGREE OF CERTAINTY OR UNCERTAINTY OF THE STATEMENT INDICATED CLEARLY?** Have appropriate statistical tests been applied to the data used in drawing the conclusion set forth in the statement? If the statement is based on a mathematical or novel conceptual model, has the model or concept been validated? Does the statement describe the model or concept on which it is based and the degree of validity of that model or concept?

4) **IS THE STATEMENT CORRECT WITHOUT QUALIFICATION?** Are there limitations of time, space, or other special circumstances in which the statement is true? If the statement is true only in some circumstances, are these limitations described adequately and briefly?

5) **IS THE STATEMENT CLEAR AND UNAMBIGUOUS?** Are the words and phrases used in the statement understandable by the decision makers of our society? Is the statement free of specialized jargon? Will too many people misunderstand its meaning?

6) **IS THE STATEMENT AS CONCISE AS IT CAN BE MADE WITHOUT RISK OF MISUNDERSTANDING?** Are there any excess words, phrases, or ideas in the statement which are not necessary to communicate the meaning of the statement? Are there so many caveats in the statement that the statement itself is trivial, confusing, or ambiguous?

7) **IS THE STATEMENT FREE OF SCIENTIFIC OR OTHER BIASES OR IMPLICATIONS OF SOCIETAL VALUE JUDGMENTS?** Is the statement free of influence by specific schools of scientific thought? Is the statement also free of words, phrases, or concepts that have political, economic, ideological, religious, moral, or other personal-, agency-, or organization-specific values, overtones, or implications? Does the choice of how the statement is expressed rather than its specific words suggest underlying biases or value judgments? Is the tone impartial and free of special pleading? If societal value judgments have been discussed, have these judgments been identified as such and described both clearly and objectively?

8) **HAVE SOCIETAL IMPLICATIONS BEEN DESCRIBED OBJECTIVELY?** Consideration of alternative courses of action and their consequences inherently involves judgments of their feasibility and the importance of effects. For this reason, it is important to ask if a reasonable range of alternative policies or courses of action have been evaluated? Have societal implications of alternative courses of action been stated in the following general form?:

"If this [particular option] were adopted then that [particular outcome] would be expected."

9) **HAVE THE PROFESSIONAL BIASES OF AUTHORS AND REVIEWERS BEEN DESCRIBED OPENLY?** Acknowledgment of potential sources of bias is important so that readers can judge for themselves the credibility of reports and assessments.
1.6.4. SOS Traditions Regarding Publication of Scientific Findings and Communication with Stakeholders

Most important scientific findings from SOS and SOS-affiliated research activities evolve gradually from hypotheses shared at SOS planning meetings, through insights (and surprises) developed and first shared with colleagues in our own institutions, and then with other colleagues during SOS Data Analysis Workshops. Agreements for joint authorship often are negotiated at these Workshops and lead to submission of abstracts for verbal presentations or posters in SOS Special Sessions at scientific meetings, such as the 1996 and 2000 Annual Meetings of the AGU and the Fall Meeting of the AAAR. Further refinements in data analysis and comparison with results of other measurements in SOS and other publicly accessible data sets are made in preparing manuscripts for submission to refereed journals. Papers on closely related topics often are grouped together and then published sequentially in SOS Special Sections of journals – such as the September 1998 and April 2000 issues of the Journal of Geophysical Research-Atmospheres.

As shown in Appendix A, about 80 refereed journal papers were published by SOS authors prior to 1995 and about 200 more between 1995 and 2000. In addition, nearly 500 abstracts, posters, and verbal presentations of SOS findings have been made at scientific meetings in this country and abroad. Mainly during the past five years, several policy-focused briefings by SOS scientists and engineers have been requested by various stakeholder groups including state, regional, federal, industrial, university, and public interest groups concerned with air quality issues.

Policy-relevant scientific findings from SOS and SOS-affiliated research activities also have been described in four major SOS summary reports:

- SOS Data Analysis Workshop Report (Fehsenfeld et al., 1993)
- The first Compendium of scientific papers from the SOS Nashville/Middle Tennessee Ozone Study (American Geophysical Union, 1999)
1.6.5. SOS Publications Archive

The SOS Publications Archive is maintained by Phyllis Garris, Librarian, at the Air Quality Library at North Carolina State University. It contains hard (paper) copies of reprints of essentially all publications from the SOS research and assessment program, copies of all the SOS summary publications listed above, and an Internet-accessible list of all refereed journal publications, titles, and copies of abstracts for presentations at scientific meetings, drafts of many manuscripts submitted for publication, and copies of briefing documents prepared by SOS scientists and engineers for various stakeholder groups.

As shown by the categorized lists of publications cited below, SOS investigators have produced refereed journal publications in 18 subject matter categories of ozone pollution research. The full references for all citations in the following list are presented in Appendix A. The references cited below are arranged first chronologically and then alphabetically by first author.

1. **Climatology of Ozone** (Aneja et al., 1992; Pielke et al., 1992; McNider et al., 1993; Sillman and Samson, 1993; Chameides, 1994; Vukovich, 1994; Pielke et al., 1995a, 1995b; Sillman and Samson, 1995; Marsik et al., 1995; Nowacki et al., 1996; Gupta et al., 1997; Pielke et al., 1997; Vukovich, 1998; Aneja et al., 2000);

2. **Meteorological factors affecting ozone** (Pielke et al., 1992; Angevine et al., 1993a, 1993b; McNider et al., 1993; Sillman and Samson, 1993; Singh et al. 1993; Angevine et al., 1994a, 1994b; Berkowitz et al., 1994; Len et al., 1994; Eastman et al., 1995; Sillman and Samson, 1995; Vukovich, 1995; Al-Wali and Samson, 1996; Gupta et al., 1997; Olszyna et al., 1997; Vukovich, 1997; McNider et al., 1998; White et al., 1999a, 1999b; Herwehe, 2000; Neff et al., 2000);

3. **Vertical distribution of ozone and precursors** (Cantrell et al., 1992; Andronache et al., 1994; Lawrimore et al., 1995; Aneja et al., 2000);

4. **Evaluations of measurement methods** (Williams and Fehsenfeld, 1991; Alvarez et al., 1993; Lee et al., 1993; Lee and Zhou, 1993; Cantrell et al., 1993; Apel and Calvert, 1994a, 1994b; Das and Aneja, 1994a, 1994b; Farmer et al., 1994; Lee and Zhou, 1994; Lee et al., 1993, 1994; Riemer et al., 1994; Buhr et al., 1995; Lee et al., 1995; Lee et al., 1996; Fischer et al., 1995; Weinstein-Lloyd and Lee, 1995; Apel et al., 1995; Bernado-Bricker et al., 1995; Buhr et al., 1995b; Oliver et al., 1996a, 1996b; Gilpin et al., 1997; Alvarez et al., 1998; Apel et al., 1998a; 1998b; Daughtrey et al., 1998; Luke et al., 1998; Parrish et al., 1998; Tanner et al., 1998; Williams et al., 1998; Apel et al., 2000; Li and Dasgupta, 2000; Parrish and Fehsenfeld, 2000);

5. **Emissions inventories** (Pierce and Woodruff, 1991; Fujita et al., 1992; Williams et al., 1992; Graedel et al., 1993; Geron et al., 1995; Monson et al., 1995; Geron et al., 1996; Klouda et
6. **Biogenic NO\textsubscript{x} emissions from soils** (Williams and Fehsenfeld, 1991; Williams et al., 1992; Meyers and Baldocchi, 1993; Valente and Thornton, 1993; Kim et al., 1994; Buhr et al., 1995; Valente et al. 1995; Potter et al., 1996; Thornton and Shurpali, 1996; Thornton et al., 1997; Davidson and Kingerlee, 1997; Potter et al., 1997);

7. **Lightning as an NO\textsubscript{x} source** (Biazar and McNider, 1995; Lawrence et al., 1995);

8. **Biogenic VOC emissions** (Chameides et al., 1988; Monson and Fall, 1989; Pierce and Waldruff, 1991; Delwiche and Sharkey, 1993; Guenther et al., 1993; Kuzma and Fall, 1993; Loreto and Sharkey, 1993a; Loreto and Sharkey, 1993b; Sharkey and Loreto, 1993; Montzka et al., 1993; Geron et al., 1994; Geron et al., 1995; Guenther et al., 1994; Harley et al., 1994; Monson et al., 1994; Goldan et al., 1995; Guenther et al., 1995a; 1995b; Monson et al., 1995; Montzka et al., 1995; Chang et al., 1996; Fang et al., 1996; Guenther et al., 1996; Harley et al., 1996; Wildermuth and Fall, 1996; Hagerman et al., 1997; Potter, 1997; Reimer et al., 1998; Wildermuth and Fall, 1996; Geron et al., 1997; Harley et al., 1997; Guenther, 1997; Helmig et al., 1998; Starn et al., 1998; Lewis et al.,1999; Guenther et al., 2000);

9. **Motor vehicle emissions** (Pierson et al., 1990; Sillman and Samson, 1990; Cadle et al., 1991; Bradow, 1992; Bishop et al., 1993; Bishop et al., 1994; Gertler and Pierson, 1994; Henry et al., 1994; Conner et al., 1995; LeBlanc et al., 1995; Bishop et al., 1996; Pierson et al., 1996; Gertler et al., 1996; Cardelino, 1998; Gertler et al., 1996; Robinson et al.,1996; Sagebiel et al., 1996; Zielinska et al., 1996);

10. **Chemical transformation processes** (Lindsay and Chameides, 1988; Sillman and Wolfsy, 1990; Hisham and Grosjean, 1991; Chameides and Lodge, 1992; Chameides et al., 1992; Cantrell et al., 1992; Cantrell et al., 1993; Lee et al., 1993; Grosjean et al., 1993a, 1993b, 1993c, 1993d, 1993e, 1993f; Casado et al., 1994; Grosjean et al., 1994; Lee and Zhou, 1993; Montzka et al., 1993; Trainer et al., 1993; Williams et al., 1993; Aneja et al., 1994; Lee and Zhou, 1994; Milford et al., 1994; Olszyna et al., 1994; Pouliota et al., 1994; Hartsell et al., 1994; Kleinman, 1994; Kleinman et al., 1994; Aneja and Das, 1995; Bertman et al., 1995; Duncan et al., 1995; Buhr et al., 1995; Goldan et al., 1995; Imhoff et al.,1995; Kleinman et al., 1995; Lee et al., 1995; Montzka et al., 1995; Roberts et al., 1995; Sillman, 1995a, 1995b; Trainer et al., 1995; Watkins et al., 1995; Aneja et al., 1996; Aneja et al., 1997; Berkowitz and Shaw, 1997; Hagerman et al., 1997; Kleinman et al., 1997; Williams et al., 1997; Frost et al., 1998; Jobson et al., 1998; Weinstein-Lloyd et al., 1998; Helmig et al., 1998; Lee et al., 1998; McClenny et al., 1998; Nouaim et al., 1998; Olszyna et al., 1998; Riemer et al., 1998; Roberts et al., 1998; Starn et al., 1998a, 1998b; St. John et al., 1998; Aneja et al., 1999; Sillman, 1999; Baumann et al., 2000; Daum et al., 2000a; Daum et al., 2000b; Goldan et al., 2000; Imhoff et al., 2000; McMillen et al., 2000; Sillman, 2000a; Sillman, 2000b; Stroud, 2000);

11. **Urban plume studies** (Aneja et al., 1992; Sillman et al., 1993; Williams et al., 1993; Duncan et al., 1995; Trainer et al., 1995; Banta et al., 1998; Kleinman et al., 1998; Nunnermacker et al., 1998; Valente et al., 1998; Daum et al., 2000a; Daum et al. 2000b; Nunnermacker et al., 2000; St. John and Chameides, 2000);
12. **Power plant plume studies** (Chang et al., 1996; Gillani et al., 1998a; Gillani et al., 1998b; Jobson et al., 1998; Ryerson et al., 1998; Senff et al., 1998; Luria et al., 2000; Nunnermacker et al., 2000; St. John and Chameides, 2000; Nunnermacker et al., 2000);

13. **Observation based modeling** (Lin and Milford, 1994; Cardelino and Chameides, 1995; Aneja et al., 2000; Cardelino and Chameides, 2000; Kleinman, 2000; Trainer et al., 2000);

14. **Other modeling studies** (Middleton et al., 1993; Sillman and Samson, 1993; Lin and Milford, 1994; Lin et al., 1994; Nicholls et al., 1995; Rozelle and Schere, 1995; Sillman et al., 1995; Zaveri et al., 1995; Al-Wali and Samson, 1996; Nowacki et al., 1996; Kasibhatla et al., 1997; Sillman et al., 1997; Kasibhatla et al., 1998; Meyers et al., 1998; Sillman et al., 1998; Houyoux et al., 2000; Karamchandani et al., 2000; Kasibhatla and Chameides, 2000; Russell and Dennis, 2000; Sillman, 2000);

15. **Indicator species studies** (Sillman, 1993; Milford et al., 1994; Kleinman et al., 1994; Kleinman et al., 1995; Sillman, 1995a; Sillman, 1995b; Kleinman et al., 1997; Sillman et al., 1997; Sillman, 1999; Tonneson and Dennis, 2000a; 2000b);

16. **Ozone management studies** (Aneja et al., 1999; Lindsay and Chameides, 1988; Lindsay et al., 1989; Sillman et al., 1989; Cardelino and Chameides, 1990; Trainer et al., 1993; Chameides et al., 1994; Cowling and Nilsson, 1996; Chameides et al., 1997; Heck and Cowling, 1997; Cowling et al., 1998; Heck et al., 1998; Saylor et al., 1998; Vukovich et al., 1999; Solomon et al., 1999; Hidy et al., 2000; Solomon et al., 2000).

17. **Ozone effects studies** (Heck et al., 1997, 1998);

18. **Characterization of PM$_{2.5}$** (Tanner and Parkhurst, 2000; von Salen et al., 2000).
1.7. **FINANCIAL AND IN-KIND SUPPORT FOR SOS AND SOS-AFFILIATED RESEARCH PROGRAMS**

During the past several years, the total costs of SOS research and assessment activities have been distributed among SOS' principal sponsoring organizations as follows:

- about $2 to $3 million per year in direct financial support and in-kind services from NOAA,
- about $1 million per year in direct financial support and in-kind services from DOE,
- about $500,000 to $1 million per year in direct support and in-kind services from TVA,
- about $1 million per year in cost sharing contributions by the SOS cooperating universities,
- about $1 million per year in 1999-2001 in direct financial support for SOS' Southern Center for Integrated Study of Secondary Pollutants (SOS-SCISSAP) by EPA's competitive grants program (EPA/NCERQA),
- about $1.4 million in 1999-2000 from EPA's Office of Air Quality Planning and Standards for SOS operation of the EPA "Initial Superset" in and around Atlanta, Georgia,
- about $1.5 million per year in in-kind services from EPA/NERL,
- about $800,000 per year in direct financial support from EPA/NERL through SOS' Cooperative and Interagency Agreements,
- about $200,000 per year in direct financial support over two years for SOS' Seasonal Model for Regional Air Quality (SOS-SMRAQ) from the eight states of the Southeastern Regional Air Resource Managers (SESARM),
- about $2 million in direct financial support and about $1 million in in-kind support from the TNRCC for the TEXAQS 2000 in 2000, for an approximate total of

**about $8 to $10 million per year in support of SOS research and assessment activities.**

In addition, in close cooperation with SOS and SOS-SCISSAP, Southern Company, other electric utilities, and EPRI have developed a series of SOS-Related research efforts that have greatly complemented and enhanced SOS and SOS-SCISSAP research and assessment efforts. These SOS-related studies include EPRI's regionally focused Southeastern Aerosol Research and Characterization (SEARCH) study (which is very closely coupled with SOS-SCION and SOS-SCISSAP), its epidemiologically-focused Aerosol Research Inhalation Epidemiological Study (ARIES), its urban-focused Assessment of Spatial Aerosol Composition in Atlanta (ASACA), and cooperative studies within the Tennessee Valley PM$_{2.5}$ Partnership Network. Thus, through its Tailored Collaboration Group (matching funds) program, the utilities and EPRI are currently providing:

**about $2 to $4 million per year for SOS-affiliated research and assessment activities.**

Also, during 1999-2001, in close cooperation with SOS scientists at Georgia Tech, the state of Georgia is investing in the Fall Line Air Quality Study (FAQS) **about $1 million per year for SOS-affiliated research and assessment activities.**

Thus, the total investments by public-sector and private sector organizations for SOS and SOS-affiliated research and assessment activities is about $11 to $15 million per year.
2. MAJOR SCIENTIFIC FINDINGS OF SOS: 1994-2000

At the time this second State of the Southern Oxidants Study report was being prepared, the research projects and field measurement campaigns and other SOS research and assessment activities were in their 12\textsuperscript{th} year. Since the inception of SOS in 1988, these programs resulted in publication of nearly 300 refereed journal papers, 39 Ph.D. dissertations and masters theses, and about 500 nonrefereed publications and presentations at scientific and professional meetings, conferences, and symposia in this country and abroad. About 200 of these peer reviewed papers, 13 additional disserations and theses, and about 200 additional nonrefereed publications were produced since 1994, when the First State of the Southern Oxidants Study report was prepared (Chameides and Cowling, 1995). A complete list of these papers is included in Appendix A.

In this section, major scientific findings in SOS and SOS-affiliated research programs are presented. With the exception of the "initial impressions" summarized in Section 2.10, this summary is based largely on peer-reviewed publications published between 1994 and 2000.
2.1. NATIONAL AND REGIONAL OZONE AIR QUALITY TRENDS, 1980-1999
William F. Hunt, Jr. and Fred Vukovich

How do we determine whether or not environmental improvement in the air is taking place? How do we take millions of hourly ozone measurements and turn them into environmental information to help decision-makers properly direct and focus the National and State air pollution control programs in the United States? For the past 25 years, the United States Environmental Protection Agency has evaluated the trends and status of the Nation’s air quality and has published the results in an annual report (USEPA, 2000). Both ambient measurements collected across the United States and emission trends, based upon engineering estimates, have been examined, focussing on the 20-year trend between 1980 and 1999 and the 10-year period between 1990 and 1999.

Progress in measuring the effectiveness of the air pollution control program is based upon examining the trends in both ambient air quality measurements and emission inventory data. Ozone is not emitted directly into the air, but is formed by the reaction of volatile organic compounds (VOCs) and nitrogen oxides (NOx) in the presence of heat and sunlight. VOCs are emitted from motor vehicles, chemical plants, refineries, factories, consumer and commercial products, and other industrial sources. Nitrogen oxides are emitted from motor vehicles, power plants, and other sources of combustion. Ozone is effected by the weather – hotter summers produce more exceedances of the ozone standard. Ozone and the precursor pollutants that cause ozone can be transported into an area from pollution sources found hundreds of miles upwind.

KEY CITATION:
2.1.1. National Ambient Air Quality Standards for Ozone

Ground level ozone has remained a pervasive pollution problem throughout the United States. Short-term (1-3 hours) and prolonged (6-8 hours) exposures to ambient ozone have been linked to a number of health effects of concern (USEPA, 1996). Table 2.1.1 summarizes the one-hour and 8-hour ozone standards. The daily maximum one-hour ozone standard requires that the expected number of days per calendar year with daily maximum hourly concentrations exceeding 0.12 parts per million (ppm) be less than or equal to one. The new daily maximum 8-hour average standard for ozone is defined as a 3-year average of the annual fourth highest daily maximum 8-hour average ozone values and must be less than or equal to 0.08 ppm.

Table 2.1.1. National Ambient Air Quality Standards for Ozone

<table>
<thead>
<tr>
<th>Primary (Health Related)</th>
<th>Secondary (Welfare Related)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of Average</td>
<td>Standard Level Concentrationa</td>
</tr>
<tr>
<td>1-hour b</td>
<td>0.12 ppm (235 µg/m³)</td>
</tr>
<tr>
<td>8-hour c</td>
<td>0.08 ppm (157 µg/m³)</td>
</tr>
</tbody>
</table>

a. Parenthetical value is an approximately equivalent concentration.
b. Not to be exceeded more than once per year on average.
c. 3-year average of annual 4th highest concentration.

The health and welfare related NAAQS(s) apply to all of our 50 States and must be achieved. Each state is required to submit a State Implementation Plan, which specifies a plan as to how each state will reduce air pollution in order to achieve the NAAQS(s). The Federal government implements a series of programs to help achieve the NAAQS(s). These programs include:

- new source performance standards for all major categories of polluting facilities;
- emission limit standards for mobile and stationary sources;
- the prevention of significant deterioration rules, the cornerstone of which is a process known as New Source Review (NSR);
- control technique guidelines for controlling air pollutants from specific industries; and
- other regulations in order to reduce air pollution emissions.

The question to ask is: "How well does the air pollution control program work, given all these control measures?"

KEY CITATION:

2.1.2. Available Ozone Monitoring Data

The ambient air quality concentrations are based upon actual measurements of pollutant concentrations. These measurements are made at monitoring sites across the United States. Emission estimates are calculated from the total tonnage of these pollutants, or their precursors, released into the air annually. [Emission estimates are derived from many factors, including the level of industrial activity, technology changes, fuel consumption; vehicle miles traveled (VMT), and other activities that affect air pollution. In 1994, EPA began incorporating direct emission measurements of sulfur dioxide and nitrogen oxides for the electric utility industry. Additional emissions information can be found at [http://www.epa.gov/oar/oaqps/efig](http://www.epa.gov/oar/oaqps/efig).

Air quality monitoring in the United States is largely conducted by state and local air pollution control agencies. In 1999, there were 705 ozone trend sites meeting the 10-year trend criteria. The trend sites were selected as national trend sites if they have complete data for at least eight of the ten years either between 1980 and 1989 or 1990 and 1999. The annual data completeness criteria for ozone require that at least 50 percent of the hours must be collected during ozone season. Because only a few sites have monitored continuously for two decades (1980-1999), the ozone trend line is composed of two segments – 441 sites with complete data for the first ten years (1980-1989) and 705 sites meeting the criteria in the most recent 10 year period.

Air monitoring sites are identified as National Air Monitoring Stations (NAMS), State and Local Air Monitoring Stations (SLAMS), Photochemical Assessment Monitoring Stations (PAMS) or other. NAMS were established to assess national policy decisions and trends. The SLAMS were used for the same purposes, but were tailored for the State's immediate monitoring needs. The principal purpose of the PAMS is to improve the monitoring of ozone and its precursor pollutants—NOx and VOCs—to make better national policy decisions (Hunt and Gerald, 1991). The PAMS objectives are to: evaluate control strategies, corroborate volatile organic compound and nitrogen oxide emission inventories, evaluate photochemical grid models, corroborate ozone attainment decisions, determine ozone, VOC and NOx trends, characterize VOCs, and assess the risk to ozone and selected air toxic pollutants.

**KEY CITATION:**

2.1.3. Trends in Ozone Concentrations

Over the past 20 years (1980-1999), ambient ozone levels have decreased 20 percent based upon one-hour and 12 percent based upon 8-hour data (USEPA, 2000a) (Figures 2.1.1 and 2.1.2). Between 1980 and 1999, emissions of VOCs have decreased 33 percent (Figure 2.1.3). During that same period, emissions of NO\textsubscript{x} increased one percent.
Ambient ozone trends are influenced by year-to-year changes in meteorological conditions, population growth, volatile organic compound to nitrogen oxides ratios, and changes in emissions from ongoing control measures. To better reflect the changes that emissions have on measured air quality trends, a method can be used to remove the effects of meteorological conditions when assessing ozone trends (NRC, 1991; Bloomfield et al., 1993). Previous Trends Reports have discussed an EPA statistical model developed by Cox and Chu (1993). Their model is based upon the Weibull probability distribution. It attempts to account for meteorological effects and helps to normalize the resulting trend estimates across years. The model, applied on an individual metropolitan area basis, includes a trend component that adjusts the annual rate of change in ozone for concurrent impacts of meteorological conditions, including surface temperature and wind speed. Figure 2.1.4 shows the model results for the 8-hour trends statistics averaged over 53 metropolitan areas.
While the ambient monitoring data reflect the year-to-year variability in ozone-conducive conditions, the meteorologically adjusted ozone trend provides a better indicator of the impact of emission changes. For 53 metropolitan areas, the meteorologically adjusted ozone trend for one-hour ozone levels shows continued improvement from 1980 through the mid-1990s. The adjusted ozone levels decreased an average of 1 percent per year through 1994. However, beginning in 1994, the improvement appears to slow.

An examination of geographical areas (Figure 2.1.5) shows a downward trend for each region of the country for the 2nd highest daily maximum one-hour O₃ level over the 20-year period, 1980-99. The Northeast and West show the greatest improvement, while the South shows the least progress.

Figure 2.1.5. Regional trend in one-hour ozone levels in each of the ten EPA Regions, 1980-99 (from USEPA, 2000).

Table 2.1.2 contrasts the 20-year and 10-year ozone trends geographically. EPA reported in its 1998 Trends Report (USEPA, 2000b) that for both the one and 8-hour ozone measurements, ozone trends increased in the Mid-Atlantic, Southeast, Central and Northwest from 1989 to 1998. The South Central States (TX, NM, OK, AR and LA) show a 3 percent decrease in the 2nd highest daily maximum one hour level and an increase of 2 percent in the 4th highest daily maximum 8-hour average. The highest increase occurred in the Southeast. The 4th highest daily maximum 8-hour average increased 17 percent, while the 2nd highest daily maximum one-hour average ozone data increased 13 percent. Overall, all Regions of the country show a decrease over the 20 year period, while four of the Regions show an increase over the 10 year period for
the daily maximum one hour values and 6 Regions show an increase in the 4th highest daily maximum 8-hour averages.

Table 2.1.2. Comparison of 20-year (1980-89) and 10-year (1989-98) ozone trends by EPA Region and Nationally.

<table>
<thead>
<tr>
<th>EPA Region</th>
<th>20 Year Trend 1980-99 2nd Highest Daily Max 1-Hour O3 Level</th>
<th>10 Year Trend 1989-98 2nd Highest Daily Max 1-Hour O3 Level</th>
<th>10 Year Trend 1989-98 4th Highest Daily Max 8-Hour O3 Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Region 1 New England</td>
<td>30% decrease</td>
<td>12% decrease</td>
<td>9% decrease</td>
</tr>
<tr>
<td>Region 2 NJ, NY, PR</td>
<td>18% decrease</td>
<td>6% decrease</td>
<td>5% decrease</td>
</tr>
<tr>
<td>Region 3 PA, MD, DE, &amp; VA</td>
<td>10% decrease</td>
<td>6% increase</td>
<td>9% increase</td>
</tr>
<tr>
<td>Region 4 Southeast</td>
<td>6% decrease</td>
<td>13% increase</td>
<td>17% increase</td>
</tr>
<tr>
<td>Region 5 Great Lakes</td>
<td>12% decrease</td>
<td>3% decrease</td>
<td>1% decrease</td>
</tr>
<tr>
<td>Region 6 South Central</td>
<td>15% decrease</td>
<td>3% decrease</td>
<td>2% increase</td>
</tr>
<tr>
<td>Region 7 Midwest</td>
<td>15% decrease</td>
<td>8% increase</td>
<td>5% increase</td>
</tr>
<tr>
<td>Region 8 Rocky Mountain</td>
<td>16% decrease</td>
<td>2% decrease</td>
<td>3% increase</td>
</tr>
<tr>
<td>Region 9 CA, AZ, NV</td>
<td>37% decrease</td>
<td>18% decrease</td>
<td>12% decrease</td>
</tr>
<tr>
<td>Region 10 Northwest</td>
<td>23% decrease</td>
<td>16% increase</td>
<td>11% increase</td>
</tr>
<tr>
<td>National Trend</td>
<td>20% decrease</td>
<td>4% decrease</td>
<td>No Change</td>
</tr>
</tbody>
</table>

Across the nation there has been little progress over the past ten years – a 4 percent decrease in the 2nd highest daily maximum one-hour O3 value and “no change” in the 4th highest daily maximum 8-hour average. One might expect that the percent increase or decrease in the 2nd highest daily maximum one hour statistic by Region and for the Nation would be greater than the percent increase or decrease for 4th highest daily maximum 8-hour average. This is expected because the ozone level for the daily maximum one-hour standard is further away from the natural background level than the level of the 8-hour standard. Among the Regional trends, 6 out of 10 regions show a decrease in the 2nd highest daily maximum one hour average versus 4 out of 10, which show a decrease in the 4th highest daily maximum 8-hour average over the past 10
years. Clearly, the trend in Regions 6 and 8 are probably too close to call, because they show both a slight decrease in the 2nd highest daily maximum one-hour statistic and a slight increase in the 4th highest daily maximum 8-hour average over the ten year period, 1989-98.

Over the last 10 years (1990-99), 8-hour ozone levels in 25 of our national parks increased nearly 8 percent. EPA (2000a) reports that nine monitoring sites in eight of these parks experienced statistically significant upward trends in the 8-hour ozone levels. The parks are Great Smoky Mountain (TN), Big Bend (TX), Cape Romain (SC), Cowpens (SC), Denali (AK), Everglades (FL), Mammoth Cave (KY), and Voyagers (MN). Most of these parks are located in the Southeastern States, which experienced a 17 percent increase in the 4th highest daily maximum 8-hour average over the 1989-98 period. For the remaining 17 parks, the 8-hour ozone levels at eight sites increased only slightly between 1990 and 1999, while seven sites showed decreasing levels and two were unchanged.

Between 1980 and 1999, the emissions of volatile organic compounds decreased 33 percent, while the NOx emissions increased one percent. This dramatic reduction occurred simultaneously with significant increases in economic growth and population. The gross domestic product increased 147 percent and the U. S. population increased 33 percent over the 1980-99 time period. The 2nd highest daily maximum hourly ozone level decreased 20 percent, while the 4th highest daily maximum 8-hour ozone average decreased 12 percent. The improvements are a result of the effective implementation of the clean air laws and regulations, as well as improvements in the efficiency of industrial technologies.

Focusing on the most recent 10-year period, 1989-98, there has been little progress over the past ten years in ozone levels – a 4 percent decrease in the 2nd highest daily maximum one-hour O3 value and “no change” in the 4th highest daily maximum 8-hour average. While there has not been deterioration in the national ozone air quality trend, there has been a lack of progress. Further, there have been regional increases in ozone levels in at least four of the EPA Regions, especially in the Southeast, where the 4th highest daily maximum 8-hour average increased 17 percent, while the 2nd highest daily maximum one-hour average ozone data increased 13 percent.

Because of this lack of progress over the past ten years, the USEPA proposed the NOx SIP Call Rule (Federal Register, 1998) in September 1997, requiring a cap-and-trade program for large sources of NOx emissions in the eastern half of the United States. It would establish a NOx
cap-and-trade program for sources in 22 eastern states, modeled after the SO\textsubscript{2} cap-and-trade program. This program would become effective in May 2003. It is the intent of this program to greatly reduce NO\textsubscript{x} emissions, especially at utilities and large sources of NO\textsubscript{x} emissions. Miller (2000) points out that a single power plant can emit as much NO\textsubscript{x} in one year as all the cars and trucks in a large metropolitan area. To illustrate this point, consider the General James M. Gavin power plant in rural southern Ohio. This facility emitted more than 110,000 tons of NO\textsubscript{x} pollution in 1996 (USEPA, 1996). In comparison, all highway vehicles (cars and trucks) in the Boston-Lawrence-Worcester, Massachusetts/New Hampshire ozone non-attainment area emitted about 125,000 tons of NO\textsubscript{x} in 1996. The NARSTO Ozone Synthesis Team (2000) suggests that the abatement of averaged ozone levels on regional scales can best be dealt with by a NO\textsubscript{x}-based strategy. They warn, however, that an increase in ozone concentrations in the urban core may occur. This is referred to as the NO\textsubscript{x} disbenefit. All things considered, the NO\textsubscript{x} SIP Call, once implemented, should have a significant impact on reducing ozone levels and should reverse the stalled trend in ozone.

2.1.4. Comparative Climatology of Ozone and Ozone Precursors Within SOS and other Regions

Regional and subregional variability in diurnal maximum ozone concentrations (DMOC) in both urban and non-urban locales within the SOS region and in other parts of the eastern United States were studied and compared with weather and climate factors. These investigations support the following conclusions.

1. Ozone accumulation in southern and southeastern states is largely decoupled from that in the northeastern US.

2. The most persistent relationship between surface ozone and weather parameters was between ozone and surface wind speed – with stagnation periods leading to the highest DMOC.

3. Interannual variations in temperature can explain about 80% of the variability in DMOC.

4. General emissions control strategies may decrease the frequency of ozone exceedance events but episodic control strategies probably will be necessary to eliminate exceedance events completely.

5. Substantial month-to-month variability in DMOC is observed within the SOS region, suggesting that different states may need to apply more stringent episodic controls in different months of the year.

6. In Baltimore, MD, weekdays in 1994-97 had about 39% more NOx, 59% more CO, and 27% more VOC than weekend days, but about 13% more ozone on weekends. Decreases in NOx emissions less than about 39% apparently will induce an ozone disbenefit in the urban core of Baltimore, but decreases in NOx emissions sufficient to avoid exceedance events in the urban core also will significantly decrease ozone exposures in nearby suburban areas.

7. Also, in Baltimore, OH reactivity with isoprene was the largest (38-40%) of the total OH reactivity with the PAMS' VOC and was the same on weekend and weekdays. OH reactivity with trimethylbenzene and toluene was 7% larger on weekdays than on weekends and thus responsible for an important part of the weekend/weekday difference. Carry-over of partially oxidized VOC either from upwind (e.g., Washington DC) sources or from previous-day oxidation (i.e., in stagnation conditions) may lead to enhanced ozone production in Baltimore.

KEY CITATIONS:


2.1.5. Conclusion—Policy-relevant Findings Regarding National and Regional Ozone Air Quality Trends

The major findings of this analysis are:

1. The national 20 year ozone trend, between 1980 and 1999, showed ambient ozone levels have decreased 20 percent based upon one-hour and 12 percent based upon the 8-hour data. Because only a few sites have monitored continuously for two decades, this trend line is composed of two segments – 441 sites with complete during the first ten years (1980-89) and 705 sites meeting the data completeness criteria in the most recent ten year period. Between 1980 and 1999, emissions of volatile organic compounds (VOCs) have decreased 33 percent. During that same period, emissions of nitrogen oxides (NOx) increased one percent. The gross domestic product increased 147 percent and the U. S. population increased 33 percent over the 1980-99 time period. Over this 20-year period, the ozone air quality improvements are a result of the effective implementation of the clean air laws and regulations, as well as improvements in the efficiency of industrial technologies.

2. Across the nation, however, there has been little progress over the past ten years – a 4 percent decrease in the 2nd highest daily maximum one-hour O3 value and “no change” in the 4th highest daily maximum 8-hour average. The emissions of VOC(s) decreased 15 percent, while the NOx emissions increased 2 percent. The U.S. population increased 10 percent and the gross domestic product increased 60 percent. The air quality improvement has not responded in the same way as the 20-year ozone trend.

3. While there has not been deterioration in the national ambient ozone trend between 1990 and 1999, there has been a lack of progress. For both the one- and 8-hour ozone measurements, ozone air quality trends in the Mid-Atlantic, Southeast, South Central, and Northwestern United States increased over the ten year period from 1989 to 1998. The highest increase of 17 percent occurred in the Southeast for the 4th highest daily maximum 8-hour measurements.

4. Because of this lack of progress over the past ten years, the USEPA proposed the NOx SIP Call Rule in September 1997, requiring a cap–and–trade program for large sources of NOx emissions in the eastern half of the United States. It would establish a NOx cap–and–trade program for sources in 22 eastern states. The NOx SIP Call, once implemented, should have a significant impact on reducing ozone levels and should reverse the “stalled” trend in ozone.
2.2. IMPROVEMENT OF PRECURSOR EMISSIONS INVENTORIES
Carlos Cardelino

Substantial uncertainties in emissions estimates and emissions inventories of ozone precursors contribute to shortcomings in the prediction and diagnosis of ozone concentrations by emission-based air quality models. SOS has taken several approaches to overcome weaknesses in emission estimates. One approach is to try to reconcile ambient measurements with emission estimates. Another approach is the development of day-specific inventories instead of the commonly used but highly imprecise typical summer day inventories. In addition to these improvements, SOS has also conducted research on ammonia emissions and on non-traditional sources of NOₓ; these results will be integrated into air quality models to study ozone and particulate matter. The results of these studies are summarized in this section.
2.2.1. Daily Variability of Motor Vehicle Emissions

In many urban areas, mobile emissions account for a significant portion of the overall emissions inventory of ozone precursors. Mobile source emissions can be characterized by analyzing traffic data measured using traffic counters. A method to study the daily variability of mobile emissions from the different types of urban and rural roads was developed by SOS. The method is based on hourly traffic volume data and emission factors, and it has been generalized to describe the daily variability of mobile emissions for the whole modeling domain. Key results of the method applied to the Atlanta metropolitan area are summarized below.

5. Interstate roads, with only 2% of the total mileage, contain 30% of the total traffic volume. Local roads with 74% of the total mileage contribute only 19% of the total traffic.

6. The temporal distribution of mobile emissions is strongly dependent on the region (urban or rural), the type of road (interstate, principal, secondary or local) and the day of the week (see Figure 2.2.1).

7. The vehicle classification distribution by road type obtained from traffic counters is significantly different from the default distribution contained within the Mobile5a computer model. When applied to a specific-day inventory, the use of observed data, as opposed to default data, produces changes in emissions that vary by 8% (VOC), 9% (CO) and 19% (NOx).

8. Compared to a typical summer day, the range of mobile emission variability is 26 to -28% for urban areas and 19 to -13% for rural areas.

KEY CITATION:
2.2.2. **Use of Survey Data for Ozone Sensitivity to Point Sources**

Photochemical modeling studies depend on the correct location and amount of emissions from point sources. SOS researchers used survey data that include daily activity logs for the largest point sources in the Atlanta region to estimate VOC and NO\textsubscript{x} point source day-specific emissions. The emissions were based on actual operating schedules rather than the more crudely estimated typical summer day emissions. The major findings of this study are summarized below.

1. The daily variability in point source NO\textsubscript{x} emissions is found to be as much as 24% with respect to typical summer day emissions.
2. Although the daily variability of point source VOC emissions is as large as 28%, their contribution to total VOC emissions is not significant.
3. Numerical simulations suggest that changes in point source NO\textsubscript{x} emissions can have an opposite impact depending on the geographical location of the sources (rural or urban areas).

Table 2.2.1. Summary of numerical simulations evaluating the impact of two power plants: Bowen and McDonough (after Chang et al., 1996).

<table>
<thead>
<tr>
<th>Description</th>
<th>Ozone Maxima</th>
<th>Number of cells</th>
<th>Number of cell-hours</th>
<th>Population</th>
</tr>
</thead>
<tbody>
<tr>
<td>Typical case</td>
<td>129</td>
<td>50</td>
<td>69</td>
<td>183,630</td>
</tr>
<tr>
<td>August 10 case</td>
<td>129</td>
<td>48</td>
<td>65</td>
<td>152,940</td>
</tr>
<tr>
<td>August 10 w/o McDonough</td>
<td>134</td>
<td>60</td>
<td>83</td>
<td>327,213</td>
</tr>
<tr>
<td>August 10 w/o Bowen</td>
<td>129</td>
<td>34</td>
<td>45</td>
<td>90,102</td>
</tr>
<tr>
<td>August 10 w/o Bowen &amp; McDonough</td>
<td>133</td>
<td>44</td>
<td>56</td>
<td>263,390</td>
</tr>
</tbody>
</table>

NOTE: “Number of cell-hours” is the number of cells that exceed ozone standard each hour summed throughout the day and “Population” is the total human population within cells experiencing ozone exceedances.

**KEY CITATION:**

2.2.3. Inverse Modeling of Emissions

Inverse modeling is a useful tool for reconciling emission inventories with direct measurements of air concentrations of precursor chemicals. Inverse methods minimize the difference between observed concentrations and concentrations obtained from air quality models. SOS applications of inverse methods include the temporal and spatial distribution of isoprene and CO emissions in the Atlanta area. Key findings of this investigation are outlined below.

1. Isoprene emissions derived from inverse modeling are 2 to 10 times higher than any of the accepted emission estimates.
2. Higher isoprene emissions significantly increase the concentration of ozone within the plumes of nitrogen oxides emitted from large point sources.
3. Uncertainties in mixing height are not likely to be responsible for the underprediction of isoprene in air quality models.
4. Inhomogeneities in the spatial distribution of emissions can severely limit the application of the inverse method.

![Image of isoprene concentration graphs](image)

Figure 2.2.2. Observed (solid circle) and model-simulated isoprene concentrations at an Atlanta monitoring station. Simulations are with (A) BEIS and (B) BEIS2 inventories: base case (open circles), and two inverse applications (square and triangles) (from Chang et al., 1996).

KEY CITATIONS:
2.2.4. Comparison of Trace Gas Concentrations and Emission Estimates

Assessing the accuracy of an emission inventory is a difficult but important step in establishing the overall accuracy of models that are used to determine ozone control strategies. A comparison between emission ratios and ambient concentrations in a source region is one of the few ways of making such an assessment. During the 1995 SOS Nashville Intensive, continuous measurements of CO, NO\textsubscript{y} and SO\textsubscript{2} and twice-a-day samples of hydrocarbons were made at a Nashville downtown location. Ratios of morning concentrations of CO, NO\textsubscript{y} and VOC were compared with the corresponding ratios derived from emission estimates for the Nashville area. Key findings of this study are summarized below.

1. Correlations between SO\textsubscript{2}, CO and NO\textsubscript{y} indicate only a minor impact from power plant emissions. Plume-like excursions of high SO\textsubscript{2} occur less than 5% of the time.

2. The observed morning ratios of VOC/CO, VOC/NO\textsubscript{x} and CO/NO\textsubscript{x} are 0.32 ppbC/ppb, 2.9 ppbC/ppb and 2.9 ppb/ppb, respectively.

3. The 1990 NAPAP emission estimates can be brought into agreement with the observed values if the VOC emission rate is decreased by 30% while the 1995 SOS inventory will agree if the CO emission rate is increased by about 35%.

4. In contrast to comparisons in other locations, no evidence of large (i.e., factor of 2 or greater) underpredictions of CO or VOCs is found.

Table 2.2.2. Comparison of observed concentrations with corresponding quantities from emission estimates (after Kleinman et al., 1995).

<table>
<thead>
<tr>
<th>Ratio</th>
<th>Observations</th>
<th>1990 NAPAP emissions</th>
<th>1995 SOS emissions</th>
</tr>
</thead>
<tbody>
<tr>
<td>VOC/CO ppbC/ppb</td>
<td>0.32</td>
<td>0.46</td>
<td>0.42</td>
</tr>
<tr>
<td>VOC/NO\textsubscript{x} ppbC/ppb</td>
<td>2.9</td>
<td>4.1</td>
<td>2.9</td>
</tr>
<tr>
<td>CO/NO\textsubscript{x} ppb/ppb</td>
<td>9.3</td>
<td>9.1</td>
<td>6.9</td>
</tr>
</tbody>
</table>

KEY CITATION:
2.2.5. NOx Emission from Soils

Soil biogenic NO\textsubscript{x} emissions are an important part of the total global NO\textsubscript{x} budget. SOS recognized that non-traditional sources of NO\textsubscript{x} should be included as part of the oxides of nitrogen budget and therefore, SOS sponsored a series of projects to characterize the magnitude and the parameters that control biogenic emissions from soils. Key findings are summarized below.

1. A model of soil NO emissions was developed based on soil temperatures. This model explains over 80% of the variation in emissions (see Figure 2.2.3).

2. The summertime contribution of soil NO to the overall NO\textsubscript{x} inventory averages 4.1% for the southeastern US with a high of 9.5 for Mississippi and a low of 2.2% for Florida.

3. Urban-metropolitan soils are not an important source of soil NO\textsubscript{x}.

4. For the Middle Tennessee non-attainment area, soil biogenic NO\textsubscript{x} contributes from 7 to 9.8% of the daily average NO\textsubscript{x} budget during the months of June through August. However, during the hottest July days the soil biogenic component can contribute over 17% of the total NO\textsubscript{x}.

![Figure 2.2.3. Soil NO\textsubscript{x} flux with soil temperature at a 5-cm depth for (A) cropland and (B) pasture (from Thornton et al., 1997).]

**KEY CITATIONS:**


2.2.6. Natural Emissions of Non-methane VOC, CO, and NOx

Natural emissions are responsible for a major portion of the chemical species that determine tropospheric oxidant concentrations. These compounds include non-methane volatile organic compounds (NMVOC), carbon monoxide (CO) and nitric oxide (NO). Natural sources include soil microbes, vegetation, biomass burning and lightning. A review of current estimates of natural emissions is summarized below (see Table 2.2.3).

1. Over 98% of the total annual NMVOC emissions are from vegetation, primarily foliage, and isoprene is the dominant compound with 35% of the total emissions.

2. Natural emissions of alkane and aromatic compounds are very low and are greatly overestimated by earlier inventories.

3. Sources of NMVOC emission from vegetation include chloroplasts, defense from specialized tissues, defense from unspecialized tissues, growth hormones, floral scents, cut and drying vegetation, and other. The total North America NMVOC flux is dominated by emissions from chloroplasts.

4. Soil and lightning each contribute about half of the annual natural NO flux. Biomass burning and vegetation are each responsible for about half of the natural CO emissions.

Table 2.2.3. Annual above canopy fluxes of NO (Tg-N), NMVOC (Tg-C) and CO (Tg-N) from natural sources in North America (after Guenther et al., 2000).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Vegetation</th>
<th>Soils</th>
<th>Lightning</th>
<th>Biomass Burning</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO</td>
<td>0</td>
<td>0.9</td>
<td>0.9</td>
<td>0.3</td>
<td>2.1</td>
</tr>
<tr>
<td>CO</td>
<td>4</td>
<td>0.0</td>
<td>0</td>
<td>6</td>
<td>10</td>
</tr>
<tr>
<td>NMVOC</td>
<td>82.2</td>
<td>1.1</td>
<td>0</td>
<td>0.6</td>
<td>83.9</td>
</tr>
</tbody>
</table>

KEY CITATION:
2.2.7. Natural VOC Fluxes from Enclosure and Ambient Measurements

A major objective of SOS and SOS-affiliated field research has been the measurement of ambient concentrations of the various hydrocarbon species that play a significant role in the production and accumulation of photochemical oxidants in both urban and rural environments. Over 90% of the total VOCs entering the atmosphere of the earth are of biogenic origin. In one project natural VOCs were measured on tethered balloon platforms between 1985 and 1996; in another project biogenic VOCs emissions were investigated at two forested sites in the southeastern US. Major conclusions are given below.

1. Ambient measurements of isoprene and monoterpane emissions are within a factor of 2 of modeled estimates (see Figure 2.2.4).

2. Concentrations of biogenic VOC decrease slowly with altitude in the mixed layer while surface layer concentrations show much more variability.

3. Isoprene concentrations in the mixed layer remained fairly constant in the middle of the day, in contrast to isoprene concentrations at canopy-level, which continued to increase until evening.

4. Daytime emissions, which increase with temperature and solar radiation, are balanced by changes in entrainment and oxidation.

Figure 2.2.4. Typical observed diurnal isoprene and monoterpane emission (µg C g⁻¹ h⁻¹) patterns from (a) post oak, (b) loblolly pine, and (c) sweetgum trees. Leaf temperature T (degrees celsius) and photosynthetically active radiation (PAR) (10 µmol m⁻² h⁻¹) are shown for reference (from Guenther et al., 1996).

KEY CITATIONS:


2.2.8. **Influence of Isoprene Emissions in Regional Ozone Modeling**

The role of biogenic hydrocarbons in ozone formation has been the subject of considerable debate since the 1970s. In order to provide better emission inventory inputs into photochemical air quality models, an improved emission algorithm (BEIS2) for calculating biogenic emission rates was developed. The key features of this new and improved emission algorithm include:

1. BEIS2 uses more temporally resolved environmental corrections (hourly versus monthly), more spatially resolved vegetative cover (county level versus 1° latitude/longitude grid cells), and more resolved vegetative emission factors (genus versus broad biome classes).
2. Higher isoprene emissions are obtained with BEIS2, which are about a factor of 5 higher than BEIS1 during warm, sunny conditions.
3. When BEIS2 is used with the RADM model, elevated concentrations of ozone went from being VOC-sensitive to NOx-sensitive across much of the RADM modeling domain.
4. The new system yields better agreement with observations. Using BEIS2 in RADM resulted in mean near-surface isoprene predictions that were slightly lower (25%) than observed.

![Figure 2.2.5](image)

**Figure 2.2.5.** Mean diurnal plot of isoprene concentrations observed and modeled near the surface of Scotia, Pennsylvania during July and August 1988. Data points represent the bin of 10 values (from Pierce et al., 1998).

**KEY CITATIONS:**


2.2.9. Sources and Importance of Ammonia Emissions

Ammonia is the most abundant alkaline component in the atmosphere and a precursor of fine particulate matter when it is converted into ammonium nitrate and ammonium sulfate. Dry and wet deposition of gases as ammonia and ammonium ion contribute significantly to the acidification and eutrophication of terrestrial and aquatic ecosystems. As a result, research on ammonia emissions has become an emerging issue in the U.S. SOS undertook studies to characterize the location and strength of the ammonia sources at the state and county level. During the 1999 Nashville field study, ammonia emission maps were used to plan the trajectories of aircraft with instrumentation to measure ammonia concentrations in the atmosphere. Key findings of the SOS study on ammonia emissions are summarized below.

1. The estimated ammonia emissions for the US are about 4,917 million kg per year. The major sources include animal waste that account for 76.8% of total emissions and fertilizer applications with 9%.

2. Minor sources include industries (5.9%), motor vehicles (5.2%), sewage treatments (1.8%), and human populations (1.4%).

3. During the last ten years, ammonia emissions have been increasing at a rate of about 0.8% per year.

Table 2.2.4. 1997 U.S. Ammonia emissions (kg NH₃ yr⁻¹) and emission density (kg NH₃ mi⁻² yr⁻¹) (after Cardelino, 2000).

<table>
<thead>
<tr>
<th>Source category</th>
<th>Ammonia Emissions</th>
<th>Emissions density</th>
<th>Percent of Emissions</th>
<th>Percent trend 1997-1987</th>
</tr>
</thead>
<tbody>
<tr>
<td>Animal waste</td>
<td>3,776,327,843</td>
<td>1,067.9</td>
<td>76.8</td>
<td>5.9</td>
</tr>
<tr>
<td>Fertilizer application</td>
<td>441,448,466</td>
<td>124.8</td>
<td>9.0</td>
<td>10.6</td>
</tr>
<tr>
<td>Human population</td>
<td>66,909,015</td>
<td>18.9</td>
<td>1.4</td>
<td>10.5</td>
</tr>
<tr>
<td>Motor vehicles</td>
<td>253,972,965</td>
<td>71.8</td>
<td>5.2</td>
<td>32.6</td>
</tr>
<tr>
<td>Industries</td>
<td>289,087,983</td>
<td>81.7</td>
<td>5.9</td>
<td>9.1</td>
</tr>
<tr>
<td>POTW</td>
<td>89,595,818</td>
<td>25.3</td>
<td>1.8</td>
<td>40.6</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>4,917,342,090</strong></td>
<td><strong>1,390.5</strong></td>
<td><strong>8.2</strong></td>
<td></td>
</tr>
</tbody>
</table>

KEY CITATION:
2.2.10. Conclusion — Policy-Relevant Findings Regarding Emissions Inventories

SOS and SOS-affiliated research on emission inventories has led to the following policy-relevant findings.

1. Significant day-to-day variability in emissions was commonly observed. Inclusion of day-specific traffic information has a major impact on mobile source emission estimates. Similarly, point source emissions based on operating schedules capture significant emission variability.

2. Location of point sources affects abatement strategies. Changes in NO\textsubscript{x} emissions from point sources can have an opposite impact on ozone levels depending on the geographical location (urban or rural) of the sources.

3. Impact of agricultural practices. The application of nitrogen fertilizer to soils and animal husbandry practices induce enhanced NO and ammonia emissions that can impact regional air quality.

4. Improvement in emission inventories. The use of inverse methodology, the inclusion of genus-specific emission factors and mechanistic-based algorithms for estimating environmental factors improves the accuracy of emission inventories.

5. Ozone sensitivity to precursors. Numerical simulations with improved biogenic emissions change ozone behavior from being VOC-sensitive to NO\textsubscript{x}-sensitive across much of the modeling domain.
2.3. OZONE FORMATION IN POWER PLANT PLUMES
James Meagher and Fred Fehsenfeld

Early efforts to decrease NO\textsubscript{x} emissions focused on motor vehicles and have resulted in dramatic improvements in automobile NO\textsubscript{x} emission rates. More recently, the EPA, in an effort to further decrease NO\textsubscript{x} emissions, has turned its attention to the electric utility sector. Fossil-fuel combustion for electricity generation contributes approximately 24\% of U.S. manmade NO\textsubscript{x} emissions. In a series of regulatory actions intended to address both ground-level ozone and acid deposition, the EPA is requiring the electric utility industry to decrease power plant NO\textsubscript{x} emissions by approximately 3 million tons per year by 2003. This decrease constitutes almost 50\% of 1997 electric utility NO\textsubscript{x} emissions, with the bulk of the decreases slated for eastern U.S. coal-fired power plants that have the greatest annual NO\textsubscript{x} emissions (see Figure 2.3.1).
2.3.1. **What is the distribution of NOx emissions from fossil-fueled power plants?**

Thousands of fossil-fueled units located throughout the country contribute to electric utility NOx emissions. However, the emissions are not uniformly distributed, with a relatively small number of power plants producing a large fraction of the total. In 1997, the last year for which data are available, the fifty power plants with the largest NOx emissions account for approximately 36% of the emissions, with the top 28 accounting for more than 25%. The location of the fifty largest NOx sources is shown in Figure 2.3.1. For the most part, the largest NOx sources are located in rural areas in the eastern U.S., many in areas with the highest natural VOC emissions. This superposition provides a fertile environment for ozone formation. SOS has conducted several field studies in this region to better understand ozone formation and distribution in the NOx plumes from these power plants.

![Map of the 50 largest NOx point sources in the U.S.](image)

**Figure 2.3.1.** The 50 largest NOx point sources in the U.S. (all are fossil-fueled power plants) for 1996 (after EPA, 1997). The annual emissions shown here can be compared to those for the Nashville urban area (Davidson county, population 1M), which are approximately 30,000 tons per year.

**KEY CITATION:**
2.3.2. **How is ozone formed in power plant plumes?**

Only one of the two major precursors required to make ozone (NO$_x$) is emitted from power plants. In the presence of sunshine when the rapidly expanding NO$_x$ plume mixes with VOCs present in the surrounding air, ozone is formed. The VOCs that participate in the ozone formation can be either natural or man-made depending upon the location of the power plant. In the early stages of plume dilution, the NO$_x$ concentrations are extremely high. They are so high, in fact, that ozone already present in the atmosphere is actually consumed in the plume, and ozone concentrations in the plume are smaller than in the surrounding atmosphere (Figure 2.3.2). As the plume grows, eventually filling the mixed layer (Figure 2.3.3), NO$_x$ concentrations become smaller and ozone is produced. Ozone production continues until all the reactive NO$_x$ is consumed or the sun goes down.

![Crosswind profiles of pollution in a power plant plume. Pollutant concentrations were measured on a NOAA research aircraft as it penetrated the power plant plume at three distances downwind.](image)

**Figure 2.3.2.** Crosswind profiles of pollution in a power plant plume. Pollutant concentrations were measured on a NOAA research aircraft as it penetrated the power plant plume at three distances downwind.
2.3.3. Do all power plants produce ozone with equal efficiency?

The chemical processes that form ozone in the atmosphere are nonlinear, which means that any change in emissions will not be accompanied by a proportional change in amount of ozone formed. We must understand the nature of this nonlinear relationship if we are to know how much decrease in NO\textsubscript{x} emissions will be required to produce a desired decrease in ambient ozone concentrations or, alternatively, what will be the effect of introducing additional sources of NO\textsubscript{x}. SOS research has therefore focused on ways to estimate the efficiency with which ozone is being formed in power plants with different NO\textsubscript{x} emission rates. In this work we have calculated the Ozone Production Efficiency or OPE for a number of power plants on different days. The OPE is defined as the number of molecules of ozone formed per molecule of NO\textsubscript{x} emitted, which provides a direct comparison of two different sources in terms of their potential to form ozone.

![Figure 2.3.3. Schematic of ozone formation in power plant plumes. A temperature inversion limits the transport of pollution out of the “mixed layer”.

The effect of NO\textsubscript{x} emission rate on ozone formation was determined using data collected in the plumes of several different coal-fired power plants located in close proximity to each other in the Southeast during the summer of 1995 (see Figure 2.3.3 for an illustration of the processes involved in ozone formation in power plant plumes). These plants had very different (more than a factor of 10) NO\textsubscript{x} emission rates and were located in a region of abundant forests with significant biogenic VOC (isoprene) emissions. Instrumented aircraft were used to study ozone production in the plumes of several different power plants on the same day (Ryerson et al., 1998) and different plants on different days (Gillani et al., 1998; Nunnermacker et al., 2000). The
measured ozone production efficiencies ranged from 0.8 to 7.0. In each case, the plants with the greatest NO\textsubscript{x} emission rates exhibited the lowest ozone production efficiencies. Model simulations of plume experiments produced somewhat higher OPEs (but lower than previous estimates) than were measured (Sillman, 2000).

The ozone production efficiency measured in these plumes varies from day to day due to changes in meteorological factors, (e.g., the temperature, the amount of sunlight, and the wind speed) that affect the abundance of isoprene in the atmosphere (Luria et al., 2000) and the rate of plume dilution. Therefore, a direct quantitative comparison between individual measurements is not possible. However, it is evident that the power plants with greater NO\textsubscript{x} emission rates produced ozone less efficiently in these studies, a direct manifestation of the nonlinear processes discussed above. Also, the data clearly demonstrate that, for large sources, the benefits of decreasing emissions of NO\textsubscript{x} are partially offset by an increase in the efficiency with which ozone is formed.

KEY CITATIONS:
2.3.4. **Conclusion — Policy-Relevant Findings Regarding Ozone Production in Power Plant Plumes**

These findings are particularly important in light of the current U.S. focus on NO\textsubscript{x} reduction as the primary mechanism for ozone management. The observed inverse relationship between ozone production efficiency and NO\textsubscript{x} emission rate has significant implications for environmental policy and management strategies related to tropospheric ozone. In particular, the results discussed above provide new perspectives that should aid in the optimization of NO\textsubscript{x} emission management plans for current and planned fossil-fueled power plants.

Current strategies for NO\textsubscript{x} emission reductions inherently assume that “all NO\textsubscript{x} is created equal”. In order to minimize costs, EPA and the States often give industry a fair amount of flexibility in terms of how and where NO\textsubscript{x} emission reductions are achieved. This policy often results in controls being applied to the sources with the greatest NO\textsubscript{x} emissions where the cost per ton of NO\textsubscript{x} removed is lowest. EPA has recently issued a rule (under section 126 of the Clean Air Act) designed to minimize the impact of ozone formed in one state on states downwind. The rule calls for NO\textsubscript{x} emission reductions at 392 large NO\textsubscript{x} sources, mostly coal-fired power plants, located in 19 states (extending from Alabama to Rhode Island) and the District of Columbia using a “cap-and-trade” program. Under “cap-and-trade” the total NO\textsubscript{x} emission reduction is fixed, but trading of emissions within the affected states is allowed. Thus, a ton of emitted NO\textsubscript{x} is “valued” equally whether it comes from a large power plant in the South or a small one in the Midwest. Our results would suggest that the OPE will vary greatly among the source types and locales being considered, and the resultant change in ambient ozone will be greatly affected by the choice of sources that are controlled under such a system.

The U.S. electric power industry is in the early stages of a massive restructuring designed to move the country away from a system of regional monopolies to a competitive market that provides open access for commercial and residential customers. The prospect of more open and competitive electricity markets has resulted in a renewed interest in distributed generation, many small (typically less than 30 MW) generating facilities located near the end user, as an alternative to large central generating stations. Incentives to promote distributed generation are included in electricity utility restructuring bills currently before the U.S. Congress. Although many technologies ranging from internal combustion engines to solar panels and fuel cells are being considered as candidates for Distributed Generation, small gas turbines appear to be the most
attractive in the near term. These modern gas turbines have impressively low NO\textsubscript{x} emissions. However, reducing the emission density by spreading the NO\textsubscript{x} emissions over a larger area, especially one with abundant VOC emissions, creates a situation that is very favorable for ozone production. Under such a scenario, the SOS results suggest that, some of the benefits associated with these lower NO\textsubscript{x} emissions will be offset by higher ozone production efficiencies.
2.4. OZONE FORMATION IN URBAN AREAS

Peter Daum and Larry Kleinman

During the last five years, SOS has conducted four major field programs centered on Nashville (1995 and 1999), Atlanta (1999), and Houston (2000). The objectives of these programs were diverse, but a common focus has been to understand the processes leading to elevated O₃ concentrations in urban areas. An overview of the field campaigns is provided in Section 1.3. In this section we summarize some of the scientific findings, concentrating on the 1995 field campaign in Nashville since the other campaigns are still in a relatively early stage of analysis.

We have very high expectations for the results of the field campaigns in 1999 and 2000. Measurement capabilities have evolved since 1995. For example, in the later campaigns instruments were deployed to determine concentrations of free radicals (OH and HO₂), NOₓ compounds important to nighttime chemistry (NO₃ and HONO), VOC compounds with 1-second time resolution, size measurements of ultra-small aerosol particles, and composition measurements for single aerosol particles. These new instruments will allow examination of photochemistry and aerosol production in unprecedented detail. Each of the cities visited by SOS has its own distinctive emissions characteristics and meteorological conditions. Conducting experiments in different venues is a deliberate strategy based on the belief that contrasts between regions constitute an important test of our understanding of the composite meteorological/chemical processes that lead to O₃ and PM formation and accumulation.
2.4.1. **Urban Plumes under Stagnation Conditions**

Stagnation conditions are a major reason for the occurrence of very high O₃ concentrations. A classic case was observed in Nashville between July 11 –13, 1995 (see Figure 2.4.1). Ozone concentrations reached 138 ppb. Vertical cross sections determined by Lidar showed that O₃ concentrations exceeded 120 ppb up to 2 km altitude, but that the O₃ hardly moved at all horizontally, instead forming a vertical column or dome of ozone over or near the city (see also Section 2.5). Findings related to urban plumes in stagnation conditions are shown below.

![Figure 2.4.1. Map of O₃ interpolated from flight data on July 11, 1995 (from Valente et al., 1998).](image)

**1. O₃ formation is VOC-limited in extreme stagnation conditions.** Observed indicator ratios show VOC-sensitive conditions in the Nashville urban plume (see Figure 2.4.2).

![Figure 2.4.2. Total peroxide to NOₓ ratio for the afternoon of July 11, 1995. Map interpolated from aircraft observations. High O₃ area can be seen from preceding figure (from Valente et al., 1998).](image)
• Under stagnation conditions, O₃ production in the Nashville urban plume starts out being VOC-limited in the morning and remains that way for the remainder of the day (see Figure 2.4.3).

Figure 2.4.3. Instantaneous O₃ production rate for downtown Nashville on July 11, 1995 as a function of the measured hydrocarbon to NOₓ OH reactivity ratio. P(O₃) calculated using a box model constrained by measured concentrations of stable species. The exhibited linear dependence is an indication of hydrocarbon sensitive O₃ formation. (from Daum et al., 2000).

2. Anthropogenic compounds (including CO) account for 2/3 of OH – VOC reactivity. As shown in Figure 2.4.4, much of the OH - VOC reactivity is apportioned to the anthropogenic component of emissions.

Figure 2.4.4. Apportionment of VOC OH reactivity for samples collected over downtown Nashville in the boundary layer on July 11, 1995 during a stagnation episode. Biogenic reactivity includes contributions from isoprene, methylvinylketone, methacrolein, and 40% of the formaldehyde. (from Daum et al., 2000).

KEY CITATIONS:
2.4.2. Urban Plumes under Advective Conditions

Winds usually limit the accumulation of pollutants in an urban area. Ozone that would be found within the city under stagnation conditions is advected away, thereby affecting a larger geographic area, albeit at lower concentration. Under advective conditions there are changes in photochemistry and optimum control measures. During the Nashville 1995 campaign there were several instances where the urban plume could be tracked over a several-hour travel time, thereby giving us a natural laboratory to follow the O₃ production process.

1. The amount of O₃ formed under stagnation and advective conditions was similar. The total amount of O₃ formed in an urban plume can be approximated as the product of NOₓ emissions times the O₃ production efficiency (OPEₓ equal the number of molecules of O₃ formed per molecule of NOₓ that reacts). OPEₓ under stagnation and advective conditions was observed to be about the same (see Table 2.4.1). Small power plants (i.e., Gallatin) have an OPEₓ similar to Nashville; large power plants (i.e., Paradise) have a lower OPEₓ. See also Section 2.2 on power plant plumes.

Table 2.4.1. O₃ production efficiencies in urban and power plant plumes.

<table>
<thead>
<tr>
<th>Date/Time(local)</th>
<th>Plume</th>
<th>OPEₓ</th>
</tr>
</thead>
<tbody>
<tr>
<td>July 11 / 1500</td>
<td>Nashville - stagnation</td>
<td>3.5</td>
</tr>
<tr>
<td>July 13 / 1430</td>
<td>Nashville - stagnation</td>
<td>4</td>
</tr>
<tr>
<td>July 13 / 1430</td>
<td>Nashville - stagnation</td>
<td>3.5</td>
</tr>
<tr>
<td>July 11 / 1500</td>
<td>Nashville - stagnation</td>
<td>4</td>
</tr>
<tr>
<td>July 18</td>
<td>Nashville - advective</td>
<td>3-4</td>
</tr>
<tr>
<td>July 3</td>
<td>Nashville - advective</td>
<td>3-4</td>
</tr>
<tr>
<td>July 7</td>
<td>Paradise</td>
<td>2</td>
</tr>
<tr>
<td>July 15</td>
<td>Gallatin</td>
<td>3</td>
</tr>
</tbody>
</table>

2. Photochemistry was rapid in the Nashville urban plume. Within 2 hours travel time from the urban center, photochemistry had removed about half of the NOₓ and half of the anthropogenic hydrocarbons.

Figure 2.4.5. Decay rate of the NOₓ concentration in the Nashville urban plume under advective conditions. Measurements from July 3 and July 18, 1995. Decay rate is consistent with a 1/e lifetime for NOₓ of ~2.1 hrs, and an average OH concentrations of 10⁷/cm³ (from Nunnermacker et al., 1998).
3. **Biogenic VOCs become more important as the urban plume is advected into the rural surroundings.** As the urban plume moved into rural areas, the biogenic apportionment of hydrocarbons to O₃ production increased (Figure 2.4.6).

![Figure 2.4.6. Estimated contribution of anthropogenic and biogenic hydrocarbons to O₃ production in the center of the Nashville urban plume. Left plot is the apportionment after transport of the urban plume approximately 2 hours downwind of Nashville. Right plot is the estimated contribution of hydrocarbon sources after approximately 4-6 hours reaction time. Data from G-1 flights of 7/3 and 7/18/1995 (after Nunnermacker et al., 1998).](image)

4. **NOₓ control is favored under advective conditions.** Model calculations indicate a tendency for NOₓ sensitivity to increase and VOC sensitivity to decrease as the meteorological situation shifts from the stagnation conditions typical of extreme episodes to more typical advection conditions (Duncan and Chameides, 1998).

**KEY CITATIONS:**


2.4.3. Ozone Transport from Urban to Rural Areas

Ozone that is formed in an urban area does not stay there. Even under extreme stagnation conditions, it is advected away within a day. Often, the advection occurs preferentially at night (see Section 2.5). As ozone has a relatively long atmospheric lifetime, ozone transported out of a city can contribute to a regional background. The next day’s photochemistry then has a higher base upon which to build. These processes were observed during the Nashville field campaigns. Model calculations show the implications on control strategies.

1. **Transport of ozone from Nashville.** Lidar cross sections and profiles and wind profiler data showed that the dome of ozone over Nashville during the July 11-13 stagnation episode mixed out and became part of the suburban and rural mixed layer the next day.

2. **Impact of urban ozone at a suburban location.** Of the 120 ppb O₃ recorded at suburban New Hendersonville (July 1, 1994), 80 ppb was due to entrainment of O₃ rich air from aloft – which was a remnant of the previous day’s photochemistry. An additional 40 ppb was added due to the current day’s urban plume (see Figure 2.4.7).

![Figure 2.4.7](image-url)

*Figure 2.4.7. Ozone measured at New Hendersonville and other ground stations. Bottom panel shows calculated O₃ production rate. From 0700 to 1000 CST, July 1, O₃ increased from essentially 0 to 80 ppb, which can only be explained by entrainment since photochemical production was nil during this period. The further increase to 120 ppb is due to intense photochemical production in the Nashville urban plume as it passed over the New Hendersonville site (adapted from Baumann et al., 2000).*
3. **Regional background and urban ozone can require different control measures.** Model calculations show that export of O$_3$ from a city is more sensitive to NO$_x$ emission decreases, even for cases where VOC emission controls more effectively decrease peak O$_3$ during pollution episodes (Duncan and Chameides, 1998).

**KEY CITATIONS:**


2.4.4. Conclusion – Policy-Relevant Findings for Ozone Formation in Urban Areas

Urban plume studies carried out under SOS have resulted in the following policy-relevant findings.

1. **Stagnation events tend to be VOC-sensitive.** In the southeastern US, the highest $O_3$ concentrations occur under stagnation conditions. Model calculations and observations show that stagnation conditions promote VOC sensitivity. In Nashville the sensitivity of peak $O_3$ concentrations is somewhere in-between the strongly VOC-sensitive condition typical of Los Angeles and the strongly NO$_x$-sensitive condition typical of rural areas. In all likelihood, a dual control strategy is required. Such a strategy will have to take into account the role of biogenic VOC emissions that cannot be controlled.

2. **Good ventilation yields NO$_x$ sensitivity.** Under more normal advective conditions, the urban plume became NO$_x$-sensitive at the point of maximum $O_3$ concentration. Ozone over the urban center can still be VOC-sensitive, but in contrast to stagnation episodes, this is no longer where peak $O_3$ occurs.

3. **Good ventilation does decrease the ambient concentration of ozone but does not decrease the total amount of $O_3$ formed.** The total number of molecules of $O_3$ formed for each molecule of NO$_x$ emitted in the Nashville urban area was observed to be almost independent of ventilation. Under stagnation conditions, this $O_3$ occupies a small volume leading to very high concentrations. Good ventilation spreads the $O_3$ and may lead to impacts in rural areas.

4. **Ozone = Plume + Background.** Each day’s photochemistry builds on a background of $O_3$ that was created in previous days. Background $O_3$ is almost always NO$_x$-sensitive. It often cannot be attributed to a single source region. Plume $O_3$, on the other hand, can be NO$_x$- or VOC-sensitive. In a stagnation episode, the $O_3$ that is formed in the urban plume during the day of the episode can be very VOC-sensitive and even increase if NO$_x$ emissions are lessened. Thus, plume and background $O_3$ can require different control measures.

5. **Biogenic VOCs are important, even in an urban center.** Observations near the center of Nashville showed that the isoprene contribution to VOC-OH reactivity is highly variable, but on average accounts for 1/4 to 1/3 of the total reactivity. This fraction increased with distance from the city center.
2.5. ATMOSPHERIC DYNAMICS AND MIXING ON URBAN AND REGIONAL SCALES
Allen White and Christoph Senff

While a thorough understanding of the atmospheric chemistry associated with the formation and destruction of atmospheric pollutants is critical in air quality research, a knowledge of atmospheric dynamics and mixing processes is equally important to gain a full understanding of the problem. Vertical and horizontal transport mechanisms as well as the temporal and spatial evolution of mixed layer height often play a critical role in the distribution of pollutants on urban and regional scales. In this section, we summarize the key findings from the SOS 95 and SOS 99 studies that pertain to atmospheric dynamics and mixing processes.

2.5.1. Daytime Transport Processes

During SOS field studies, a number of meteorological processes contributed to horizontal and vertical transport of pollutants during the daytime. A schematic summarizing many of these processes is shown in Fig. 2.5.1. SOS used a variety of ground-based and airborne observing systems to study transport mechanisms. Key findings are summarized below.

1. **Horizontal Advection.** We found that synoptically driven winds were the dominant daytime horizontal transport mechanism. Mesoscale circulations caused by topography or land use differences also contribute to daytime transport.

![Figure 2.5.1. Transport between the surface and the atmospheric boundary layer (ABL) and between the ABL and free troposphere: A. fluxes from nearly homogeneous surfaces to ABL, B. fluxes from inhomogeneous surfaces to ABL, C. transport across capping inversion (Z_i) by entrainment/detrainment and cumulus venting, and D. direct injection to troposphere caused by horizontal variations in boundary-layer depth.](image-url)
2. **Boundary-layer Venting.** Under light wind conditions, we observed substantial (~40%) horizontal variations in daytime mixing height due to the urban-rural contrast in the surface energy balance (the “urban dome”). The dome allowed venting of urban emissions aloft, making them available for horizontal transport but unavailable for vertical mixing downwind of the dome during the day (refer to D in Fig. 2.5.1).

3. **Convection.** Cumulus clouds vented pollutants from the boundary layer and reduced the sunlight available for photochemistry. Because direct measurements of cumulus venting are difficult to obtain experimentally, we were unable to quantify this process during SOS. The deep vertical mixing associated with convective storms may also have resulted in stratosphere/troposphere exchange.

4. **Subsidence.** Synoptic scale subsidence associated with high pressure strengthened the boundary-layer capping inversion, thereby inhibiting vertical transport of momentum and pollutants and cumulus convection. This behavior, combined with the stagnant conditions resulting from relaxation of the synoptic-scale pressure gradient, allowed pollutants to accumulate locally during the day (Banta et al., 1998).

5. **Morning Transition.** The morning transition caused photochemically aged pollutants from the residual layer to interact with pollutants emitted at night into the shallow nocturnal boundary layer. During the 1999 SOS Nashville Intensive, the breakup of the nocturnal inversion occurred at an urban site 1-2 h earlier than at three rural sites. In the humid environment during the SOS field studies, surface water vapor mixing ratio was often an excellent meteorological tracer for the timing of the morning transition (see Fig. 2.5.2).

**Figure 2.5.2.** 1-min time series of CO and NOy concentrations, the concentration ratio of NOx to NOy, and water vapor mixing ratio (rmix) measured near the surface on 15 July 1999 at the Dickson, Tennessee site. The early morning increase in rmix is due to surface evaporation. The sharp transition in rmix near 0920 CDT occurs after the nocturnal inversion is fully eroded and as the mixed layer grows rapidly through the residual layer and entrains drier air from aloft. The CO and NOy concentrations decrease because nocturnal surface emissions of these gases were confined to the shallow nocturnal boundary layer. The NOx/NOy ratio decreases because the residual layer contains photochemically aged air from the previous day.

**KEY CITATIONS:**


2.5.2. Nighttime Transport Processes

During the night, the effect of surface friction is confined to a shallow layer (10s of meters) near the surface. In general, vertical motions not associated with convective storms are considerably weaker at night than during the day. Thus, during SOS, nocturnal transport tends to redistribute pollutants horizontally rather than vertically. Key features are summarized below.

1. **Low-Level Jet.** At night, the winds above a shallow (10s of meters) layer at the surface accelerated as the atmosphere decouples from the surface.

2. **Inertial Oscillation.** The nocturnal winds rotated in time in accordance with the principles of the inertial oscillation. McNider et al. (1998) demonstrated the persistent nature of this phenomenon using wind spectra obtained from wind profilers deployed during the SOS95 Nashville Intensive. Under sufficiently weak synoptic forcing, the low-level jet and inertial oscillation dominated nocturnal transport. Trajectories derived from the wind profiler network deployed during SOS95 demonstrated the combined effect of these important features (see Fig. 2.5.3).

3. **Vertical transport is suppressed at night.** In the absence of convective storms, the atmosphere stabilized at night, which suppressed any significant vertical transport. In many cases, intermittent turbulence has been observed in the nocturnal boundary layer, which may be linked to wind shear associated with the low-level jet. The effect of intermittent turbulence on pollution levels at the surface is an important topic of current SOS research.

**KEY CITATIONS:**


Figure 2.5.3. Overnight forward trajectories calculated from the network of 915-MHz boundary-layer wind profilers deployed during SOS95. Winds were averaged over the 400-m vertical intervals shown in the key. Trajectories were calculated from an origin centered on Nashville, at 36.2°N, 86.8°E (after Banta et al., 1998).
2.5.3. Variations in Mixing Height

During the SOS95 and SOS99 studies, it was found that the daytime mixing height can vary considerably in the Nashville, TN area, especially when comparing the urban and adjacent rural areas. As mixing height is an important parameter affecting air pollution concentrations, this finding has significant implications for the regional distribution of ozone and particulates. Key results are summarized below.

1. **Remote sensors provide reliable measurements of mixing height.** A comparison of mixed layer depth estimates deduced from wind profiler and airborne lidar data showed very good agreement under clear or partly cloudy conditions (White et al., 1999). This result confirmed that radar wind profilers and lidars are well suited to measure the depth of the mixed layer and its variability.

2. **Mixing height variability is tied to land use differences.** Variations in mixing height are related to differences in surface characteristics, such as soil and vegetation type as well as surface moisture (see Fig. 2.5.4). During SOS99 Nashville Intensive, these different surface characteristics were reflected in varying energy, ozone, and carbon fluxes at the surface.

![Figure 2.5.4](image)

Figure 2.5.4. Time height cross section of aerosol backscatter gradient indicating the top of the mixed layer measured with the NOAA/ETL airborne lidar during midday on 12 July 1995 during a northwest to southeast transect over Nashville, TN (city of Nashville is in center of panel). The urban heat island over Nashville is clearly visible at flight times near 11:30 LST. Over forested areas to the northwest of Nashville (left side of panel) the mixed layer is strongly suppressed, while over suburban and agricultural terrain to the southeast (right side of panel) the mixed layer is only slightly shallower than over the city.

3. **Differences in mixing height are most pronounced under light wind conditions.** Under stagnant conditions, air parcels tend to dwell over regions of one surface type, which allows surface heating differences to express themselves as variations in mixing height. Stronger flow moves air parcels over many surface types, thus producing a more uniform mixing height.
4. **Urban heat island.** The strong differences in surface heating between the Nashville urban area and the surrounding agricultural and forested areas resulted in significantly deeper mixed layers over the city, especially under stagnant conditions. We frequently observed urban mixing heights of 2 km or more, which was as much as 800 m higher than the mixing heights over adjacent rural areas (see Figs. 2.5.4 and 2.5.5).

![Nashville 99 profilers July 4](image)

Figure 2.5.5. Hourly measurements of mixed layer depth on 4 July 1999 from the wind profiler network deployed in and around Nashville, TN during SOS 99. The wind profiler at Cornelia Fort airport shows a maximum mixed layer depth of about 2.1 km while all other profilers deployed in rural areas around Nashville detect peak mixed layer heights of only about 1.5 km.

5. **Model prediction of mixing depth.** We found that the Pennsylvania State National Center for Atmospheric Research Mesoscale Model 5 (PSU/NCAR MM5) has difficulty accurately predicting mixing depths under both stable and unstable atmospheric conditions. Deficiencies in the atmospheric radiation parameterizations are believed to have caused excess energy in the model’s surface layer. MM5’s response to this additional input resulted in daytime mixed layers that were too deep.

**KEY CITATIONS:**


2.5.4. Vertical Distribution of Ozone, Precursors, and Aerosols

The vertical distribution of ozone, precursors, and aerosols is influenced to a large extent by the dynamical processes described above. The key findings are:

1. **The vertical distribution of pollutants in the daytime mixed layer.** Mixing processes due to convective or mechanical turbulence acted to smooth out vertical inhomogeneities in the daytime boundary layer. Figure 2.5.6 shows a high-ozone layer near the surface mixing vertically as convective turbulence increased over the course of the morning.

![Figure 2.5.6. Series of vertical profiles of ozone concentration measured with the NOAA/ETL airborne ozone lidar on the morning of 12 July 1995. The ozone profiles are each spaced about 50 min apart, starting at 7:30 CDT and showing the vertical redistribution of ozone as the mixed layer grows.](image)

2. **The vertical distribution of pollutants at night.** Due to a lack of vertical mixing (see Section 2.5.2) pollutants tended to form horizontal layers or patches that persisted throughout the night until they were mixed out by the growing boundary layer the next morning. Fig. 2.5.7 depicts the cross section of a power plant plume that had been injected into the stabilizing evening atmosphere. In the absence of any significant vertical mixing the power plant plume stayed confined to a thin vertical layer.

3. **Pollutant levels in the free troposphere are affected by long-range transport or stratosphere-troposphere exchange processes.** Ozone sonde and aircraft measurements from the Nashville 95 and 99 campaigns showed that levels of ozone and other pollutants in the free troposphere were highly variable and were primarily affected by regional to continental-scale advection of clean or polluted air masses. Another significant process contributing to high tropospheric ozone levels is the intrusion of stratospheric air. Through entrainment processes (see Section 2.5.1) pollutant concentrations in the lower free troposphere can impact the air quality in the atmospheric boundary layer and at the surface.
Figure 2.5.7. Cross section of Cumberland power plant plume measured with the NOAA/ETL airborne ozone lidar on the evening of 4 July 1999 at about 10 km downwind of the power plant. The plume is easily identified by its low-ozone signature. Note that the plume is confined to the layer between 800 and 1200 m ASL.

KEY CITATIONS:
2.5.5. **Conclusion — Policy-Relevant Findings Regarding Dynamics and Mixing on Urban and Regional Scales**

Meteorological studies carried out under SOS have resulted in the following policy-relevant findings:

1. **Daytime Transport.** During the day, synoptic winds control horizontal transport. In the absence of synoptic forcing, vertical transport mechanisms such as convection, entrainment, subsidence, venting become increasingly important.

2. **Nighttime Transport.** Under sufficiently weak synoptic forcing, the low-level jet and inertial oscillation dominate nocturnal transport while vertical transport is suppressed. Thus, nocturnal transport tends to redistribute pollutants horizontally rather than vertically.

3. **Variations in Mixing Height.** Daytime mixing height variability is tied to differences in land use, with the most prominent differences in mixing height being observed between urban area and surrounding rural regions. Remote sensors (lidar, radar) provide reliable estimates of mixing height for air pollution applications.

4. **Vertical distribution of Ozone, Precursors, and Aerosols.** The vertical distribution of pollutants in the boundary layer is most uniform during the day. Under sufficiently weak synoptic forcing, the vertical distribution of pollutants at night is inhomogeneous because of the stable stratification of the atmosphere. Pollutant levels in the free troposphere are primarily affected by long-range transport or stratospheric intrusions.
2.6. GAS PHASE MEASUREMENT TECHNOLOGIES - DEVELOPMENT AND INTERCOMPARISON OF TECHNIQUES  
Eric Apel and David Parrish

Full understanding of the photochemistry that produces ozone and PM$_{2.5}$ requires ambient measurements of the precursors, intermediates (radicals as well as more stable species), and products. These measurements must be made with high and well-defined sensitivity, accuracy, precision, and specificity, and with fast time response (particularly ~ 1 Hz for aircraft measurements). The achievement of these goals is an evolutionary process requiring careful instrument development and operation in the field. This section summarizes the major progress of the SOS research program in this area.
2.6.1. Major Advance: Chemical Ionization & Proton Transfer Mass Spectrometry

The combination of mass spectrometry with chemical ionization (CIMS) potentially provides a sensitive and specific measurement technique for many atmospheric species. SOS-sponsored work includes the development, testing, and deployment of CIMS techniques for the measurement of HNO₃, isoprene, and ammonia as well as the deployment and testing of proton transfer (PTR-MS) instruments. The PTR-MS instruments can detect most gas-phase organic species with excellent time response, but their sensitivity and specificity are limited for many compounds by the manifold of organic species and fragment ions with similar masses. Highlights of this work are summarized below.

1. Specific HNO₃ Measurement Developed. A CIMS instrument to measure gas-phase HNO₃ was developed and demonstrated to be sensitive with fast response (detection limit of approximately 10 pptv at 1 Hz), accurate, precise, and interference-free. It has been tested in a ground-based intercomparison and deployed on aircraft during SOS 1999 and 2000 field intensives.

2. PTR-MS Deployed and Tested. PTR-MS instruments have been deployed at ground sites and on aircraft along with other instruments for measurement of several organic species. Intercomparison of the coincident measurements will help to define the capabilities of the PTR-MS instruments.

3. CIMS Isoprene and Ammonia Measurements Developed. CIMS techniques for measurement of isoprene and ammonia have been developed and tested in ground-based intercomparisons. These techniques promise to provide sensitive and fast aircraft measurements of those species. The selectivity of the isoprene technique must be tested by comparison to other techniques.

KEY CITATIONS:
2.6.2. Major Advances: Odd Hydrogen Radical Techniques

The hydroxyl radical (OH), the main oxidant in atmospheric chemistry, cycles rapidly with the hydroperoxyl radical (HO₂), initiating the production of ozone and other pollutants. A now widely accepted measurement technique for OH and HO₂, together called HOₓ, is laser-induced fluorescence in detection chambers at low pressure. This technique was applied for the first time to continuous, 24-hour measurements on 10-meter tall towers in Nashville in 1999 and at TEXAQS 2000 in Houston. In addition, a new, unique instrument was developed to measure the OH loss rate due to reactions with other atmospheric chemicals. This new instrument, the Total OH Loss-rate Measurement (TOHLM), was successfully deployed for the first time in Nashville in 1999. The combination of HOₓ measurements and TOHLM provides powerful new diagnostics for understanding and testing the oxidation chemistry of any environment.

1. **First continuous OH and HO₂ measurements in urban environments.** The measurements, when compared to models, test the fundamental atmospheric chemistry that underpins chemical transport models. For Nashville SOS, OH and HO₂ measurements agree to within a factor of two with model calculations near midday, but tend to be larger than models in the evening, at night, and for periods when nitrogen oxides are especially abundant. These observations indicate unidentified HOₓ sources and questions about HOₓ-NOₓ chemistry.

2. **Total OH Loss-rate Measurement tests the completeness of measured VOC inventories.** The presence of unmeasured VOCs is indicated if TOHLM-measured OH loss rates are greater than those calculated from the sum of VOC measurements and OH reaction rate coefficients. Preliminary Nashville observations indicate that OH loss rates are about twice those calculated, suggesting unmeasured VOCs.

**KEY CITATION:**
2.6.3. Non-Methane Hydrocarbons (NMHCs): Intercomparisons of Techniques

NMHCs, emitted from a variety of sources, are precursors to ozone and PM$_{2.5}$, and some species are considered toxins. NMHCs are the primary photochemical fuel in urban and many rural areas whereas carbon monoxide and methane play this role in regions remote from sources. Biogenic NMHCs dominate the VOC chemistry in many highly forested regions and even in urban areas situated in regions surrounded by forests, as is the case in most cities located in the SOS domain (southeastern U.S.) [e.g., Chameides et al., 1997]. Anthropogenic NMHCs dominate in most other urban areas.

1. Accuracy of NMHC Measurements Tested. Because of the large role of NMHCs in ozone formation, it is imperative that measurements accurately reflect the true atmospheric composition. SOS has taken a leadership role in the atmospheric science community and has partnered with the NOAA Climate and Global Change Program in conducting “The Non Methane Hydrocarbon InterComparison Experiment” (NOMHICE). This experiment was designed to assess the accuracy of analytical methods used to determine mixing ratios of atmospheric non-methane hydrocarbons (NMHCs).

2. NMHC Measurements Intercompared in the SOS Network. To help ensure quality measurements and to understand where there are problems, intercomparisons of NMHC measurements are conducted in the SOS network before and during every field study. Prior to the Nashville 99 Field Study nine measurements were intercompared. For each measurement, a set of canisters were simultaneously collected at the Cornelia Ft. site in Nashville, TN and distributed to 4 groups for analysis. Figure 2.6.1 shows the mean ratio of each laboratory’s analysis of a given compound to that of the reference laboratory (EPA-Lonneman). It is apparent that for some species, the accuracy of the analyses is good (agreement to within 11% for all groups), but for some species there were errors up to a factor of 5. Some of the problems could be corrected during the experiment. For example, the discrepancy of the Argonne data for i-pentane was determined to be due to an overlap with another peak and corrected. The precision of the measurements of the individual species by the different laboratories is indicated by the standard deviations of the ratios. These standard deviations ranged from very good (±3%) to quite poor (factor of 3).

3. High Quality Multi-Component Standards Developed. Eight identical standards containing 100 NMHC were developed and tested for the TexasAQS 2000 study. These standards were used as a common calibration source for all participants in the study.
Figure 2.6.1. Comparison of the mean ratios of selected NMHC measurements from 4 different SOS measurement groups using EPA-Lonneman results as reference.

**KEY CITATIONS:**


2.6.4. Formaldehyde Technique Development and Intercomparisons

Formaldehyde (CH$_2$O) is a primary emission product from internal combustion engines and is produced in the atmosphere by the photochemical oxidation of methane and non-methane hydrocarbons (NMHCs). It is the most abundant gas-phase carbonyl compound in both urban areas and the remote troposphere. Formaldehyde is extensively connected with the odd hydrogen (HO$_x$ = H+OH+HO$_2$) and odd nitrogen (NO$_x$ = NO + NO$_2$) chemical cycles. It is also a major source for HO$_2$ and for CO in air not strongly perturbed by anthropogenic sources. Consequently, accurate measurements of formaldehyde are critical to understanding the overall tropospheric chemistry leading to hydrocarbon oxidation, the processes controlling the odd hydrogen cycles and nitrogen cycles, and the global budgets of OH and CO.

1. Two Measurement Techniques Developed. SOS has encouraged the development of fast and sensitive techniques to measure formaldehyde. Two techniques, tunable diode laser absorption spectroscopy (TDLAS) and coil/2,4-dinitrophenylhydrazine (CDNPH), have emerged which satisfy the necessary criteria for ground-based and aircraft-based measurements. These techniques have been used extensively in SOS field studies. The TDLAS technique can provide 1-second averages, while the CDNPH technique has been limited to averages of at least 1 minute.

2. Two Field Intercomparisons Completed. A blind intercomparison of six ambient formaldehyde measurement techniques was conducted at the National Center for Atmospheric Research (NCAR) in Boulder, CO, from May 29 to June 3, 1995. It was concluded that gas phase standards should be employed with any of the measurement techniques, and the cartridge measurement methods are limited by long collection periods, generally lower precision, and the incomplete understanding of potential interferences from ozone and possibly other compounds. Airborne CH$_2$O measurements by TDLAS and CDNPH techniques indicated that, on average, both instruments measured identical ambient CH$_2$O concentrations to better than 0.1-ppbv over the 0 to 0.8-ppbv-concentration range. However, significant differences, larger than the combined 2σ total uncertainty estimates, were observed in 29% of data set. It is clear that careful attention must be paid to the behavior of CH$_2$O in the inlet for accurate airborne measurements.

3. CH$_2$O Gas Phase Standards Developed. Through SOS support, formaldehyde standards have been produced in high-pressure cylinders at the ppmv level. Techniques have been developed, including FTIR and GC-FID, to verify the concentration of the standard. Long-term stability tests are presently being conducted.

KEY CITATION:
2.6.5. Carbonyl Technique Development and Intercomparisons

Aldehydes and ketones and other oxygenates are produced by the oxidation of hydrocarbons, and some are emitted directly. Until recently, this compound class has received much less attention than its VOC counterpart, the NMHCs. This is largely due to difficulties encountered in measuring these compounds. SOS has taken a leading role in developing carbonyl standards, carbonyl measurement techniques, and evaluating the techniques with intercomparisons. Through these studies, it is becoming apparent that the carbonyls and other oxygenates may be more ubiquitous than previously thought, and hence contribute significantly to photochemical processes in the troposphere.

1. The first quantified and verified carbonyl standards. Carbonyl standards have been prepared gravimetrically with both calibrated permeation sources and in specially treated aluminum cylinders. Techniques such as atomic emission detection (AED) (Apel et al., 1998a) and FTIR have been applied to verify the accuracy of the standards. Table 2.6.1. demonstrates the verification of a prepared standard.

Table 2.6.1. Quantification of Standards Results

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<td>3.2 ± 0.4</td>
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<tr>
<td>Propanal</td>
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<td>n.d</td>
<td>n.d.</td>
</tr>
<tr>
<td>Butanal</td>
<td>3.02 ± 0.03</td>
<td>n.d</td>
<td>n.d.</td>
</tr>
</tbody>
</table>

*analysis based on calibration factors from permeation tubes
n.d. - not determined

2. Intercomparison completed. Cartridge–based (Si-Gel and C18) and GC-MS measurements have been intercompared through SOS. Serious discrepancies were found and more work is needed to resolve these differences.

3. New techniques developed. A new relatively fast-response (15 minute cycle) GC-FID technique has been developed to measure carbonyls and other oxygenates aboard aircraft. A new GC-MS technique is currently being developed to measure carbonyls with a 5-minute time response.

KEY CITATIONS:

2.6.6. NO$_2$ and NO$_y$ Technique Development and Intercomparisons

The oxides of nitrogen (NO and NO$_2$) are precursors of ozone and PM$_{2.5}$, and the total oxidized nitrogen family (NO$_y$) in an air parcel represents the total emissions of these precursors that remain in the atmosphere. Improvements in the measurement of these species are summarized below.

1. Improved NO$_2$ measurements by photolysis-chemiluminescence. A new photolytic converter utilizing the focused UV output from a high-pressure mercury (Hg) arc lamp was developed and tested. The new configuration permits simple and accurate retrieval of ambient NO$_2$ data at very high time resolution, is more specific, provides increased sensitivity, and is less expensive to operate than previous photolytic converter designs.

2. Validation of an aircraft inlet for HNO$_3$ and NO$_y$. Rapid and quantitative sampling of NO$_x$ species, including HNO$_3$, has been demonstrated using a short, heated Teflon inlet. In flight, standard addition calibrations of HNO$_3$ at the aircraft inlet demonstrate freedom from significant surface adsorption of HNO$_3$, which has significantly compromised measurements through other aircraft inlets.

3. Intercomparisons of ground-based NO$_2$ and NO$_y$ measurements. Intercomparisons during SOS field intensives have demonstrated that laser-induced fluorescence, differential optical absorption spectroscopy, and photolysis-chemiluminescence techniques are all capable of accurately quantifying atmospheric NO$_2$ above 1 ppbv. Further, MoO and Au converters were shown to be capable of accurately measuring NO$_y$ above 2 ppbv in the urban and suburban environments typical of the SOS region. These studies further concluded that generation of reliable NO$_2$ or NO$_y$ data still demands skilled operators and dedicated, critical oversight during the measurement process.

KEY CITATIONS:
2.6.7. Organic Nitrate Technique Development

Several advances have been made in the measurements of organic nitrates through the course of SOS. Emphasis has been put on improving separation and quantitation of compounds that are of biogenic origin, and on developing rapid methods for aircraft measurements.

1. Measurements of peroxyacyl nitrates (PANs). Gas chromatographic methods for PANs have been refined to provide rapid and sensitive measurement. Aircraft-based instrumentation was developed to measure four of the major compounds of interest, PAN, PPN, PiBN, and MPAN, every 3.5 min. The measurement of PANs by proton-transfer reaction mass spectrometry (PTR-MS) was deployed during the Nashville 99 intensive (Hansel and Wisthaler, 2000). While still in the development stage, this method has the potential to provide rapid (10 sec) measurements of PAN aboard aircraft.

2. Development of PAN calibration systems. Two different calibration methods for PAN have been developed: a diffusion source and photochemical production of PAN in acetone/air/CO/NO mixtures. The diffusion system relies on an NO$_x$ measurement for calibration, while the photochemical source relies on a known, efficient conversion of an NO standard to PAN. The two were compared during the TEXAQS 2000 study and were found to agree within 5%.

3. Development of organic nitrate measurements. An automated system for the measurement of the organic nitrates produced from OH radical attack on isoprene was developed and deployed at the Dickson site during SOS 99. These compounds result when the peroxy radicals derived from OH reaction with isoprene, react with NO to produce a set of 8 isomeric RONO$_2$ species. The maximum concentrations of the sum of these species were in the 100-200 pptv range, much higher than observed in a previous study. Comparison of these two data sets provides a good opportunity to examine the NO$_x$-dependence of this aspect of isoprene photochemistry.

KEY CITATIONS:
2.6.8. Carbon Monoxide Technique Development and Intercomparisons

Carbon monoxide is a long-lived gas primarily emitted in automobile exhaust, which makes it a useful tracer for urban pollution plumes. The result of an SOS effort to develop an instrument for aircraft measurements of this species is summarized below.

1. Development of an instrument based upon vacuum UV resonance fluorescence of CO.

An instrument was developed that is capable of fast (~1 Hz), accurate (~5%), and precise (~1 ppbv) measurement of CO from an aircraft platform. Intercomparisons with other techniques demonstrate that it is highly specific with no identified interferences (see Figure 2.6.2).

![Figure 2.6.2. Time series of coincident 5-second-average measurements of CO. The solid lines give tunable diode laser absorption (darker) and the vacuum ultraviolet fluorescence (lighter) results and the dotted line indicates the aircraft altitude. The features labeled 1 through 4 are intercepted urban plumes.](image)

KEY CITATION:
2.6.9. Conclusion — Policy-Relevant Findings Regarding Gas Phase Measurements

1. Chemical Ionization & Proton Transfer Mass Spectrometry can provide accurate and sensitive measurements for a wide variety of species. Instruments based on CIMS have been developed that are capable of fast (~1 Hz), accurate (~5%), and precise (~ ±0.1 ppbv) measurement of HNO$_3$, isoprene, and NH$_3$. PTRMS instruments can detect most gas-phase organic species, including peroxyacyl nitrates, with excellent time response, but compared to CIMS instruments, their sensitivity and specificity are more limited.

2. The technology exists for investigating odd hydrogen radicals in urban atmospheres. Instruments have been developed to continuously measure ambient concentrations of OH and HO$_2$, as well as the OH loss rate in urban atmospheres. They have been deployed in Nashville 1999 and TEXAQS 2000. The resulting data sets will be invaluable for characterizing the sources and sinks of these critical species.

3. A critical need of the atmospheric chemistry community is a formal intercomparison of NMHC measurement techniques. Work carried out during SOS demonstrates that for many NMHC species, large uncertainties remain in their measurements. The importance and ubiquity of measurement errors can be evaluated only through such intercomparisons.

4. The technology exists for the accurate measurement of formaldehyde. Two techniques have been developed for the measurement of ambient CH$_2$O concentrations. The TDLAS technique can provide 1 Hz time response. An airborne intercomparison showed that, on average, the two techniques agreed to better than 0.1 ppbv at sub-ppbv concentrations. However, the observed differences were larger than could be explained by uncertainty estimates.

5. Significant progress has been made in the development of the technology for the accurate measurement of other critical atmospheric species. A great deal of effort has been invested in new technology and in improving existing technology. Important advances have been made in the measurement of carbonyls, NO$_2$, NO$_y$, organic nitrates, and carbon monoxide.
2.7. OBSERVATION BASED ANALYSIS  
Larry Kleinman, Carlos Cardelino, Sandy Sillman, Gail Tonneson

A challenge that the atmospheric sciences community faces is to translate the measurements made during field programs into knowledge about the processes responsible for elevated pollutant concentrations and the efficiency of possible control measures. The traditional way of proceeding is to use field observations to validate emissions based models. A complementary approach, which has been pioneered by the SOS community, is to use Observation Based Analysis—a family of techniques that attempts to relate questions about processes and emission controls directly to measured concentrations. The promise of observation-based methods is that by bringing in the actual atmospheric concentrations there is less reliance on ill-characterized emissions, computational demands are lessened, and an element of reality is imposed on the problem.

Measurements are intrinsically local in that they provide information about the state of an air mass at the time and place that the observations occur. From local measurements we hope to do two things: 1) Deduce rates and sensitivities which cannot be measured, for example the production rate of O₃ and its sensitivity to NOₓ and VOCs. 2) Deduce the effects of emission controls, which depend on the entire time history of the air mass.

Observation based analysis establishes a link between processes and observations. This linkage is one that an emissions based model must reproduce to give credible predictions on emission controls. Observation based techniques thereby suggest criteria for evaluating model performance that goes beyond the usual matching of O₃ concentration fields.
2.7.1. O₃ Production Rate and Sensitivity

The comprehensive sets of measurements obtained at surface sites and from aircraft allow one to calculate the local rate at which O₃ is produced and the dependence of this rate on precursors. Analytic formulas provide a framework for generalization and a theoretical rational for Indicator ratios (see Section 2.7.2).

1. Ozone Production Rate, P(O₃). Consistency between different methods of determining P(O₃) is an important test of theoretical understanding and measurement procedures.

2. Ozone Production Rate – NOₓ and VOC Sensitivity. The SOS community has developed two complementary ways of analyzing the local rate and sensitivity of O₃ production: by means of a radical budget and by means of radical propagation efficiency. These methods yield insights and useful formulas. Generalizations provide the basis for Indicator Ratio methods.

- **Radical Budget.** Photochemistry under NOₓ-sensitive conditions preferentially forms peroxides; under VOC-sensitive conditions NOₓ compounds are preferentially formed. The sensitivity of P(O₃) to NO and VOCs is given by a simple analytic function of "LN/Q", the fraction of free radicals removed by reacting with NOₓ.

![Figure 2.7.1. Diurnal profile for P(O₃) calculated from data collected during the ROSE campaign at a rural site in Alabama in June-July, 1990. P(O₃) calculated using a steady state model (SSM), photostationary state (PSS), radical budget (RB), and from peroxy radical concentrations measured with a chemical amplifier (CA). Vertical bars indicate variability of average hourly values. (Frost et al., 1998).](image1)

![Figure 2.7.2. The relative sensitivity of O₃ production rate to [NO] and [VOC] as a function of the fraction of radicals reacting with NOₓ. Solid lines are analytic formulas. Data points are from constrained steady state box model calculations driven from observations taken during the 1995 Nashville campaign. (Kleinman et al., 1997).](image2)
- **Radical Propagation Efficiency.** \( \text{O}_3 \) is formed in a chain reaction. A simple version is:

\[
\begin{align*}
\text{OH} + \text{VOC} & \rightarrow \text{HO}_2 \\
\text{HO}_2 + \text{NO} & \rightarrow \text{OH} + \text{NO}_2 \\
\text{NO}_2 + \text{h}_\text{\<}\text{\<} + \text{O}_2 & \rightarrow \text{O}_3 + \text{NO}
\end{align*}
\]

Numerical calculations show that the \( \text{O}_3 \) yield is maximized when the chain length is long. Radical loss processes limit the chain length. At low \( \text{NO}_x \), \( \text{HO}_2 \) radicals combine to form peroxides; at high \( \text{NO}_x \), \( \text{OH} \) reacts with \( \text{NO}_2 \) forming \( \text{HNO}_3 \). The combination of these two loss reactions causes a maximum in \( \text{P(O}_3) \) at a particular \( \text{NO}_x \) concentration. The ratio of the peroxide to \( \text{HNO}_3 \) production rate tells us whether the atmosphere is on the low or high \( \text{NO}_x \) side of the maximum.

Figure 2.7.3a and b. A trajectory model, simulating Atlanta, GA was used to calculate \( \text{O}_3 \) (left panel) and \( \text{OH} \) radical chain length (right panel) as a function of initial \( \text{NO}_x \) and VOC concentration. Emissions were proportional to initial concentrations. Note that the \( \text{O}_3 \) ridgeline (bold diagonal line) is also a maximum in \( \text{OH} \) chain length. (Tonnesen and Dennis, 2000).

**KEY CITATIONS:**


2.7.2. Effects of Emission Controls: NOx vs. VOC sensitivity

1. Indicator Ratios. The local analysis described in 2.7.1 shows that under NOx-sensitive conditions, peroxides are preferentially formed as a by-product of O₃ production; under VOC-sensitive conditions NO₂ is preferentially formed. Observed concentration ratios containing these compounds thereby contain information on whether O₃ was formed under NOₓ- or VOC-sensitive conditions. An emissions-based model is used to determine the value of the indicator ratio that corresponds to the transition between NOₓ- and VOC-limited conditions. {See SOS I, Sec. 2.5.1}

Measured indicator ratios in the Nashville urban plume (O₃/NO₂ and H₂O₂/NO₂) are close to the values associated with the transition between NOₓ- and VOC-sensitive chemistry. In contrast, indicator ratios suggest that Atlanta is NOₓ-sensitive and Los Angeles is VOC-sensitive.

Figures 2.7.4a. and b. Variation of O₃, NO₂, and peroxides in the Nashville urban plume and surrounding rural areas on the afternoon of July 13, 1995. Panel (a) contains observations from the G-1 aircraft; Panel (b), Eulerian model predictions. Ozone varies from relatively low concentrations in surrounding rural areas to a maximum concentration in the Nashville urban plume. High values of O₃/NO₂ are associated with NOₓ sensitive chemistry in rural areas; low values with a transition between VOC and NOₓ sensitive chemistry where peak O₃ occurs. O₃/(2*H₂O₂ + NO₂) and O₃/(2*Peroxide + NO₂) are "test ratios" which according to theory should be relatively constant. The close agreement between model and observation in this case provides a measure of validation for the use of NOₓ – VOC indicators (from Sillman et al., 1998).
2. The Observation Based Model (OBM). The Observation Based Model provides an independent check on the precursor relationships predicted by emission-based air quality models. The OBM utilizes atmospheric observations (instead of emission inventories) to drive a photochemical model and infer sensitivities of ozone in an urban atmosphere to changes in the emissions of either VOC, NO\textsubscript{x}, or CO. The OBM was used to analyze data gathered at three photochemical assessment monitoring sites (PAMS): Washington, DC, Bronx, NY, and Houston, TX. Results of the analysis are summarized below.

- Natural hydrocarbons, primarily isoprene, represented a significant fraction of the total hydrocarbon reactivity and significantly degraded the efficacy of VOC emission reductions as an ozone mitigation strategy.

- Afternoon NO concentrations typically fell to levels at or below the limit of detection of the PAMS instrumentation and, as a result, it is not possible to determine whether ozone was more sensitive to reductions in anthropogenic hydrocarbons or nitrogen oxides.

KEY CITATIONS:


Figure 2.7.5. Variation in OBM-calculated relative incremental reactivities (RIRs) for nitric oxide (NO), anthropogenic hydrocarbons (AHC), natural hydrocarbons (NHC), and CO at the Bronx, New York site as a function of the assumed minimum afternoon NO concentration (from Cardelino and Chameides, 2000).
2.7.3. Process Based Evaluation of Emission Based Models

An evaluation of models used to establish ozone control policy must include a comparison between observed and predicted \( O_3 \) concentration fields. But models can have \( O_3 \) predictions that are substantially identical yet predict different sensitivities to \( NO_x \) and VOCs. Sillman et al. (1997) have shown that alternate model predictions on \( O_3 \) sensitivity can be distinguished one from the other according to their predictions of indicator ratios. The premise developed within the SOS community is that there is a robust relation between indicator ratios and \( O_3 \) sensitivity so that predicting these ratios correctly is strong evidence that a model can accurately predict the effects of emissions controls.

In a process based evaluation:

- Models should be evaluated by how well they perform for specific ratios (\( O_3/NO_x \), \( H_2O_2/HNO_3 \)) that are closely linked with \( NO_x \) or VOC sensitive chemistry
- The evaluation should be based on measurements that are concurrent with peak \( O_3 \) in the event.
- An evaluation should be done for a series of plausible model scenarios that give different results for \( O_3 – NO_x – VOC \) sensitivity.

Figure 2.7.6. Peak \( O_3 \) and concurrent \( NO_y \) in the Atlanta urban plume on August 10, 1992. The X's represent helicopter measurements at 600m elevation, 4:00-5:00 pm, located within 4 km of the location of measured peak \( O_3 \). Bold letters represent domain-wide peak \( O_3 \) and concurrent \( NO_y \) at 600m elevation, 4:00-5:00 pm for different model scenarios. The line represents the transition between \( NO_x \) and VOC sensitive chemistry based on \( O_3/NO_y \). Note that only 2 model scenarios are consistent with both \( O_3 \) and \( NO_y \) observations. Both scenarios are \( NO_x \)-sensitive (from Sillman et al., 1997).

KEY CITATION:
2.7.4. Conclusion – Policy-Relevant Findings for Observation Based Analysis

Use of observation-based methods to evaluate effects of emission controls has resulted in the following policy-relevant findings:

1. **Both NO\textsubscript{x} and VOC controls needed in Nashville.** Indicator species ratios show that peak O\textsubscript{3} levels in Nashville are neither strongly VOC sensitive or NO\textsubscript{x} sensitive, but rather are an intermediate case where the optimum control strategy will involve reductions in both categories of precursors.

2. **Weight of evidence.** State Implementation Plans for meeting O\textsubscript{3} standards can use methods other than the traditional emission based modeling approach to demonstrate that progress is being made. Indicator Species methods and the Observation Based Model are complementary approaches to emission based models. These techniques are well-grounded in theory and bypass many of the difficulties associated with conventional modeling approaches.

3. **Models can give right O\textsubscript{3} for wrong reason.** The traditional method of demonstrating skill with a regulatory model is to duplicate within some tolerance limits, the observed patterns for O\textsubscript{3}. This, however, is no guarantee that a model can accurately predict effects of emission controls. Process oriented tests of model performance provide a more robust evaluation of model performance.

4. **Ubiquity of biogenic hydrocarbons.** Significant daytime concentrations of isoprene from biogenic sources are found in urban areas that degrade the efficacy of anthropogenic hydrocarbon reductions in controlling ozone levels.

5. **Afternoon NO concentrations.** If data from monitoring networks are to be used to diagnose ozone precursor relationships, these networks will need to use instrumentation capable of reliably quantifying NO concentrations at the sub-ppbv level.
2.8. EMISSIONS BASED MODELING
Richard McNider, Robert Imhoff, and Prasad Kasibhatla

Emissions based modeling has always been at the core of the SOS programs. While the emphasis in SOS clearly has been observations, it was always intended that the emissions based models would serve as a synthesis point for the observations and as a means to test model performance and fidelity. Because of the delay in actually getting observational and supporting auxiliary data sets in place, many of the modeling efforts have involved sensitivity studies and in improving model components or processes.
2.8.1. **Strengths and Limitations**

2.8.1.1. **Auxiliary Emissions Based Modeling Activities**

In the last 5-7 years the SOS program has focused on field observation activities, thus the program level of support for emissions based modeling from the core budget of SOS has been relatively small. At the same time, the SOS program has facilitated and nurtured a substantial number of emissions based modeling activities funded outside the core EPA budget by other agencies, EPA grant programs, or through in-house activities by SOS cooperators within EPA and NOAA. The SOS modeling community fostered these activities through workshops, observational data support, and intellectual contributions. Some of these activities are discussed below in the larger context of SOS contributions.

These separately funded and collaborative programs are described below.

6. **The Ozone Transport Assessment Group (OTAG)** carried out an assessment of the role of transport in ozone episodes using emissions based models. Tennessee Valley Authority (TVA) and EPRI played a major role in this activity. One of the four OTAG episodes centered around the July 1995 episode, which included the Nashville 1995 Intensive period. Both TVA and University of Alabama at Huntsville (UAH) utilized special meteorological data collected during the intensive to evaluate winds in the model. In addition, several SOS investigators and groups contributed time and effort in the review and analysis of these simulations.

7. **Southeast States Air Resources Managers (SESARM) Seasonal Modeling of Regional Air Quality (SMRAQ).** Microelectonics Center of North Carolina (MCNC), Duke University, and Georgia Tech developed a very innovative program to test the fidelity of emissions based models in a seasonal context rather than an episodic mode. This program was fostered by SOS and funded by the States in the Southeast with some contribution from utilities. SOS investigators played a major role in design and review of this modeling effort and the 1995 field program observations were a key conceptual opportunity for model evaluation for this activity.

8. **Southern Appalachian Mountain Initiative (SAMI).** Georgia Tech, TVA, UAH, Alpine Geophysics, and other groups are carrying out a comprehensive study of air quality in the Southern Appalachians. This program was funded by the States in the Southeast, the U.S. EPA, and Congressional appropriations. The core understanding of Southeast modeling issues and supporting data were key to the conceptual design and evaluation of this activity. Several SOS investigators contributed to this effort.

9. **EPA Competitive Grants Programs.** Several SOS investigators have been successful in winning emissions based modeling grants from EPA Headquarters. The SOS connectivity has almost certainly helped during the policy relevance review portions of this competitive process. Specifically, UAH won activities related to satellite assimilation, plume-in-grid
modeling and coupled chemical, large eddy simulations. University of Michigan won grants related to developing indicator species.

10. NOAA and EPA In-House Modeling Programs. Both the NOAA Aeronomy Laboratory and EPA Research Laboratory at RTP have conducted large domain regional simulations and also small domain plume studies. These studies have been spurred in part by the SOS observational program, and SOS scientists have been involved in the planning and evaluation of these modeling activities.

2.8.1.2. SOS Community Modeling Activities

While the SOS program early on saw the long-range utility of coupling the robust observational program with a strong emissions based modeling component, it was clear that because of program priorities and the distributed nature of SOS that a new paradigm was needed for the modeling program to be viable.

In conjunction with EPA’s NERL Modeling Branch, UAH coordinated a workshop in April 1999 to explore and define a structure for an SOS Modeling Program. At the workshop, overviews of SOS modeling activities were given by a variety of SOS investigators. A broad discussion was held concerning the future and structure of an SOS Modeling Program. From this discussion the concept of a distributed SOS Community Modeling built around the use of MODELS3 was formulated. This structure was based on the premise that no one organization possessed all the skills, talents and infrastructure necessary to carry out a state-of-the-art emissions based modeling program. However, if each university (or partner such as TVA) could contribute in the areas that they have expertise, then the combined skills and talents were there. For example, UAH might support the meteorological modeling component, while GIT might contribute in the area of emissions modeling and University of Michigan in the area of chemical mechanisms.

This SOS Community Modeling Framework has begun. UAH is taking the lead in coordination and putting the Models3 framework in place. Preliminary meetings have been held with GIT and TVA to plan the emissions development process. While the heavy field program load in the past year has limited the attention to this community modeling program, it is expected that such a distributed community modeling program is the proper framework for SOS modeling investigators to make substantial contributions in the Nashville, Atlanta, and Houston field program settings.
2.8.2. Photochemical Mechanisms

The Carbon Bond IV Mechanism (CB4) has been the primary photochemical mechanism used in regulatory settings for testing and setting strategies by local, State, and Federal regulators. Investigators under the SESARM activities explored the role of a seemingly small modification in the CB4 mechanism related to organic peroxy radicals that affect organic nitrate formation. They demonstrated that the simulated large distribution of ground-level ozone is extremely sensitive to this modification, especially in regions of relatively low NOx emissions. The change effectively reduces the rate of formation of organic nitrate in the atmosphere, thus that portion of the NOy that is removed as active in ozone formation.

Previous tests of this mechanism change in the Northeast had shown only modest changes in ground level ozone (5-10 ppb). However, this study showed that in the Southeast this mechanism change could alter ground level ozone by 10-25 ppb. The authors also stressed that the sensitivity of ozone to this mechanism change increased the importance of understanding the nitrate budget in the Southeast.

In a similar vein as this study, Biazar (1996) also showed extreme sensitivity to the handling of organic nitrates in the modeling framework especially in the inclusion of deposition losses for MPAN. Once organic nitrates are formed, the rate of removal of nitrogen in the system through surface deposition losses compared to thermal decomposition freeing the nitrogen for subsequent ozone formation. With the inclusion of deposition losses of MPAN in a rural environment, nitrogen was rapidly removed from the system, leading to much lower ozone levels.

KEY CITATIONS:
2.8.3. **Role of Temperature in Ozone Production**

Observational studies of ozone have shown a strong positive dependence with increasing temperature. SOS investigators explored the causality of this relationship employing a photochemical model. Their study concluded that in the model a significant portion of the ozone-temperature relationship is associated with temperature dependence in the chemistry mechanism, especially in the thermal decomposition of PAN and its homologues. The thermal decomposition evidently increases the available NOₓ for photochemical production. Although not mentioned specifically, at lower temperatures the greater partitioning into PAN and other organic nitrates allows more efficient surface removal.

While the study relates the primary ozone/temperature relationships in the model to the chemical mechanisms it did note that isoprene emission dependence also plays a role. It also noted that ozone/temperature dependence in the model is less than in observational studies postulating that other mechanisms such as anthropogenic emissions dependence on temperature as a factor.

**KEY CITATION:**
2.8.4. Regional Surface Ozone Predictability

In order to determine model performance outside of the traditional episode mode, the results and performance of a seasonal photochemical model for the eastern U.S. was carried out for the summer of 1995. The model was the MAQSIP Model driven by the MM5 meteorological model in a data assimilation mode with the MM5 reinitialized every five days. Primary emphasis was placed on model performance in rural areas.

In an analysis of the seasonal model results, a comparison of daytime average ozone produced by the model with observed values, showed virtually no bias and a relatively strong correlation at both low and high concentrations. On the other hand, when model performance on a day-to-day basis was examined, the results showed that on many days the model showed very little skill. This seemed especially true of some of the higher domain average ozone days. The large paired-in-space-and-time errors may have been due to not having modeled clouds at the right place and time.

Figure 2.9.1. Day to day variation in the Pearson correlation co-efficient (solid line) and the observed domain-mean 10am- 5pm average surface ozone concentration (dashed line) (from Kasibhatla and Chameides, 2000).
In addition to this study, SMRAQ investigators have teamed with investigators in the Northeast to co-evaluate modeling for the Eastern U.S. by the NARSTO NE modeling team for the month of July 1995, which overlaps the SMRAQ. This study concluded that predictions of ozone are insignificant on the intra-day time scale, high for the diurnal component, low for the amplitude of the diurnal component and highest yet for the synoptic scale. The modeling results show that the higher frequency (several-day or less) mesoscale characteristics are not well replicated in the models. Thus it was suggested that for regulatory purposes longer-term simulations may be preferred to episodic simulations.

KEY CITATIONS:
2.8.5. Meteorological Predictability

Meteorological models are utilized to produce the physical atmosphere to carry out photochemical simulations and control strategy tests. The characteristics of the meteorological model in large part control model performance especially for paired-in-space-and-time statistics. Joint studies of meteorological model performance for the SMRAQ 1995 seasonal modeling and the Northeast NARSTO July 1995 modeling were carried out looking at meteorological model performance. SMRAQ used the MM5 model, and the NARSTO NE study used the RAMS model. These studies showed that in both models the higher frequency intra-day fluctuations were not well correlated with observations. Correlations were highest for the longer time scale (synoptic) components. In a separate study of the temporal spectral characteristics of profiler data taken during Nashville ‘95, it was shown that models underestimate the magnitude of the diurnal/oscillations compared to observations. This study also argued that there is an inherent spectral gap in models where the spectral energy at spatial scales less than several model grid scales and above the PBL scale is not included in the simulations. This conclusion is evidently in keeping with the MM5 and RAMS results.

KEY CITATIONS:
2.8.6. Control Strategy Sensitivity

In this study the Regional Oxidant Model (ROM) was used to carry out a sensitivity study examining the relative sensitivity of changes in ozone to reductions of VOCs and NO\textsubscript{x}. A simulation period July 2-10, 1988 was used. A very deliberate and methodical set of reductions of NO\textsubscript{x} and VOC emissions in 25% increments both separately and concurrently were carried out. The initial state was based on 1988 emissions. A comparison of modeled versus observed ozone patterns showed relatively good skill, but the point-to-point comparisons were less favorable, showing large scatter. ROM underpredicted daily maximum O\textsubscript{3} for most of the distribution. There did seem to be tendency for bias toward underprediction in the Southeast. This bias was absent in the Northeast, but scatter was greater.

![Response surface plots of maximum ozone (ppb) to NO\textsubscript{x} and VOC emission reductions on July 4, 1988 for (a) western Gulf Coast, (b) Southeast, (c) interior Northeast, (d) Northeast Corridor, (e) Lake Michigan, (f) Ohio Valley, and (g) eastern Great Lakes Region (from Roselle and Shere, 1995).

The sensitivity study showed that NO\textsubscript{x} reductions led to significant reductions of maximum ozone over large areas. VOC reductions did reduce maximum ozone near major urban areas.
However, reducing NO$_x$ by 50% in general had a larger impact than a 50% reduction in VOCs. These results indicate that much of the Eastern U.S. is NO$_x$-limited. While some of the northern subregions (Northeast Corridor and Lake Michigan) were VOC-limited at least some of the time, the Southeast was predicted to be NO$_x$-limited for the entire distribution. Because the anthropogenic VOC emissions were believed to be underestimated generally, the sensitivity to NO$_x$ emissions could be even greater than the model indicated. Because of the large-scale grid resolution (18.5 km), the authors caution against application of the results near large NO$_x$ and VOC sources.

**KEY CITATION:**
2.8.7. Model Performance Evaluation Using Chemical Signals

Comparison of UAM and UMICH model results with observations were carried out during the 1992 Atlanta Intensive. Two days were examined in detail, 10-11 August. Vertical variation of primary organic species was used to assess the extent of vertical mixing of the model. The model underestimated isoprene, but overestimated reaction products of isoprene such as HCHO. Meteorology could be manipulated within the range of uncertainty to alter the modeled ratio of O3/NOy from too low to too high. Most of the model domain showed peak O3 sensitivity to NOx and little sensitivity to ROG. However the locations downwind from Atlanta, characterized by the highest peak O3, also include ROG-sensitive chemistry. Peak O3 was more sensitive to NOx in all cases. The O3/NOy ratio was used as a test for O3-NOx-ROG sensitivity. Scenarios created to force the system into ROG sensitivity tended to estimate O3 correctly but underestimated the O3/NOy ratio.

Net ozone production efficiencies (OPE) which have been reported based on observed O3/NOz slopes likely overestimate the true net OPE. This is due to the rapid deposition of NOz species, especially HNO3. Model results were consistent with a dry deposition velocity of HNO3 and H2O2 of 5 cm s\(^{-1}\), which is higher than values commonly used (2.5 cm s\(^{-1}\)) but are consistent with measurements of differential loss rates between SO2 and NOy observed by the helicopter in power plant plumes. The modeled OPE for various sources were compared, taking into account the NO2 loss. The OPE for Nashville and a small power plant, Gallatin, were similar at about 3.2 to 5, while the OPE for the much larger Cumberland power plant ranged from 2 to 3. The indicator ratios in the Nashville urban plume indicate that the chemistry is intermediate between VOC- and NOx-limited. The authors could not firmly distinguish between the two alternatives.

KEY CITATIONS:


2.8.8. Role of Mixing Processes in Emissions Based Models

In a study using UAM-IV in Atlanta, it was found that air pollution concentrations depend strongly on vertical diffusivity used in UAM-IV modeling. Vertical mixing is believed to be overestimated during the day by the normal procedures used in UAM-IV. The calculated vertical diffusion coefficient, $K_v$, exceeds measured and comparable literature values. Although generated using the UAM-IV model and the UAM-IV $K_v$ parameterization, the results show that a large error potential is possible in air quality grid models due to $K_v$ parameterization. Varying the $K_v$ made little difference to the surface $O_3$ concentrations, but did change significantly the vertical profile of $O_3$ concentrations. Over urban areas, the surface $NO_y$ concentration is increased using lower $K_v$'s due to the high subface source strength. For reactive hydrocarbons such as isoprene, lower $K_v$'s can more than double the surface concentrations in the model, improving the comparison with measurements.

There has been considerable discussion about vertical profiles during several of the SOS observational campaigns and their consistency with modeling results such as the study above. When comparing model profiles to observed profiles it is very important that the observed profiles are averaged for long periods since the first order closure models are based on ensemble statistics in which the effect of individual eddies have been averaged out. Otherwise significant structure in the vertical profiles even in a convective boundary can exist. Large-scale fluctuations about the long-term mean can be manifested especially in the deep boundary layers in the Southeast. In an effort to understand the appropriate averaging time for reactive pollutants in convective boundary layers a coupled large eddy (LES)/photochemical model was built and tested for the Southeast. It allows one to look at the variation in the vertical profiles of reactive compounds such as isoprene and $NO_x$ for different averaging times. It also allows one to address the question of whether the fluctuations that do exist in the real atmosphere but don’t exist in a first order closure model have any impact on the ultimate chemical solution. In probably the first LES study of this kind using a complete chemical mechanism, it was shown that isoprene profiles have to be averaged for several hours to produce a statistically stationary profile. It also showed that in large part first order closure models can be trusted within the deep boundary layers of the Southeast, i.e., there was agreement between the LES and first order closure models. It did suggest however that the chemistry can evolve quite differently in the LES and first order closure just outside the boundary layer.
KEY CITATIONS:
2.8.9. Conclusion – Policy-Relevant Findings for Emissions Based Modeling

1. Photochemical Mechanisms. For the Southeast, the changes to the CB4 mechanism will make the sensitivity to NO\textsubscript{x} reduction strategies greater than with the previous CB4 mechanism. It is then imperative that some understanding of the fidelity of this mechanism be had either from observations or from other more complete mechanisms. Nitrogen losses through surface deposition of organic nitrates (MPANS, PANS) may make a substantial difference in the sensitivity to NO\textsubscript{x} control strategies.

2. Role of Temperature in Ozone Production. Since this study demonstrates that ozone/temperature dependence is tied to the lifetime of organic nitrates then correctly handling these rates is critical to assessing the efficiency of NO\textsubscript{x} reduction control strategies. At present there is also new regulatory approach to give urban areas credit for reductions in temperatures. It is critical that the temperature/ozone relationships are faithfully replicated to test these credits.

3. Regional Surface Ozone Predictability. In the past, most control strategy demonstrations have attempted to use models to simulate specific episodes, usually the design day for a city or region. This study shows that a model’s skill in replicating any specific episode may not be great. The danger is that the tuning of a model to fit a given episode may forfeit the fundamental integrity of the model relationships. Based on the seasonal results, the authors propose that perhaps control strategy tests would best be carried out for longer-term simulations.

4. Meteorological Predictability. The use of episodic models for control strategy tests is brought to question. The meteorological models evidently have relatively poor skill at replicating higher frequency intra-day variations. Thus, individual episodes may not be well characterized by the models, leading to bias in photochemical results or control sensitivity. Rather, it argues that sensitivity and control strategy tests should be carried out on longer time scale simulations.

5. Control Strategy Sensitivity. The study by Roselle and Schere (1995) was one of the first to explore ozone sensitivity to NO\textsubscript{x} and VOC reductions on regional scales. While the ROM model has perhaps been supplanted by higher-resolution, newer-generation models, the basic results shown in this study probably still prevail and are consistent with regional observations carried out under SOS for rural NO\textsubscript{x} sensitivity.

6. Model Performance Evaluation Using Chemical Signals. These studies demonstrate the power of vertical concentration profiles, indicator ratios, and ozone production efficiencies in diagnosing model outputs. Simply achieving an acceptable statistical performance for ozone is not sufficient to ensure that control actions taken based on model results will have the desired effectiveness.

7. Role of Mixing Processes in Emissions Based Models. The coupled LES chemical models results show that the turbulence paradigm that most air quality models are based upon, i.e. first order closure, can be trusted even within the deep boundary layers of the Southeast. However, details on how the first order closures (K profiles) are formulated can make a difference in model results. Thus, additional work is needed to ensure that the K-profiles imposed actually in models reflect the appropriate turbulent intensities and scales in actual boundary layers.
2.9. SOS CONTRIBUTIONS IN OZONE EFFECTS RESEARCH
Walter Heck and Cari Furiness

Ozone remains an intractable air pollution problem in North America, Europe, and many other parts of the world. The negative effects of ozone on human health are well known. Ozone also has been considered the most insidious and ubiquitous air pollutant affecting the vegetative component of crop, forest, and natural ecosystems. During the past five years, SOS has not participated in direct ozone effects research, either on plants or animals. However, several efforts were undertaken to utilize existing data on ozone’s impacts on ecosystems: (1) to formulate recommendations for a secondary standard for ozone; (2) to assess the critical needs for research on the ecological effects of ozone; and (3) to synthesize the data available for assessing ozone impacts on ecosystems in the SOS region. Key findings of each of these efforts are summarized here.

2.9.1. Recommendations Regarding the Secondary Standard for Ozone – Ecological Effects

SOS sponsored a workshop in January 1996 with the primary purpose of developing consensus statements pertinent to a Secondary Standard for ozone from a broad group of ecologists and air quality scientists. Key statements from the workshop are listed below.

8. The public is generally unaware of the sensitivity of plants to ozone.
9. Plants are more sensitive to ozone than humans and should have a more restrictive standard.
10. The effects of ozone on plants are both cumulative and long-term.
11. Workshop participants recommended that the SUM06, summed over a running 90-day maximum, using values from a 12-hour (0800-1959) daily window, be accepted as the form for the Standard.
12. A SUM06 value between 15 and 20 ppm-hrs was recommended as the most prudent choice for a Secondary Ozone Standard.
13. The Secondary Standard recommended was different in both form and value from the Primary and Secondary Standards that were promulgated by EPA.

KEY CITATION:
2.9.2. Recommendations Regarding Ozone Ecological Effects Research Needs

SOS organized an EPA-sponsored workshop in May 1997 to assess future research needs related to ozone effects on ecological systems. Key outcomes of the workshop are listed below.

1. A detailed listing of research needs was developed for crop, forest and natural systems (see Table 2.10.1).

2. Participants recommended that EPA take primary responsibility for developing and managing research that would address its specific needs for undertaking another review of the Secondary Standard.

3. Without the recommended research, EPA will not be in a position to address the need for a long-term, cumulative Secondary Standard for ozone and will not find such a standard acceptable.

4. Participants recommended that other agencies (e.g., USDA/ARS and FS) should accept the lead in directing and managing research that fits into their own environmental missions. This should include research needed to understand how ozone affects crop, forest, and natural ecosystems and developing models to help predict expected losses from ozone exposure.

5. EPA and other federal agencies should work cooperatively in their respective responsibilities.

6. In general, research programs should develop integrated teams that include research scientists, statisticians, economists, and policy analysts, among others, in the planning stages for the research.

Table 2.10.1. Research tasks, identified as needed during the workshop, that should be led by EPA in collaboration with other agencies such as USDA-Agricultural Research Service, USDA-Forest Service, USDOI-Fish and Wildlife Service, and USDOI-National Park Service.* **

<table>
<thead>
<tr>
<th>Crop Systems</th>
<th>Forest Systems</th>
<th>Natural Systems</th>
<th>Research Across Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>METHODOLOGY - OPEN-TOP CHAMBER EFFECTS</td>
<td>SCALING OF SEEDLING-SAPLING RELATIONSHIPS</td>
<td>FOLIAR INJURY AS AN ENDPOINT - AN ASSESSMENT TOOL</td>
<td>EXPOSURE INDEX</td>
</tr>
<tr>
<td>INTERACTIONS - OZONE/ABIOTIC</td>
<td>OZONE GRADIENT STUDIES - USING NATURAL GRADIENTS</td>
<td>OTHER INDICATORS - BIOINDICATORS FOR NATURAL SYSTEMS</td>
<td>OZONE MONITORING NETWORK - RURAL</td>
</tr>
<tr>
<td>ECONOMIC LOSSES - VALIDATE CROP LOSS ESTIMATES</td>
<td>OZONE GRADIENT STUDIES - USING NATURAL GRADIENTS</td>
<td>VALE</td>
<td>VALUATION DETERMINATION - ECONOMIC TECHNIQUES</td>
</tr>
</tbody>
</table>

* The research highlighted above is essential before a reasonable review of the ecological components of the Secondary Standard can be accomplished. It is also probably essential before EPA will accept a long-term, cumulative standard. The research is mission oriented and will be accomplished better and more rapidly through the use of cooperative agreements and interagency agreements than through competitive granting mechanisms.

** See text of document for details of research tasks.

KEY CITATION:
2.9.3. **Recommendations for Assessing the Impact of Ozone on Ecological Systems in the Southeast**

Following the two workshops described above, an extensive literature review was conducted to identify literature that could be used in the development of an assessment of the ecological effects of ozone in the SOS region. The review included a determination of what has been done and/or is in the process of being done to assess the impact of ozone on ecological systems in the Southeast. The study was also designed to identify what needs to be done to produce a complete assessment of ozone impacts on ecological systems in the Southeast. Key findings of this report, funded by NOAA, are listed below.

1. Current environmental research likely is compromised by a lack of understanding of how ozone affects the response of plants to other factors in the environment.
2. Over 5500 references, relating to ozone effects on ecological systems were surveyed, and 963 were found to be of potential value in undertaking a complete assessment of effects in the Southeast.
3. Nine programs were identified that were designed to undertake some level of effects assessment that could be used in the Southeast.
4. No program has adequately assessed the effects of ozone on ecological systems in the Southeast.
5. Summary statements from the report include:
   - Ambient concentrations of ozone in the Southeast cause visible injury to sensitive species of crop, forest, and natural ecosystems.
   - Ambient concentrations of ozone in the Southeast can decrease yields of sensitive species of crop, forest, and natural ecosystems.
   - Agricultural crop losses across the country were estimated at $1-5 billion in 1988.
   - Southern commercial loblolly pine was estimated to show 2 to 5% annual growth reduction at current levels of ozone. This could result in a 10% reduction in stemwood biomass over a ten-year period.
   - Growth reduction in forest species at ambient ozone levels in the eastern USA appears to be in the range of 1-25% per year.
   - Forest growth losses have not been quantified on an economic basis, either based on loss of productivity of commercial forests or based on degradation of non-commercial assets of Southeastern forests.

**KEY CITATION:**
2.9.4. SOS Interactions with the Health-Effects Research Community

Only a few SOS scientists have participated directly in field or laboratory research designed to determine the direct or indirect impacts of ozone or fine particulate matter on humans or vegetation. Most of the persons are participants in the SOS-affiliated ARIES Program sponsored by the Southern Company and EPRI (see Section 1.4, Item 4 and Section 2.10.6). In the future, SOS is committed to continue to work with ARIES and to develop liaison relationships with organizations that are involved in human health effects research.

During the Nashville/Middle Tennessee Ozone Study, scientists from the Harvard School of Public Health used personal ozone monitors to characterize individual human exposure to ozone. During SOS work in Atlanta, an EPRI-sponsored study was conducted to study the correlation between air quality and pediatric emergency room visits for asthma.

SOS maintains strong ties with the ozone ecological health effects community. As described in the sections above, SOS has brought together scientists for workshops to discuss issues of importance to ecological effects of ozone, and utilized existing knowledge about the ecological health effects of ozone to develop pertinent summary statements, to identify gaps in knowledge, and to identify the data needs to allow an adequate assessment of ozone impacts on ecosystems in the SOS region. The next phase of SOS will incorporate a larger research and assessment component dealing with ecological effects of ozone.

In the case of PM$_{2.5}$, a major SOS-affiliated research effort has been undertaken to begin to determine the epidemiological effects of PM$_{2.5}$ and other air pollutants in Atlanta; the results should be applicable to the SOS study region and the nation as a whole. The Aerosol Research Inhalation Epidemiology Study (ARIES), which began data collection in July 1998 and finished the first phase of field monitoring in August 2000, is described in Section 1.4.

Although there are no known direct effects of PM$_{2.5}$ on plants, there may be indirect impacts as a result of decreased insolation with regional haze caused by PM$_{2.5}$. Certainly decreases in visibility represent a significant welfare effect of PM$_{2.5}$ and are important aspects for consideration in determination of a secondary standard.
2.9.5. Conclusion – Policy Relevant Findings Regarding Ozone Effects on Ecological Systems

1. Ozone at ambient concentrations causes visible damage and growth reductions in certain sensitive species of crop, forest, and natural ecosystems.

2. Agricultural crop losses across the country were estimated at $1-5 billion in 1988.

3. Growth reduction in forest species at ambient ozone levels in the eastern USA appears to be in the range of 1-25% per year.

4. Scientists have recommended that the SUM06 (the number of hours in which ozone concentrations are above 60 ppb), summed over a running 90-day maximum, using values from a 12-hour (0800-1959) daily window, be accepted as the form for the secondary standard. 15 – 20 ppb-hr was recommended as a protective value of the standard.

5. EPA should take primary responsibility for developing and managing ecological research that will address its needs for undertaking another review of the Secondary Standard. This research should include: a more comprehensive rural ozone monitoring network; development of appropriate exposure indices for plants; economic valuation and validation of forest, crop, and natural ecosystem losses from ozone; development of ozone bioindicators for natural systems; methods for scaling of results from seedlings to mature plants, up to the landscape level.

6. Although much research has been done on the effects of ozone on plants, a complete assessment of the impacts of ozone on crop, forest, and natural ecosystems in the SOS region has not been done. Several efforts have been completed or begun that may provide useful information for development of a full assessment of ozone impacts in the Southeast.
2.10. "INITIAL IMPRESSIONS" FROM SOS PM\textsubscript{2.5} AND OZONE FIELD MEASUREMENT STUDIES IN 1999-2000

As in other carefully focused scientific research programs, most "major scientific findings" from SOS and SOS-affiliated research develop gradually (often over months or even years of time) through five stages of evolution:

1. Hypotheses shared at SOS planning meetings,
2. "Initial impressions" derived from carefully planned field observations that are first shared with colleagues in our own institutions and with SOS sponsoring organizations,
3. "Emerging insights" (and sometimes major surprises!) shared with additional colleagues during SOS Data Analysis Workshops,
4. Plans for joint authorship and submission of abstracts for verbal presentations or posters at open scientific meetings,
5. Further refinements in data analysis and interpretation, partly in response to critical comments received at scientific meetings, and comparison with results of other investigations inside and outside of SOS, and finally
6. Submission of manuscripts to refereed journals where "major scientific findings" that are "consistent with available scientific evidence and contradicted by no important evidence" are the raison d'etre for acceptance by both the journal and the scientific community at large.

Results from most SOS field studies initiated in 1999-2000 are in stages 2-4 in this six-step process. Thus, we offer the following brief summaries of some sample results from nine specific SOS and SOS-affiliated investigations.

- Nashville '99 PM\textsubscript{2.5} and Ozone Study
- Atlanta Initial Supersite Study
- Texas 2000 Air Quality Study
- SOS Center for Integrated Study of Secondary Air Pollutants
- Southeastern Aerosol Research and Characterization Study
- Aerosol Research Inhalation Epidemiological Study
- Assessment of Spatial Aerosol Composition in Atlanta
- Tennessee Valley PM\textsubscript{2.5} Partnership Network
- Georgia Fall Line Air Quality Study
2.10.1. Nashville '99 PM$_{2.5}$ and Ozone Study

After the third SOS Data Analysis Workshop held in March 2000, about 75 SOS scientists submitted a total of 36 abstracts for presentation in two SOS Special Sessions at the 2000 Fall Meeting of the American Geophysical Union. The moderators, titles, and senior authors of these abstracts are shown below – 12 for verbal presentations on Sunday morning December 17, 2000 and 24 for poster presentations on Monday morning December 18, 2000. These 36 titles give a good idea of the wide range of topics from which "initial impressions" have been gained from analysis and interpretation of measurements made during the SOS' Nashville '99 study. During the AGU meeting, additional progress was made in forming multiple-investigator teams that will prepare detailed manuscripts for submission for publication in the *Journal of Geophysical Research-Atmospheres* and other refereed journals. Each of these 30-40 manuscripts will contain carefully crafted statements of scientific findings that are "consistent with all scientific evidence and contradicted by no important evidence" developed inside or outside of SOS.

### Fall 2000 Meeting of American Geophysical Union

**Southern Oxidants Study (SOS) Ozone and Particulate Matter Pollution Studies**

**Nashville'99 Studies – Verbal Presentations**

**Sunday Morning, December 17, 2000, 8:30 a.m. – Noon**

**Moderators: Jim Meagher and Fred Fehsenfeld**

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<tr>
<th>Time</th>
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<th>Senior Author</th>
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<tr>
<td>8:30</td>
<td>The Vertical Structure and Downwind Chemistry of the Nashville Urban Plume</td>
<td>Carl Berkowitz</td>
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<td>8:45</td>
<td>Production Rates and Yields of Ozone in Refinery, Urban, and Power Plant Plumes</td>
<td>Thomas Ryerson</td>
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<td>9:00</td>
<td>Rates and Efficiencies in Nashville and Phoenix</td>
<td>Peter Daum</td>
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<td>9:15</td>
<td>Particle Characteristics and Dynamics in Power Plant and Urban Plumes</td>
<td>Charles Brock</td>
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<td>9:30</td>
<td>Urban Plume With Airborne Lidar During SOS99</td>
<td>Christoph Senff</td>
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<td>9:45</td>
<td>Nocturnal Transport and Mixing of Pollutants Observed During SOS-99 in Nashville</td>
<td>Robert Banta</td>
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<td>10:00</td>
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<td>10:20</td>
<td>The Impact of Solar Irradiance Errors on the MM5 Surface Energy Balance During the Nashville Southern Oxidants Studies</td>
<td>Robert Zamora</td>
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<td>10:35</td>
<td>Analysis of Motor Vehicle Emissions During the Nashville/Middle Tennessee Ozone Study</td>
<td>Robert Harley</td>
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<td>10:50</td>
<td>Decrease in Emission Ratios of Carbon Monoxide to Nitrogen Oxides in Two Urban U.S. Areas over the Past Decade</td>
<td>David Parrish</td>
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<td>11:05</td>
<td>OH and HO2 Variations During Summertime Nashville Southern Oxidant Study in 1999</td>
<td>Monica Martinez</td>
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<td>11:20</td>
<td>The Influence of the Nighttime Inversion on the Chemistry of Nitrogen Oxides During the 1999 SOS Field Study in Nashville</td>
<td>Jochen Stutz</td>
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<tr>
<td>11:35</td>
<td>Fast Response VOC Measurements at Cornelia Fort Airport</td>
<td>Armin Hansel</td>
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## Fall 2000 Meeting of American Geophysical Union
### Southern Oxidants Study (SOS) Ozone and Particulate Matter Pollution Studies
#### Nashville'99 Studies – Poster Presentations
#### Monday Morning, December 18, 2000, 8:30 a.m. – Noon
#### Moderator: Leonard Newman

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<td>A11B-19</td>
<td>The SOS Nashville 99 Field Study: Scientific Objectives and Study Design</td>
<td>James Meagher</td>
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<td>A11B-20</td>
<td>The Morning Transitions Observed During SOS99</td>
<td>Allen White</td>
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<td>A11B-21</td>
<td>Urban Effects on Mixing Depth and Cloudiness -- Nashville 1999</td>
<td>Wayne Angevine</td>
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<td>A11B-22</td>
<td>Changes in Ozone Measurements due to a Gust Front Passage</td>
<td>Lisa Darby</td>
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<td>A11B-23</td>
<td>Airborne Formaldehyde Measurement on a NOAA WP-3 Aircraft during the 1999 SOS Summer Field Experiment</td>
<td>Yin-Nan Lee</td>
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<td>A11B-24</td>
<td>Aircraft Observations of PANs Over the Southeastern United States during SOS 99</td>
<td>Frank Flocke</td>
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<td>A11B-25</td>
<td>PAN and Related Compounds at the SOS 1999 Nashville, TN Study</td>
<td>James Roberts</td>
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<td>A11B-26</td>
<td>Airborne In-Situ Measurements of Non-Methane Hydrocarbons during the SOS 1999 Summer Field Campaign</td>
<td>Paul Golden</td>
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<td>A11B-27</td>
<td>Comparison of oxy-VOC and PAN measurements at Cornelia Fort Airport</td>
<td>Armin Wisthaler</td>
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<td>A11B-28</td>
<td>Isoprene and its Oxidation Products, Methacrolein and Methyl Vinyl Ketone, at an Urban Forested Site during the 1999 Southern Oxidant Study</td>
<td>Craig Stroud</td>
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<td>A11B-29</td>
<td>Evaluation of the NOx Dependence of BVOC Oxidation Using Field Site Data and a Simple HOx Model</td>
<td>Dennis Barket</td>
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<td>A11B-30</td>
<td>Detailed Analysis of the NOx Dependence of Isoprene Nitrate Formation</td>
<td>John Grossenbacher</td>
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<td>A11B-31</td>
<td>NMOC Measurements in Downtown Nashville</td>
<td>Paul Doskey</td>
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<td>A11B-32</td>
<td>The Utility of Measured Carbon Dioxide as a Conserved Tracer of Precursors in Tropospheric Photochemistry</td>
<td>Richard Dissly</td>
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<td>A11B-33</td>
<td>Measurements of O3, HCHO, NO2, HONO and NO3 by Differential Optical Absorption Spectroscopy during the 1999 SOS Field Study in Nashville</td>
<td>Bjoern Alicke</td>
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<td>A11B-34</td>
<td>A Comparison of Inferred Nitric Acid Mixing Ratios by an NOy Difference Technique to a Selective Measurement by SiF5 Chemical Ionization Mass Spectroscopy</td>
<td>Dennis Nicks</td>
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<td>A11B-35</td>
<td>Tropospheric Ozone Pollution Transport Traced From the TOMS (Total Ozone Mapping Spectrometer) Instrument During the Nashville-1999 Campaign</td>
<td>A. Thompson</td>
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<td>A11B-36</td>
<td>Ozone Sensitivity to NOx and VOCs in the Nashville Urban Plume</td>
<td>Lawrence Kleinman</td>
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<td>A11B-37</td>
<td>Inferences about Peroxy Radicals and Ozone Production at Cornelia Fort Airpark, Nashville, TN during the 1999 Southern Oxidants Study</td>
<td>J. Thornton</td>
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<td>A11B-38</td>
<td>Comparisons of a Photochemical Box Model to Observed OH, HO2, NO2, and PO3 in Nashville During the 1999 Southern Oxidants Study</td>
<td>Gregory Thornton</td>
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<td>A11B-39</td>
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<td>John Frost</td>
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<td>Ozone Production from Canadian Wildfires During the 1995 Southern Oxidant Study</td>
<td>Stuart McKeen</td>
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<td>A11B-41</td>
<td>Comparison of Ozone Measurements in Urban Environments</td>
<td>Eric Williams</td>
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<td>A11B-42</td>
<td>Informal Comparison of In-Situ and Long Path Measurements of NOx during the 1999 Southern Oxidant Study</td>
<td>P. Wooldridge</td>
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<td>A11B-43</td>
<td>Sensitivity of Ozone and Peroxide Formation in the Lombardy Region, Italy</td>
<td>Josef Dommen</td>
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2.10.2. SOS' Atlanta Initial Supersite Study

Similarly, the 75 or so SOS scientists in the Atlanta Supersite Study, after initial presentation of results at the March 2000 SOS Data Analysis Workshop, submitted a total of 7 abstracts for presentation in an SOS Special Session at the Annual Meeting of the American Association of Aerosol Research in St. Louis, Missouri in November, 2000. They also submitted 30 additional abstracts for presentation in two other SOS Special Sessions at the Annual Fall Meeting of the American Geophysical Union in San Francisco, California in December 2000. The moderators, titles, and senior authors of abstracts from both meetings are shown below. These 37 titles give a good idea of the wide range of topics from which "initial impressions" and can be gained from SOS' Atlanta Initial Supersite Study in August 1999.

American Association of Aerosol Research, Annual Meeting,
St. Louis, Missouri, November 6-10, 2000

Session 12C – ATLANTA SUPERSITE STUDY

12C1 Trends in Single Particle Size and Chemical Composition During the Summer in Atlanta GA, RYAN J. WENZEL, Univ of California/Riverside, Don-Yuan Liu, Univ of California/Riverside, Kimberly A. Prather, Univ of California/Riverside

12C2 Measurement of Fine Particulate Organic and Elemental Carbon in the 1999 Atlanta Supersite Experiment, HO-JIN LIM, Rutgers Univ, Barbara J. Turpin, Rutgers Univ

12C3 Measurements Of Density Of Atmospheric Particles Using the TDMA-APM Technique, Xin Wang, Univ of Minnesota, PETER MCMURRY, Univ of Minnesota, Kensei Ehara, National Research Lab of Metrology

12C4 Continuous On-Line Measurement of Aerosol Ammonium and Ammonia-Gas with the Steam Jet Aerosol Collector (SJAC), J. Slanina, ECN, HARRY M. TEN BRINK, Netherlands Energy Research Found, Rene Otjes, ECN, Piet Jongejan, ECN, Minn Hu, Peking University

12C5 Measurements of 3 to 10 NM Size Distributions In Atlanta: Implications For Nucleation Mechanisms, PETER MCMURRY, Univ of Minnesota, Keung-Shan Woo, Univ of Minnesota, Da-Ren Chen, Univ of Minnesota, David Y.H. Pui, Univ of Minnesota

13C2 Characterizing PM$_{2.5}$ in Atlanta, 1999-2000, Andre’ Butler, Georgia Institute of Technology, Michael Andrew, Georgia Institute of Technology, ARMISTEAD RUSSELL, Georgia Institute of Technology, Eric S. Edgerton, Atmospheric Research and Analysis Inc, Benjamin Hartsell, Atmos Research and Analysis Inc

10B4 Classification Analysis of Atlanta PALMS Single Particle Data: The Ambient Relative Humidity Dependency of Nitrate in Tropospheric Aerosols, SHAN-HU LEE, NOAA Aeronomy Lab, Ann M Middlebrook, NOAA Aeronomy Lab, Daniel M. Murphy, NOAA Aeronomy Lab, David S. Thomson, NOAA Aeronomy Lab, Matt Warshawsky, NOAA Aeronomy Lab, Rebecca Washenfelder, NOAA Aeronomy Lab
### Fall 2000 Meeting of American Geophysical Union

**Southern Oxidants Study (SOS) Ozone and Particulate Matter Pollution Studies**

**Atlanta Supersite Study – Verbal Presentations**

**Sunday Afternoon, December 17, 2000, 1:45 – 5:00 pm**

**Moderators: Bill Chameides and C. S. Kiang**

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<th>Senior Author</th>
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<tbody>
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<td>13:45</td>
<td>Comparison of Integrated Samplers for Mass and Composition</td>
<td>Paul Solomon</td>
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<td>14:00</td>
<td>Intercomparison of Semi-Continuous Techniques For Measurement of Sulfate and Nitrate at the EPA Atlanta Supersite, August 1999</td>
<td>Rodney Weber</td>
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<td>14:15</td>
<td>An intercomparison of Particle Mass Spectrometers during the Atlanta SuperSite Experiment</td>
<td>Ann Middlebrook</td>
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<td>14:30</td>
<td>Hourly Chemical Composition Profiles for Fine Particulate Matter during the Atlanta Supersite Study, August 1999</td>
<td>Susanne Hering</td>
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<td>14:45</td>
<td>Daily Sampling of PM$_{2.5}$ in Atlanta: Results of the First Year of the Analysis of Spatial Aerosol Composition</td>
<td>André Butler</td>
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<td>15:00</td>
<td>Meteorological Conditions and the Identification and Characterization of Interesting &quot;Events&quot; During the Atlanta '99 Supersite Experiment</td>
<td>James St. John</td>
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<td>15:15</td>
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<td>15:30</td>
<td>Particulate NH$_4$, NO$_3$, OC and EC During the Atlanta SuperSite Experiment</td>
<td>Eric Edgerton</td>
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<td>16:00</td>
<td>Measurement of Aerosol Radiative Properties During the Atlanta SuperSite Study</td>
<td>Michael Bergin</td>
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<td>16:15</td>
<td>Single Particle Size and Chemical Composition Using ATOFMS During the Summer in Atlanta, GA</td>
<td>Ryan Wenzel</td>
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<tr>
<td>16:30</td>
<td>Size-Resolved Chemical Composition of Urban Aerosol in Georgia and Texas</td>
<td>Jose Jimenez</td>
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<td>16:45</td>
<td>Composition of Individual Ultrafine Particles during August 1999 in Atlanta, Georgia</td>
<td>Kevin Rhoads</td>
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<td>Poster #</td>
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<tr>
<td>A11B-1</td>
<td>An Overview of the Objectives and Design of the Atlanta '99 SuperSite Experiment</td>
<td>William Chameides</td>
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<tr>
<td>A11B-2</td>
<td>Chemical and Meteorological Characteristics of the Jefferson Street Monitoring Site</td>
<td>Eric Edgerton</td>
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2.10.3. Texas 2000 Air Quality Study (TexAQS 2000)

[Adapted from notes prepared by staff of the Texas Natural Resource Conservation Commission (TNRCC) during a conference call with SOS senior scientists shortly after completion of the field measurements for the Texas 2000 Air Quality Study.]

Peter Daum from Brookhaven National Laboratory was the Lead Scientist for TexAQS 2000. At the conclusion of the field campaign, he prepared a closing message for the 250 study participants, which included the six "initial impressions" listed below. While Daum and the other senior scientists in TexAQS 2000 were willing to share these initial impressions, they cautioned that these statements are indeed "initial impressions" and should be regarded as very preliminary.

Message from Peter Daum:
"On behalf of the entire TexAQS Science Team, I would like to extend our thanks to all the fine scientists and engineers who made the dream of TexAQS 2000 a reality. More than 250 of us worked many long and tireless hours over the past six weeks. As a consequence, I believe we have collected the largest, most comprehensive, and most sophisticated air quality data set in history. Certainly, we have collected sufficient air quality and meteorological information to begin to address ozone and fine particle air quality management issues for Houston and other parts of the eastern half of Texas. There are several initial impressions that I found most interesting and would like to share them with you:

1. It appears that ozone is produced more efficiently by emissions from the Houston ship channel area than from other urban Houston emissions.

2. During episodic conditions, ozone formation from ship channel emissions can occur very rapidly, at rates of up to 100 ppbv per hour for several hours.

3. Concentrations of highly reactive hydrocarbons can be very high in and around the ship channel. These may have a significant role in exceedances of the ozone standard.

4. Biogenic emissions of reactive hydrocarbons do not appear to play a particularly important role in Houston area ozone production. While they may play an important role in other parts of east Texas, they didn't seem to overtly influence Houston area ozone during TexAQS 2000."

5. Accumulation mode fine particle loadings generally seemed lower than loadings found in previous studies in Nashville, Philadelphia, and New York.

6. There is no question that Houston's meteorology plays an important role in production, accumulation and transport of secondary air pollutants. Although we experienced but one classic land breeze/sea breeze episode during TexAQS 2000, it is evident that, in the absence of large scale meteorological forcing conditions, the air which stagnates over Galveston Bay
in the morning is often pushed inland by the sea/bay breeze in the mid-afternoon with interesting air quality consequences.

Senior scientists from both NOAA and DOE also added five additional "initial impressions."

1. Power plant plumes in the eastern part of Texas have higher efficiencies of ozone production in areas with higher isoprene production than in areas of lower isoprene emissions.

2. NOAA scientists saw high concentrations of pollution in some haze layers (in the boundary layer) that appeared to have been transported over long distances.

3. Occasionally NOAA scientists found layers in the free troposphere (i.e., above the daily mixed layer) that were transported from forest fires in the northwest U.S. and Canada.

4. Some power plant plumes in the eastern half of Texas appeared to have unexpectedly high concentrations of carbon monoxide (CO). We hope to use the data from these plumes to assess NOx loss using CO as a conservative tracer.

5. On an August 28 flight it appeared from a preliminary look at the data that each of the refining and chemical complexes to the south and west of Houston was contributing rapid, incremental production of 25 to 30 ppbv of ozone in the plumes from each complex. It will take careful analysis of data from all such flights to develop a more complete picture of the contribution of these facilities to ozone production under different meteorological conditions.
2.10.4. SOS Center for Integrated Study of Secondary Air Pollutants (SOS-SCISSAP)

William Chameides and Karsten Baumann of Georgia Tech provide leadership for this important study, which is designed to compare and contrast the chemical composition of PM$_{2.5}$ samples collected at three sites in the SOS region: Atlanta, GA and Hendersonville and Dickson, TN. Measurements were made at these sites using a custom-designed three-channel Particle Composition Monitor and associated ion chromatograph and gas-chromatograph/mass spectrometer instruments that together permit determinations of total particle mass as well as the following chemical constituents: NH$_3$, HNO$_3$, HONO, SO$_2$, Na$^+$, Ca$^{++}$, NH$_4^+$, Cl$^-$, NO$_2^-$, NO$_3^-$, SO$_4^{=}$, total elemental carbon, total organic carbon including formic, acetic, and oxalic acids, other speciated organic compounds, and trace metals.

SCISSAP data provide evidence for the following initial impressions:

1. A clear seasonal pattern is shown with respect to total fine mass (PM$_{2.5}$) at the three sites, with averages being highest during the summer.

2. The urban site (ATL) exhibits the highest mass concentrations, possibly due to higher emissions of primary particles and/or PM$_{2.5}$ precursors. Comparisons among all sites support the hypothesis that fine particle pollution, like ozone pollution, is a regional phenomenon across the Southeastern United States and is only partially influenced by spatially confined local sources.

3. As opposed to sulfate and unidentified mass, the total organic mass concentration does not show significant seasonal variation.

![PM2.5 Seasonal Averages](image)

Figure 2.10.1. Seasonal averages of PM$_{2.5}$ measured at urban (ATL), suburban (HV), and rural (DX) sites in ‘99-'00.
4. Gaseous precursors for gas-to-particle conversion, i.e., NH$_3$, HNO$_3$, and SO$_2$, are highest in the urban environment where we also see highest PM$_{2.5}$. Acidic gases exhibit a seasonal trend with lowest values in winter.

Figure 2.10.2. Seasonal averages of gases measured at urban (ATL), suburban (HV), and rural (DX) sites in ’99-‘00.

5. Calculation of net inorganic acidity reveals relatively well neutralized aerosols, with slightly acidic conditions in summer and slightly basic conditions in fall and winter (but being more completely neutralized in fall and winter).

Figure 2.10.3. Seasonal averages of acidity measured at urban (ATL), suburban (HV), and rural (DX) sites in ’99-‘00.
2.10.5. Southeastern Aerosol Research and Characterization Study (SEARCH)

Deployment of the SEARCH PM network began in early 1998 and continues today as new technologies are brought to bear.

An unprecedented data set, consisting of daily PM$_{2.5}$ measurements (mass and composition), was collected at all SEARCH sites during calendar year 1999. A summary of these data was requested by and presented to EPA in late 2000. This summary has also been shared with collaborating state and local agencies. These data were submitted to the NARSTO data archive in January 2001.

The following figures and findings derive from SEARCH research. More detail and references to publications of findings from SEARCH can be found at [http://www.atmospheric-research.com](http://www.atmospheric-research.com) in the SEARCH Fact Sheet produced by EPRI, from which the following statements are derived.

Key observations to date include:

1. Carbonaceous material (elemental and organic carbon) and sulfate are the dominant components of PM$_{2.5}$ (see Figure 2.10.5).

2. There is significant season-to-season, day-to-day, and hour-to-hour variability in the concentration and composition of PM$_{2.5}$ (see Figure 2.10.7).

3. PM$_{2.5}$ concentrations are significantly higher at urban sites than at regionally representative rural sites. This phenomenon is largely explained by differences in carbonaceous material (higher concentrations in urban areas).

4. Methodological issues (e.g., sampling frequency and blank correction) and natural sources of PM$_{2.5}$ (e.g., sea-salt, African dust, fires) can have a determining effect on attainment status of a monitoring site.

5. Initial data from continuous mass and speciation monitors demonstrate the importance of real-time information for understanding sources and processes leading to PM$_{2.5}$ formation. (see Figure 2.10.7).
Some additional impressions are given below in the context of the following figures.

1. Sites in or near larger cities may exceed NAAQS for PM$_{2.5}$. Rural and smaller cities may attain, but are at risk. Inter-annual variability is largely unknown at present.

![Map showing PM$_{2.5}$ concentrations](image)

Figure 2.10.4. Mean PM$_{2.5}$ for 1999 using Federal Reference Method (FRM) (ug/m$^3$). Note: TEOM annual average is also shown for the Center site. FRM value is suspect due to low sample recovery.

2. Methodological issues and natural sources of PM$_{2.5}$ can have a determining effect on the attainment status of a monitoring site.

### Issues Affecting PM$_{2.5}$ Measurements (based on SEARCH observations)

- **Bias & Uncertainty**
  - Blank correction (0.6 ug/m$^3$)
  - Carbon artifacts (+/- 2 ug/m$^3$)
  - Nitrate loss (0.6 ug/m$^3$)
  - Sampling Schedule
    - 3-day (+/- 0.3 ug/m$^3$)
    - 6-day (+/- 0.4 ug/m$^3$)
    - Wed./Sat. (+/- 0.3 ug/m$^3$)
  - Inter-laboratory (under evaluation)
  - FRM vendor (under evaluation)

- **Natural & Other Sources** (Note: upper limit estimates)
  - Sea salt
    - 0.2 ug/m$^3$
  - North African Dust
    - 0.5 ug/m$^3$
  - Wood Smoke
    - 1.0 ug/m$^3$
3. Organic matter exceeds sulfate in urban areas but are equivalent in rural areas. Total carbon exceeds sulfate at all sites.

Figure 2.10.5. Relative composition of PM$_{2.5}$ in 1999 at SEARCH sites.

4. Differences in PM$_{2.5}$ between urban and rural areas are largely explained by differences in carbonaceous material (i.e., higher concentrations in urban areas).

Table 2.10. Differences (µg/m³) between urban-rural site pairs in 1999.

<table>
<thead>
<tr>
<th>Site Pair</th>
<th>Delta PM$_{2.5}$</th>
<th>Delta SO$_4$</th>
<th>Delta NH$_4$</th>
<th>Delta OM</th>
<th>Delta EC</th>
<th>Delta Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>JST/YRK (GA)</td>
<td>5.3</td>
<td>0.6</td>
<td>0.3</td>
<td>2.1</td>
<td>1.2</td>
<td>4.2</td>
</tr>
<tr>
<td>BHM/CTR (AL)</td>
<td>6.4</td>
<td>0.9</td>
<td>0.4</td>
<td>2.9</td>
<td>2.0</td>
<td>6.2</td>
</tr>
<tr>
<td>PNS/OLF (FL)</td>
<td>2.3</td>
<td>0.1</td>
<td>0.1</td>
<td>1.1</td>
<td>0.5</td>
<td>1.9</td>
</tr>
</tbody>
</table>
5. There is significant day-to-day variability in PM$_{2.5}$ concentration. Elevated concentrations occur throughout the year, not just in summer.

Figure 2.10.6. Daily PM$_{2.5}$ at urban (upper) and rural (lower) sites (µg/m$^3$).
6. Continuous methods illustrate important variability of pollutants and provide powerful tools for source identification and understanding aerosol formation processes.

   a. Continuous particulate carbon data show buildup under nocturnal boundary layer.

   **Figure 2.10.7.** Continuous particulate carbon data from Atlanta SuperSite experiment.

   b. Combination of continuous gas and particle measurements yields insight into sources of primary particles.

   **Figure 2.10.8.** Continuous total carbon and CO data from Atlanta SuperSite experiment.
2.10.6. Aerosol Research Inhalation Epidemiological Study (ARIES)

This epidemiologically focused study was centered in Atlanta, Georgia during 1998 and 1999. It sought to determine if statistical relationships could be established between a variety of health risk indicators (such as emergency room visits, asthma attacks, billings for visits to doctors and other health professionals, reports of chronic obstructive pulmonary disease, etc.) and various relevant measures of air quality (such as gaseous pollutant concentrations; various features of ambient particulate matter including: particle number and size distribution; major cations, anions, and acidity; elemental and organic carbon; specific elements; water soluble transition metals; mold spores; pollen grains, etc).

Highlights from these studies include the following summary statements, which are taken from the ARIES Fact Sheet produced by EPRI. More detail and references to publications of findings from ARIES can be found at http://www.atmospheric-research.com.

1. Detailed characterization of PM$_{2.5}$ in Atlanta demonstrates the quantitative importance of carbonaceous matter.
2. There are discrete episodes of elevated ultrafine particle numbers that are believed to be tied to anthropogenic emissions.
3. PM$_{2.5}$ composition varies from hour-to-hour, day-to-day, and season-to-season. Sulfate comprises the largest fraction of PM$_{2.5}$ in summer, while carbonaceous matter comprises the largest fraction in the spring, fall and winter.
4. To date there are no statistically significant associations between mortality in Atlanta and any air quality variable. These results are based on first year results; adding the second year of data is expected to provide further insights with increase statistical power.
5. Morbidity results are presently available only for hospital emergency room admissions data. To date no air quality variable has been associated with increased asthma or chronic obstructive pulmonary disease (COPD) admissions. Increased cardiovascular admissions have been associated with several air quality variables including: carbon monoxide (CO); PM$_{2.5}$ elemental carbon (EC); PM$_{2.5}$ organic carbon (OC), and PM$_{coarse}$ mass (i.e., the "coarse" fraction of PM$_{10}$ or the difference between PM$_{10}$ and PM$_{2.5}$).
2.10.7. Assessment of Spatial Aerosol Composition in Atlanta (ASACA)

This study was undertaken at Georgia Tech under the leadership of Ted Russell and his graduate students. The objectives were to determine how daily and weekly PM$_{2.5}$ samples collected in various parts of Atlanta varied among three major locations – Jefferson Street (JST), Fort McPherson (FT), and Tucker (TU) (see map in Figure 1.6). André Butler's recently completed Ph.D. dissertation includes the following important insights from analysis of the first 12-months' observations in the ASACA study -- March 1999 through February 2000:

1. PM$_{2.5}$ mass showed little spatial variability but substantial temporal variability with highest values in summer, lowest values on Mondays, and highest values at night and during morning rush hours.

2. Organic carbon (OC) and elemental carbon (EC) in PM$_{2.5}$ showed little spatial variability but substantial temporal variation with:
   a) Peak values of OC in summer, lowest values on Mondays, and significant secondary aerosol contributions (40-80 percent), and
   b) Peak values of EC in winter and August (which proved to be anomalous among summer months) and lowest values of EC on weekends.

3. Major inorganic ions showed little spatial variability but substantial temporal variation with:
   peak SO$_4^{2-}$ values in summer, peak NO$_3^-$ values in winter, and peak values of NH$_4^+$ in summer associated with high values of SO$_4^{2-}$ and NO$_3^-$. 

In further summary:

- Spatial variability during 1999 was much smaller than temporal variability in all PM$_{2.5}$ attributes at all three ASACA test sites,
- Organic carbon (OC) and SO$_4^{2-}$ were the dominant compositional fractions of PM$_{2.5}$,
- Substantial seasonal variation was observed in PM$_{2.5}$ mass, OC, EC, SO$_4^{2-}$, and nitrate with peak values of mass and OC in summer but peak values of nitrate and EC in winter months,
- Secondary formation mechanisms appeared to dominate SO$_4^{2-}$ and OC accumulation in PM$_{2.5}$,
- A slight increase in PM$_{2.5}$ mass occurred from Monday through Friday of most workweeks,
- Power generation, construction, and mobile sources all appeared to be important contributors to PM$_{2.5}$ in Atlanta in 1999,
- In all 12 months of 1999, the Atlanta Supersite location (Jefferson Street site) was representative of all the ASACA sites tested in Atlanta, and
- August 1999 (the time of the SOS Atlanta Supersite Study) should be recognized as a month of unusually high concentrations of PM$_{2.5}$ at all ASACA sites in Atlanta.
2.10.8. Tennessee Valley PM2.5 Partnership Network

The 12-station Tennessee Valley Partnership Network (see map in Figure 1.4) has been measuring seasonal trends in mass and chemical composition of PM$_{2.5}$ since May 1997 and is expected to continue its affiliation with SOS so long as the Partnership Network and SOS continues to exist -- at least through 2006 and probably beyond.

As shown in Figure 2.10.8, although the mass of PM$_{2.5}$ varied considerably among the 12 sampling sites, essentially all sites showed summer-time maxima in particle mass. Thus, the seasonal trends observed in the data for the urban ASACA network are also observed in the rural, suburban, and even the remote sites in the Tennessee Valley Partnership Network.

![Figure 2.10.8. Monthly mean PM2.5 mass at twelve principal monitoring sites (see Figure 1.4) in Tennessee Valley Partnership Network during 1997-2000.](image-url)
2.10.9.  Georgia Fall Line Air Quality Study (FAQS)

This comparative study of ozone and PM$_{2.5}$ concentrations in and around three ozone Near Non-Attainment cities within the state of Georgia began field measurements during the summer of 2000 (see map in Figure 1.7 with Augusta to the east, Macon in central Georgia, and Columbus to the west).

Initial impressions from FAQS' first-year Pilot Study suggest that:

1. Regional sources of ozone and PM$_{2.5}$ precursors constitute a large part of the Near-Non-Attainment problem in all three cities;
2. Local areas may simultaneously contribute to and be affected by high concentrations of ozone across the southeastern region -- this is most evident in Augusta and Columbus;
3. In Macon, like Atlanta, the underlying regional air quality sometimes may be dwarfed by local effects;
4. High ozone concentrations in each of the three Fall Line cities appear to be associated most frequently with light or stagnant winds;
5. Total hydrocarbon concentrations and isoprene fractions observed in the three cities were similar in relative magnitude to those observed in previous studies of Atlanta suggesting controls on NOx emissions may be needed to reduce ozone concentrations; and
6. Fine particulate matter in all three cities was composed largely of organic carbon and sulfates.
2.10.10. Conclusion -- Potential for Future Progress through Comprehensive Analysis and Publication of Results from these SOS and SOS-Affiliated Investigations

As indicated at the beginning of this section, the scientists and engineers of SOS and SOS-affiliated research programs have a long way to go before full advantage can be taken of the rich data and information resources accumulated in the nine research programs described above.

At the end of 1995, when the SOS Nashville/Middle Tennessee Ozone Study had just been completed, we said to all who would listen that "we have both a moral and a scientific responsibility to analyze, interpret, and publish the results of these investigations." It took us nearly four years to fulfill those promises. The first SOS Special Section of JGR-Atmospheres contained 31 papers; it was published in September 1998 and was followed two months later by 6 additional papers. The Second SOS Special Section of JGR-Atmospheres was published in April 2000; it contained 13 additional papers. In July 1999, we published the First SOS Compendium Volume deriving from the Nashville/Middle Tennessee Ozone Study; it contained 48 papers from JGR-Atmospheres and Geophysical Research Letters by 149 authors. The Second SOS Compendium Volume will contain 15 papers by nearly 50 SOS authors.

Our intention, especially in 2001-2003, is to follow the same general path of progress for each of the nine SOS and SOS-affiliated research activities described above. In publishing the results of our PM$_{2.5}$ research studies, our hope is to work with leaders in the American Association of Aerosol Research and other professional societies in much the same way we have worked with leaders in the American Geophysical Union to publish our earlier research results, mainly on ozone and other oxidants.

But as outlined in Chapter 3 of this report, we also intend to expand our intellectual horizons, our graduate and post-doctoral educational aspirations, and our public-service responsibilities—so that, by the end of 2006 we will have served, even more effectively than we have in the past, some of the important air-quality management challenges and needs of our region, and through our continuing contributions to NARSTO, also meet some of the important air-quality management needs of our sister nations in North America and elsewhere around the world.

We welcome all who are interested to join us in these research, assessment, and communication tasks. And if you can not join us, we hope you will help us obtain the resources necessary to fulfill these goals and aspirations.
3. SOS AND SOS-AFFILIATED RESEARCH IN THE FUTURE—CONTINUING EVOLUTION OF SOS AND ITS AFFILIATED OZONE AND PARTICULATE MATTER RESEARCH PROGRAMS TO THE SOUTHERN AIR QUALITY SCIENCE, EFFECTS, AND MANAGEMENT STUDY (SOS-SAQSEMS)

During the past 12 years, the Southern Oxidants Study (SOS) has become an important source of policy-relevant findings in ozone pollution research. But this research also has shown that the 10 states of the SOS region continue to have some of the United States' most recalcitrant oxidant and PM$_{2.5}$ pollution problems. In addition, SOS has demonstrated that the South continues to be an ideal natural laboratory for policy-relevant scientific study of the photochemistry of ozone and PM$_{2.5}$ and their separate and combined effects on public health, regional haze, ecosystem health and productivity, and the economic vitality of rural and urban areas throughout this region.

The SOS experience also has proven the effectiveness of the SOS collaborative research paradigm—substantial progress in scientific and public understanding of ozone and PM$_{2.5}$ pollution can be achieved through well-focused and well-disciplined collaboration and cooperation among scientists and engineers in a wide array of research universities, federal, regional, state, municipal, and private sector research and regulatory organizations.

But SOS research has demonstrated the need for continuing evolution in: patterns of thought, definition and prioritization of objectives, analysis and publication of policy-relevant scientific findings, translation and packaging of these findings for use by air-quality managers, and adaptation to new realities in both organizational and financial arrangements for research and outreach to air-quality managers. Learning to cope with these new realities is essential if significant and enduring progress in cost-effective management of ozone and PM$_{2.5}$ pollution is to be achieved. This is true in any ozone or PM$_{2.5}$ non-attainment area, in any given state or

### 3. SOS in the Future

- SOS will continue successful collaborative research paradigm with evolution of oxidant and particulate matter research program into Phase III as SOS-SAQSEMS
- SOS-SAQSEMS will incorporate research and assessment of health and environmental effects
- SOS-SAQSEMS will increase economic and policy analysis
- SOS-SAQSEMS will increase participation of stakeholders, especially air quality managers in region
group of states, or across the North American continent, but it is especially true in the South
given the severity of our air-quality management problems.

As shown in the Major Scientific Findings part (Chapter 2) in both the original State of the
Southern Oxidants Study document (Chameides and Cowling, 1995) and the present document,
SOS has made a number of critical advances in understanding the sources and fate of air
pollutants in the South, many of which have major implications worldwide. Critical findings by
SOS and SOS-affiliated researchers include, among others:

1. Identifying many reasons why past air pollution management efforts have been much less
effective than planned,
2. The role of forest trees and other natural sources of ozone and PM$_{2.5}$ precursors in forming
ozone and PM$_{2.5}$,
3. Development of instrumentation and methods to characterize the atmosphere,
4. Developing observation-based methods for evaluation and improvement of emissions
inventories and air quality models, and
5. Understanding the interactions among regional and urban natural and mobile sources of
precursors, urban plumes, and power plant plumes in determining rural and urban exposures
to ozone.

Air quality managers at the local, state and national levels cite these "Policy Relevant
Findings in Ozone Pollution Research" as being valuable in their efforts to "provide good
government" by improving air quality management, particularly in the South. Current air quality
management efforts, e.g., SAMI, rely heavily on results from SOS and affiliated research.

Such fundamental improvements in what we know about air pollution in the Southeast are
critical. This region has a serious regional ozone pollution problem—a number of cities
experience ozone exposures above the “old” National Ambient Air Quality Standard (120 ppbv
for one hour) for human health and vegetation. A new standard was promulgated in 1997 (80
ppbv for eight hours) and is now undergoing legal challenge and review. If implemented, it will
cause a number of other "near-non-attainment" cities and large parts of the rural South to exceed
the new National Standard (EPA, 2000) as well. Ozone currently damages plants, e.g., crops,
forests, and natural vegetation all over the South.

An even greater problem for the region is fine particulate matter, so called PM$_{2.5}$ (particulate
matter with a diameter less than 2.5 microns). These microscopic particles are the cause of
regional haze throughout the SOS region and are suspected to be an important cause or
contributing cause of excess deaths and increased morbidity nationally. For this reason, a new National Standard for PM$_{2.5}$ (also under legal review) was promulgated in 1997. While supporting data are sparse, it is suspected that many, if not most, large and medium-sized cities in the Southeast will be above the new PM$_{2.5}$ standard, largely because the region as a whole has relatively high PM$_{2.5}$ concentrations. Relatively small increases in PM$_{2.5}$ exposures due to local emissions (e.g., traffic, construction work, industrial sources, and cooking of food) raise the local concentrations above the legal threshold. Particulate matter damages more than health. It also impairs visibility, decreases photosynthesis in some crops, forests, and natural vegetation, and alters local weather and climate. Recent research suggests that these small particles may decrease rainfall amounts and change the local hydrologic cycle. Recent droughts and interstate water resource concerns highlight the importance of this issue.

Addressing both ozone and PM$_{2.5}$ problems is critical to the region's economic and social well being because of a need to protect human and environmental health and also to sustain and encourage economic growth. Further, air quality management in the Southeast must be approached from a regional perspective. It is apparent that both ozone and particulate matter and their natural and anthropogenic precursors do not heed state boundaries, and the whole region (including the relatively “pristine” areas of the southern Appalachians) has remarkably high ozone and PM$_{2.5}$ pollutant concentrations.

Envisioned is a five year Phase III of SOS, titled the Southern Air Quality Science, Effects and Management Study (SOS-SAQSEMS). The new name highlights evolution of a largely atmospheric science-focused regional air quality study to one that keeps its strong atmospheric scientific foundation, but evolves still further to include additional activities dealing with understanding the effects of air pollutants impacting the Southeast, and how to best manage our air quality. It is proposed to include five activities/topic areas: Measurements and Monitoring, Ecological and Other Environmental Effects, Health Effects, Emissions and Atmospheric Modeling, and Economic and Policy Analysis. The objectives of the next five years will be to:

- Enhance our present understanding of the chemical meteorology and chemical climatology of ozone and particulate matter in the Southeast, including quantification of the role of individual regional and local natural and anthropogenic sources that impact air quality.
- Use observation-based and emissions-based methods along with other top-down and bottom-up approaches to determine and improve the accuracy of present and future estimates of
those regional and local emissions actually present in the air and which lead to accumulation of ozone, other oxidants, and PM$_{2.5}$ pollutants in the region.

- Quantify the transport of pollutants and chemical precursors into and through the region.
- Better understand the linkages between air quality, particular components of particulate matter, and both public health and environmental impacts including regional haze.
- Develop and provide the information and tools, e.g., air quality and emissions models, needed for identifying effective strategies to protect human and environmental health.
- Conduct comparative economic analyses of alternative regional and local control measures to identify economical and environmentally effective strategies for management of ozone and PM$_{2.5}$ pollution.

As currently envisioned, core funding for SOS-SAQSEMS would be from the southeastern and south central states and EPA, at a roughly 50-50 split, and would total about $4.5 million per year in addition to the $2-4 million per year currently being invested in SOS-affiliated research and assessment activities by EPRI, the Southern Company, TVA, and others. The joint funding is modeled after other successful projects with similar goals in other parts of the US. Additional funding also will be developed from other stakeholders (e.g., the USDA, NIH, NSF, DOI, DOE, DOD, and other regional concerns such as the forest products and other agriculture-related industries).

What should the stakeholders expect after these additional five years? Not all questions will be answered, as the atmosphere and health effects (both environmental and human) are just too complex. However, it is quite realistic to believe that the region will gain a set of technologies and information to provide better air quality management at both the local and regional level. We will have a better understanding of how to protect human health in the Southeast. There will be a better understanding of how air pollutants are impacting crops, forests, natural vegetation and the tourism industry that is so important, especially in mountain regions of the South, and what can be done both technically and economically to minimize these adverse effects. There will be a better scientific, technical, and economic foundation for the region to proceed with developing regional strategies for air pollution management. We will better understand the role of pollutant transport into and out of the region.

During this third phase of SOS (2001-2006), SOS-SAQSEMS will continue analysis of the many field programs conducted to date, and also will develop, evaluate, set up, and apply models that the state and local agencies (as well as other stakeholders, including the scientific
community) can and will use for air quality planning and analysis. The models will be based on much more accurate emissions inventories than are currently available, in part using direct measurements of the amounts of ozone and PM$_{2.5}$ precursor chemicals actually present in the atmosphere of rural and urban areas to identify emissions inventory problems. Such a foundation will be available to the region, both sooner and more economically than would be possible from individual efforts by the states and other affected parties, and the extensive testing will provide greater confidence in their use.

Working directly and cooperatively with stakeholders throughout the region will get these technologies to the states and industries of the region much sooner, in a way that is more directly focused on the realities of their specific ozone and PM$_{2.5}$ health, ecological, and regional haze problems, and at a much lower cost than if done individually. In addition, all the public and industrial stakeholders will be familiar with the approaches that others are using to develop efficient and cost-effective pollutant management strategies and tactics. Further, there will be better-informed guidance on how best to protect human and environmental health or deal with regional haze in their specific localities. Likewise, each of the states and the region as a whole will have additional insight about how a state’s or industry’s strategy fits into a regional picture, and what set of pollutant-management measures provides the greatest benefits—both locally and regionally and both environmentally and economically. Such information will be key to greater economic development and environmental improvement in the region, and will have the effect of laying a foundation for more efficient and cost-effective regional air resource management approaches.
3.1. SOS-SAQSEMS STUDY COMPONENTS

3.1.1. Measurements and Monitoring

SOS has built an international reputation for conducting state-of-the-science field studies, developing and deploying advanced monitoring technologies, and analyzing and publishing the results of those measurements. These aspects of SOS will continue to be central to the SOS-SAQSEMS program, especially during 2001-2003. In previous years, SOS has been involved in or affiliated with a number of intensive field measurement and monitoring programs: e.g., in Atlanta in 1990-1992 and again in 1999; in Nashville in 1994, 1995, and 1999; in the eastern half of Texas through TEXAQS 2000; in the Tennessee Valley PM2.5 Partnership Network since 1993; in the regionally-focused SEARCH and urban-focused ASACA research and monitoring studies; and in the 3-city 3-year-long Fall Line Air Quality Study (FAQS) in Georgia beginning in 2000. Likewise, SOS researchers have been affiliated with the epidemiologically focused ARIES program. SOS also participated in development of the Southern Center for the Study of Air-Borne Pollutants and Health Effects (SoCSAPHE) PM Centers proposal together with the University of Miami and Emory University. The third phase of SOS will continue and strengthen such collaborative efforts, for example, to field studies to help evaluate exposure of populations more accurately, and have detailed knowledge of which sources are contributing to specific components of the air pollutant mixture. From this, more detailed source-health impact assessments can be conducted.

Especially during 2003-2006, SOS-SAQSEMS will participate in targeted field measurement campaigns, most likely in other regions of the Southeast. Targets of opportunity and focus would include providing additional information for use by the health and ecological effects and regional haze research communities. For example, in determining pollutant exposures of crops and forests, and both NH$_4^+$ and NO$_3^-$ loadings to streams and estuaries are of special importance outside of the major cities. Further, information on air pollutants in rural areas, in particular PM$_{2.5}$, is key to identifying optimal controls for urban areas since particulate matter is
transported so efficiently. Health effects related field studies, and measurement work, will be
designed to address specific health questions, e.g., what part of the PM$_{2.5}$ (or even if it is PM$_{2.5}$)
is most responsible for health impacts. This may well involve the development of a technology
to measure a particular component of the PM$_{2.5}$, and deploy the instruments in target locations
for exposure assessment. These continuing measurement and modeling studies will also serve to
further resolve any lingering atmospheric chemistry and transport questions from prior
experiments.

This portion of the project is expected to require $1 million per year in the initial three years,
decreasing in the latter two years. This is on top of the work currently being conducted in the
region over the next few years, supported by local industries, state, local, and national agencies,
and others. At the present time, the funds would be leveraged approximately two to one, and
such a commitment would provide assurance that some of the current projects can be fully
utilized in the future. Further, this continuing work will be key to developing a chemical
climatology of the region to better understand long term changes and impacts, building upon the
detailed measurements to date.

### 3.1.2. Analysis and Interpretation of the Atlanta PAMS Data

Atlanta is the only PAMS site in the southeastern states and very little analysis and
interpretation of these data has so far been accomplished [much to the mutual chagrin of both
EPA-OAQPS and the Georgia Environmental Protection Division (GA EPD). Thus, a
significant opportunity for getting these valuable data analyzed, interpreted, published, and used
would be to apply the skills in the SOS scientific community to this important task. In fact, Bill
Hunt, former leader of the PAMS program nationally, is presently on an Interagency Personnel
Act (IPA) assignment as a Visiting Professor in the Department of Statistics at NC State
University and has been working with several students in the Department in analyzing PAMS
data in the states of Connecticut and New Jersey. Hunt has indicated a keen interest to work
with others in SOS, including Carlos Cardelino of Georgia Tech and Fred Vukovich of SAIC
(see Section 2.1.4.) to ensure that effective use is made of the Atlanta PAMS data. The GA EPD
is currently negotiating a contract with Carlos Cardelino of Georgia Tech to conduct further
analysis of the Atlanta PAMS data. This is an example of how SOS financial resources and
scientific competence can help attract additional funding from state and regional stakeholders.
3.1.3. Environmental Effects

Agriculture and forestry are major economic drivers in the Southeast. Both ozone and particulate matter have important adverse effects on these sectors of society in the Southeast. The extent of these impacts is not well quantified, and further, some of the larger potential impacts are just being identified. For example, particulate matter is altering regional climate. First, particulate matter leads to increased cooling in the region (this may be a benefit). Studies now suggest that it may also lead to decreased rainfall, altering the hydrological cycle, which has ramifications on the regional use of water resources. Decreased solar radiation reaching the ground will decrease photosynthesis, and thus inhibit growth and development of crops, forests, and natural vegetation, though the extent is unknown.

We know from controlled exposure studies that ozone concentrations above 60 ppbv decrease growth and yield of many species of crops, forests, and natural vegetation. We also know that the magnitude of ozone effects on yield varies greatly with various species of plants. But we do not know enough about actual ozone exposures in rural areas, in large part because most ozone monitors are placed in and around urban areas rather than in rural and remote areas, especially at high elevations. Thus, more ozone monitoring in rural areas and more emphasis on modeling of rural ozone exposures based on measurements at existing nearby (mostly urban and rural monitoring sites) along with traditional air quality modeling and statistical analysis (e.g., kriging) would be a cost-effective way to quantify exposures and estimate economic impacts on crops, forests, and natural vegetation. Another element of estimating effects on a regional basis is the calculation of the actual ozone dose experienced by various species of plants based on micrometeorological conditions, soil type, moisture status, etc.; a modeling component that incorporates various types of information, likely in a geographical information system, will be developed.

Ozone stresses plants, though to an amount that is highly dependent on species. Particulate matter can decrease photosynthetically active radiation and reduce temperatures regionally. Given the high regional levels of particulate matter and ozone, it is important to better quantify the extent of impacts to crops and forest in the region. The first step in quantifying regional impacts would be an assessment of the impacts that are currently known. From that information, field studies will be planned to characterize air pollution impacts to specific crops and forests in...
specific areas of the region. Results of those studies would then be used to analyze the impacts on such systems. A particular thrust of the study would be on studying regional climate and hydrologic cycle impacts.

This portion of the study is estimated to require approximately $1 million per year in funding from the southeastern states-EPA combination, and addition funding would be generated from other agencies (e.g., USDA, NSF and DOI) with related missions. Total funding would be envisioned at about $2 million per year.

3.1.4. Health Effects

While the Southeast has some of the highest PM$_{2.5}$ exposures in the nation, we are also one of the only areas without an EPA-funded PM-center devoted to studying health effects. The SoSCAPHE proposal outlines the types of research that are needed in the SOS region. It would build upon the atmospheric research currently being conducted in this region, as well as additional studies performed as part of SOS-SAQSEMS. In particular, SEARCH/ARIES (a utility funded project), ASACA, and others are developing a detailed, long term record of air pollution in the region that can be used to support health effects studies. SOPHIA (also utility funded, a predecessor to ARIES), used historical information to do just that. Such studies are based upon long-term records, and continuation will increase the power of their results. Further, the current studies are not able to look at personal exposure. This portion of SAQSEMS would provide funding critical to alleviating these two limitations. Required funding would be $1.5 million per year, from EPA and the states, and it is anticipated that additional funding of approximately $1-2 million would be identified from other sources (e.g., NIH and EPRI).

3.1.5. Emissions and Atmospheric Modeling

Air quality models are used both for scientific and management purposes, and they will be so used in Phase III of SOS. As in the first two phases of SOS, air quality models have been employed to understand the state of the atmosphere and to develop source-air quality relationships. They have been used to identify which classes of emissions (VOC or NOx) are best for reducing ozone. As such, their role is key.

In this phase of SOS, we plan to continue to use and advance state-of-the-science air quality models for addressing science questions, and also to provide them to the regional stakeholders
for their use in air quality management. It is the intent to have the models ready for use to evaluate control strategies at the regional and local levels, having previously conducted extensive evaluation to ensure their use with confidence and acceptance by others (e.g., EPA, affected industries, environmental groups). Confident use of observation-based and emissions-based air quality models requires continuing comparison of ambient measurements with emissions inventories for the region, fully characterizing the meteorology during episodes that lead to high concentrations of air pollutants (and in the case of PM$_{2.5}$, periods when concentrations are not that high), and extensive evaluation, e.g., with detailed measurements taken as part of SOS during this and prior phases, as well as routine monitoring. During the first two years of the study, significant effort would be given to working with the states and local industries to inventory emissions of ozone and PM$_{2.5}$ precursors. Such information would then be used, along with meteorological fields, to conduct air quality modeling of a variety of periods for use in developing quantitative emissions-source-air quality relationships in the region over a suite of meteorological regimes. The models and their inputs will then be for use by regional stakeholders. Required funding is estimated to be about $1 million per year at first, and escalating in the latter years, and would rely on significant cooperation with related state agencies in charge of emissions inventorying and related industries. It is suspected (evidence already exists) that there will be a significant interest by stakeholders in the region to utilize the products from this portion, and contribute to their further development, testing, and application.

3.1.6. Economic and Policy Analysis

The final step in this third phase of SOS-SAQSEMS will be to use the air quality model results from above to evaluate local and regional policies to quantify their cost and benefits, and how such costs/benefits are distributed in the region. Further, the policy analysis would look at how attainment/non-attainment issues impact the region’s development. This activity would begin modestly at the start, and would increase to about $500 thousand per year in the latter stages. Again, much of the more applied modeling will be funded by regional stakeholders interested in specific aspects of the problem (e.g., individual state source impacts).
3.2. FURTHER JUSTIFICATION FOR SOS-SAQSEMS

While SOS has a very positive history, the name no longer is descriptive of the types of activities required for the Southeast region over the longer term. Ozone and other oxidants, alone, are no longer the only air-quality problems. The region is concerned with ozone, particulate matter, and possibly air toxics, all of which share a common set of precursors. Second, during the next five years, SOS-SAQSEMS should move towards improved understanding of the health and environmental effects of air quality and development of both the technical means and the economic optimization of air quality management.

The Southeast region will continue to have air pollution in the future; thus, the question is how best to manage the atmosphere as a resource. However, the South is still an appropriate domain over which to examine the problem due to the unique characteristics of this region. Thus, a new title — SOS-Phase III - the Southern Air Quality Science, Effects and Management Study (SOS-SAQSEMS), is suggested. The program will continue to involve researchers from across the nation, with particular emphasis on those in the southeastern state study region, including Alabama, Florida, Georgia, Kentucky, Louisiana, Mississippi, North and South Carolina, Tennessee, and Texas, and, with the addition of Virginia and West Virginia. All 12 of these states share transboundary air pollution problems. University, federal, state, and industry researchers in these states have shown an ability to work together effectively during the 12 years of the first two phases of SOS.

During the past 12 years, stimulated and encouraged by the 1991 NRC report, the Southern Oxidants Study (SOS) has played a central role in understanding the dynamics of ozone in the Southeast, though scientific findings have been of both national and international significance.

First, SOS researchers have shown that the relative role of natural and anthropogenic sources to ozone formation differ between the Southeast and other regions, though biogenic sources are
important worldwide to varying degrees. Without this improved understanding, the region’s ability to effectively manage ozone would have been severely hampered, less effective, and even more costly.

SOS researchers also have discovered critical flaws in information used by air quality managers to develop air quality management strategies. A number of instruments have been developed that can better probe the chemical nature of the atmosphere. Various field studies and analyses have led to better understanding of emissions in the Southeast, how they differ from emissions in other regions, and that ozone accumulation in the Southeast is a regional phenomenon that is substantially different in character from that in either the northeastern states, midwestern states, or southern California. In summary, SOS has laid a substantially better scientific foundation for ozone pollution management in the Southeast, and demonstrated that many features of the ozone problem are unique to the region.

The last decade has also been historic on the national regulatory front. The Clean Air Act Amendments of 1990 were passed, with parts being based in part on work done by SOS researchers during the years before SOS was initiated in 1988. More recently, two new standards were promulgated: one tightening the National Ambient Air Quality Standard (NAAQS) for ozone, another setting a new standard for PM$_{2.5}$ (particulate matter with a diameter less than 2.5 micrometers, or about 20 times smaller than the width of a human hair). While these two standards are now undergoing legal review, they represent a major change in the air quality management landscape, particularly in the Southeast. Outside southern California, the Southeast region has the highest concentrations of PM$_{2.5}$ in the nation. Many cities in the South have PM$_{2.5}$ concentrations that exceed the proposed National Standard. Again, all indications to date suggest that the problem is largely regional, with pollutant sources being spread throughout the region and transported hundreds of miles from one state to the next. Also, there are preliminary indications that, like ozone in our region, biogenic sources (including forest trees and both crop and animal agriculture) are major contributors of particulate precursors—VOC, NH$_4$, and other organic forms of airborne nitrogen compounds. Ambient measurements also indicate that a number of areas within the southern region that have been in compliance with the old ozone standard will not be so fortunate with the new standard.
Further economic development of the South will be impacted by our inability to maintain air quality within those standards, or show progress toward those goals. One further set of rules is also going to impact the southern region, that being the NOx-SIP call, requiring drastic decreases in emissions from electricity generating plants. The Southeast enjoys some of the cheapest electricity in the nation, and such rules will significantly increase the current rates.

While the NOx-SIP call places new economic constraints on all eastern states, the objective of the "call" is to protect public and environmental health. Some estimates suggest that thousands of people will die from high PM$_{2.5}$ exposures each year. Also, a high correlation has been found in some but not all epidemiological studies between ozone and respiratory problems (e.g., pediatric asthma). Given our high exposures to ozone and PM$_{2.5}$, the southern region should be particularly concerned with how to better manage air quality problems to improve both human health and environmental quality. Air pollutant impacts are not limited to human health. Ozone above about 60 ppbv inhibits photosynthesis in many species of crops, forests, and natural vegetation. PM$_{2.5}$ decreases the enjoyment of scenic vistas in many part of the South and leads to soiling of windows, fabrics, and building exteriors. PM$_{2.5}$ may also be leading to regional climate modification, decrease of light exposure and thus photosynthesis in crop and forest vegetation, changes in rainfall amounts and other alterations of the hydrologic cycle, and changes in the frequency and severity of extreme weather events. These observed and/or potential changes in air-quality-related values suggest that further action dealing with our regional air quality problem is needed, and soon. However, such management actions must be well founded in scientific understanding of how the atmosphere works, sound understanding of how air pollutants affect the health and well-being of our society, and how alternative strategies of air quality management affect the economic vitality and quality of life in society.

For example, for years many air quality managers spent most of their resources decreasing emissions of one of the two major ozone precursors, volatile organic compounds (VOCs). It now appears that focusing on the other major precursor, nitrogen oxides (NOx), would have been more effective in many parts of our region. A similar mistake may be made in addressing the PM$_{2.5}$ problem. PM$_{2.5}$ is composed of many different constituents, including sulfate (largely from power plants), organic matter (from a multitude of sources), and various metals. It is not known which components of PM$_{2.5}$ are the primary cause or major contributing causes of human health impairment. This lack of knowledge about the causal constituents of PM$_{2.5}$ has led to air
quality standards being based on PM$_{2.5}$ mass. If our strategy is to meet any particular air-quality standard, it is possible that the region may spend billions to decrease emissions of the wrong part of the problem. Thus, there is a need to have our approach to air quality management tied to achieving the ultimately desired endpoints: improving human health and decreasing other undesirable environmental impacts (e.g., visibility impairment and decreased yields of crops, forests, and natural vegetation).

The above points argue that the Southeast should take the lead in a more aggressive approach to air quality management, based on addressing the issues cooperatively from a regional perspective, and directly targeting improved human health and environmental quality. SOS has laid a very strong scientific foundation. The next step is translation and packaging of scientific knowledge in ways that air quality managers can understand and use as tools for making wise choices among alternative air-quality management options. In part, this requires reaching out to new communities that have not played as large a part in SOS as in the past—in particular health and environmental effects researchers and the air quality management community. The latter community includes local, state, tribal and national agencies, affected industries, and environmental organizations in the region. With their participation, the next five years of SOS have the potential to provide the region with the knowledge and tools to help improve health and environmental quality while furthering economic development in the region.

During the first three years (2001-2003) of SOS-SAQSEMS (2001-2006), significant attention will be given to analysis, interpretation, presentation, publication, translation, and packaging of policy-relevant scientific findings from ozone and PM$_{2.5}$ field research campaigns conducted in 1998-2000. [Judging from the 100+ refereed journal publications SOS scientists and engineers published in 1998-2000 on the basis of the 1994-1995 Nashville/Middle Tennessee Ozone Study, it is reasonable to project that the total yield of papers published in 2001-2003 based on the seven major field research campaigns completed by SOS and SOS-affiliated research scientists in 1998-2000 (see list below) would be at least 200 refereed journal publications and about 300 additional non-refereed publications and presentations at scientific meetings.]

Especially during 2001-2003, progress in SOS-SAQSEMS will be based largely on the approach effectively used in SOS to date—large research teams working cooperatively to characterize the atmosphere in the region, in this case working primarily with the results of the fields experiments conducted to date and those planned in the next few years. Without such data, it is quite possible to miss key pieces of knowledge about which processes are driving and controlling ozone and PM$_{2.5}$ accumulation in the region. Such data is then analyzed, both by the original SOS science team, and others who bring additional expertise especially in the areas of observation-based and emissions-based modeling, public health and ecological exposures and effects, and economic analysis of alternative pollutant-management strategies. Public health and ecological effects researchers will help identify the types of measurements needed to link air quality with human exposure, public health, environmental, and visibility impacts. Environmental effects researchers will use the measurements, along with other methods, to associate both specific sources with specific impacts and multiple-pollutant exposures with both local and regional sources of precursor chemicals. Another evolution will be for researchers specializing in emissions estimation to cooperate with both state and industrial stakeholders in...
developing detailed emissions inventories for the 12-state SOS region. These inventories, along with the results from the field experiments, will be used by researchers and state and industrial stakeholders to develop, evaluate, and then directly apply these improved air quality models as part of the informational background for ongoing air quality management decisions. In order to provide additional information to air quality managers in the region, SOS-SAQSEMS will include environmental policy analysts to provide additional guidance on what pollutant control measures will provide the greatest benefits both within specific industries, states, and multi-state parts of the SOS region and throughout the region as a whole.

This period will also see the beginning of the evolution of SOS as described above. However, as the list of studies in the last few years by SOS and SOS-affiliated researchers suggests, considerable effort will need to be made to complete the analysis and publication/translation of results from the nine SOS and SOS-Affiliated studies listed below:

- **SOS-SCISSAP (Southern Center for Integrated Study of Secondary Air Pollutants)** — a 25-investigator, ground-based regional, urban/rural aerosols characterization study led by Bill Chameides at Georgia Tech during the 30 months from June 1998 through December 2001. SOS-SCISSAP was funded through a grant to Georgia Tech from EPA-NCERQA with subcontracts to other SOS investigators in various parts of the region.

- **SEARCH (Southeastern Aerosol Research and Characterization)** study — a ground-based, 8-site, regional, urban/rural gas/aerosol characterization study patterned after SOS-SCISSAP and led by John Jansen of the Southern Company and Alan Hansen of EPRI. Since 1996, SEARCH was implemented through an EPRI Tailored Collaboration Contract with Eric Edgerton of Atmospheric Research and Assessment (ARA) Inc. This long-term study began within SOS in June 1992 and was continued from June 1996 through 2000 by the Southern Company and EPRI. The SEARCH study was recently authorized for continuation from 2001-2006.

- **ARIES (Aerosol Research Inhalation Epidemiological Study)** — a ground-based epidemiologically focused, human-health/aerosol-exposure study led by Tina Bahadori and Alan Hansen of EPRI during the 24-month period May 1998-June 2000.

- **ASACA (Assessment of Spatial Aerosol Composition in Atlanta)** — a ground-based urban/rural aerosol characterization study in the Atlanta metropolitan area led by Ted Russell of Georgia Tech. This study has been largely funded by the Southern Company for a 29-month period extending from March 1999 to August 2001, and is expected to continue beyond that date.

- **SOS-NASHVILLE ‘99** — a 150-investigator, ground- and aircraft-based, integrated study of ozone-formation and aerosol-formation processes in urban plumes and power plant plumes in the 10-state region surrounding Nashville, TN. This study was led by Jim Meagher of the NOAA Aeronomy Laboratory during July 1999.
• **SOS-ATLANTA SUPERSITE** — a 75-investigator, multi-institutional, ground-based instrument intercomparison study of methods for determination of the chemical composition and physical characteristics of PM$_{2.5}$ in Atlanta. This intensive study was sustained through funding provided by both EPA-NERL and EPA-OAQPS. The study was led by Bill Chameides of Georgia Tech during August 1999.

• **TEXAQS 2000** — a 250-investigator, multi-institutional, ground- and aircraft-based study of the unique interactions between petrochemical industry emissions, the Houston urban plume, and sea-breeze- induced meteorological factors that lead to accumulation of ozone and PM$_{2.5}$ in the Houston metropolitan area and the eastern half of Texas. This six week intensive field measurement campaign was led by Peter Daum and Larry Kleinman of the Brookhaven National Laboratory in cooperation with Jim Price and others of the Texas Natural Resources Conservation Commission (TNRCC) and David Allen of the University of Texas and Matt Fraser of Rice University through the Gulf Coast Aerosol Research and Characterization (GC-ARCH) study — the so-called "Houston Supersite" part of EPA's six-city PM Supersite Program led by Paul Solomon and Rich Scheffe of EPA-NERL and EPA-OAQPS. The GC-ARCH program began in March 2000 and will continue through December 2002.

• **TENNESSEE VALLEY PM$_{2.5}$ PARTNERSHIP Network** — a dozen or so investigators working under the general leadership of Bill Parkhurst of TVA are maintaining indefinitely a long-term monitoring network to characterize PM$_{2.5}$ in various parts of the Tennessee Valley region. At present this Partnership Network includes 2 remote sites, 1 regional background sites, 3 suburban sites, and 6 urban sites. Additional sites are planned for the future (see map in Section 1.4).

• **FALL LINE AIR QUALITY STUDY (FAQS)** — this detailed study of three “near-non-attainment” cities in the state of Georgia (Augusta, Macon, and Columbus) was initiated in 1999 under the general leadership of Michael Chang with significant participation by several SOS faculty and graduate students within the Schools of Earth and Atmospheric Sciences and Chemical Engineering at Georgia Tech. The FAQS study will continue at least through the 2002 calendar year.
3.4. CONTINUING EVOLUTION OF SOS-SAQSEMS IN THE LONGER TERM (2003-2006)

The objectives of SOS-SAQSEMS beginning during the short term (2001-2003) but accelerating during the long term (2003-2006) should be to:

- Enhance present understanding of the chemical meteorology and chemical climatology of ozone and particulate matter in the Southeast, including quantification of the role of individual regional and local natural and anthropogenic precursor emissions sources that impact air quality.

- Use field-observational and hybrid modeling methods to determine the accuracy of present estimates of those regional and local emissions actually present in the air and which lead to accumulation of ozone, other oxidants, and PM$_{2.5}$ pollutants in the region.

- Quantify the transport of pollutants and chemical precursors into and through the region.

- Better understand the linkages between air quality, particular components of particulate matter, and both public health and environmental impacts including regional haze.

- Provide the tools, e.g., air quality and emissions models, needed for identifying effective strategies to protect both human and environmental health.

- Conduct comparative economic analyses of alternative regional and local control measures to identify economically and environmentally effective strategies for management of ozone and PM$_{2.5}$ pollution.

At the end of the five year period, the states and other air quality managers in the region will have an improved understanding of the science of ozone and PM$_{2.5}$ accumulation in the 12-state region and the tools needed to deal much more effectively with their individual air pollution problems — both from a local as well as a regional perspective. Further, the work would lay the foundation for more effective national policies and management approaches.

The proposed five year SOS-SAQSEMS study will require base funding of about $4.5 million per year, and following examples from other areas of the country, would be supported by the states in the region and the EPA (at about a 50-50 split). It is expected, as is evidenced by activities in this region and elsewhere, that other interested stakeholders in the region would add
on to the study, supporting work of direct interest to themselves, though usually of importance to others.

An example is the current work being conducted by Southern Company, characterizing PM levels in the region, and the use of that data to drive health effects analysis. Likewise, TVA is conducting a range of studies on air quality in the area. In California, oil and auto companies and utilities have contributed significantly to the air quality studies that have been used to help provide state-of-the-science models and air quality data sets that are being used for air quality management in that state. Individual states also would likely contribute to studies germane to their specific part of the region, for example if a specific city is found to have a problem that appears to be of limited spatial extent, though needs to identify what solutions exist, that city or state would be expected to contribute to the work — as has occurred in 1999-2002 with the three-city Fall Line Air Quality Study in Georgia.

In many ways, the evolution of SOS is already underway as exemplified by the SEARCH/ARIES, SAMI and FAQS studies. The region is beginning to recognize the need to understand better, the science behind the air quality problem it now faces, and to identify the real impacts and possible solutions. SOS has set itself up to take a leadership role in further improving the scientific foundation of those studies, and other derivatives, and at the same time make sure that the scientific fundamentals get translated for use in policy setting and effects research.

3.5. Continuing role of SOS Investigators in NARSTO (FORMERLY, THE NORTH AMERICAN RESEARCH STRATEGY FOR TROPOSPHERIC OZONE).

SOS' role as a significant constituent part of NARSTO began in 1991 shortly after publication of the National Research Council (NRC) report on “Rethinking the Ozone Problem in Regional and Urban Air Pollution.” NARSTO was created in 1993 in response to the 10th and final recommendation in the "Rethinking" report. This recommendation called for creation of a “coherent and focused national program for the study of tropospheric ozone and related aspects of air quality” that "emphasizes high-quality science and is relevant to policy but not driven by policy considerations." In fact, SOS was mentioned specifically on page 11 of the Executive Summary of the "Rethinking" report as an example of the kind of regional research program that was needed on a national level.
From the beginning of the planning processes that led to creation of NARSTO in February 1993, SOS scientists and engineers have played a prominent role in the working groups on modeling, measurements, emissions, and other topics leading to the creation of NARSTO.

During 1997-98, NARSTO developed plans for a NARSTO Scientific Assessment of the tropospheric ozone issue. Bill Chameides, Chief Scientist for SOS and Ken Demerjian, State University of New York, served as co-chairs of the Science Team that prepared the 2000 NARSTO Assessment Document -- An Assessment of Tropospheric Ozone Pollution -- A North American Perspective (NARSTO, 2000). Nineteen SOS scientists served as senior authors or co-authors for nine of 24 NARSTO Critical Review Papers (NARSTO Special Section, Atmospheric Environment, 2000; [http://www.cgenv.com/Narsto](http://www.cgenv.com/Narsto)). Also, 58 of the 195 other scientific papers cited in the NARSTO Assessment Document were prepared by SOS scientists and engineers and included scientific findings from SOS.

Several SOS scientists have been asked to join the Analysis and Assessment Team for the 2001 NARSTO Scientific Assessment on PM$_{2.5}$. Thus, SOS-SAQSEMS will continue in 2001-2006 to be an important part of other NARSTO research, research-coordination, and scientific-assessment activities.

Just as SOS found inspiration and guidance for much of its ozone-focused research in the National Research Council “Rethinking” report, SOS has found similar inspiration and guidance for its PM$_{2.5}$ research in the National Research Council’s two recent reports on “Research Priorities for Airborne Particulate Matter” (NRC, 1998, 1999).

**KEY CITATIONS:**
APPENDIX A. PAPERS PUBLISHED OR PRESENTED BY SOS SCIENTISTS AND ENGINEERS FROM 1988-2000

Peer-Reviewed Publications


Ph.D. Dissertations and M.S. Theses


Non Peer-Reviewed Publications and Presentations


Chameides, W.L. and E.B. Cowling (comp.) 1994. Key scientific contributions by SOS scientists (additional "Papers to be provided"). Southern Oxidants Study, Raleigh, NC. Various pagings.


Cowling, E. 1996. Avoiding the necessity for a second NRC report on rethinking the ozone problem in urban and regional air pollution during the years between 2002 and 2017. Statement before the EPA Clean Air Act Scientific Advisory Committee. EPA Auditorium, Research Triangle Park, NC, March 21, 1996.


Fehsenfeld, F.  1996.  An aircraft view of the regional transport of plumes.  SOS Nashville data analysis workshop, Raleigh, NC.  May 1996.


APPENDIX B. PRINCIPAL INSTITUTIONS AND INVESTIGATORS IN SOS

The alphabetized lists of more than 80 organizations and nearly 500 persons shown below indicate the wide variety of public and private-sector institutions, organizations, and personnel that contribute to the success of the Southern Oxidants Study in 1994-2000. The individuals listed include two general groups:

1) Scientists, engineers, graduate students, and postdoctoral fellows who are actively engaged in SOS field measurement campaigns, and, in most cases, also join in authorship of SOS scientific contributions – mainly in refereed journals. These persons are listed without asterisks;

2) Contact- and liaison-persons who play active roles in providing financial and/or in-kind (cooperative) support for SOS or are active users of SOS data, information, publications, and policy briefings. These persons are identified by asterisks (*).

Aerodyne Research, Inc., Billerica, Massachusetts
Manjula Canaragatna, Charles Kolb, John Jayne, Jose Jimenez, Phil Silva, M. Stolzenburg, Douglas Worsnop

Aerosol Dynamics, Inc., Berkeley California
Susanne Hering

Atmosphere Research and Analysis, Inc., Durham, North Carolina
Eric Edgerton, Benjamin Hartsell

Baylor University, Waco, Texas
Sergio lvarez, Joshua Anderson, Jerry Begbie, Jimmy Flynn, Guelmy Garcia, Keith Hewson, Clint Owens, Max Shauck, Tim Sinclair, Steve Stanford, Matt Tilghman, Grazia Zanin

Boston College, Boston, Massachusetts
K. Purvis

Bringham Young University, Provo, Utah
D. J. Eatough, M. K. Modley

Clarkson University, Potsdam, New York
Phil Hopke, Alexander Polissar, Xinhua Song

Colorado State University, Fort Collins, Colorado
Bill Durham, Jim Slusser

Duke University, Durham, North Carolina
Prasad Kasibhatla, D. L. Wright, S. Yu

Emory University, Atlanta, Georgia
Dana Farber, Howard Frumken, Judy Hughes, Mitchell Klein, Krista Metzger, Page Talbert, Know Todd, Dennis Tolsma

Environ Corporation
Mary Roberts

Environment Canada, Downsville, Ontario, Canada
Jan Bottenheim, Chris Hilme, Douglas Lane
EPRI (formerly Electric Power Research Institute), Palo Alto, California
Tina Bahadori, Alan Hansen, Pradeep Saxena, Peter Mueller*, Ron Wyzga

Georgia Institute of Technology, Atlanta, Georgia

Harvard University, Cambridge, Massachusetts
George Allen, Petros Koutrakis, Jennifer Logan, Helen Suh, Steve Wolfsy

Mantech Environmental Technology, Research Triangle Park, North Carolina
Tad Kleindienst, K. Kronmiller, David Stiles

Mercer University, Macon, Georgia
Andre Butler

NARSTO (formerly North American Research Strategy for Tropospheric Ozone), Pasco, Washington
Jake Hales*

National Aeronautics and Space Administration
Marshall Space Flight Center, Huntsville, Alabama
Dale Quattrochi, David Rider

Goddard Space Flight Center, Greenbelt, Maryland
A. M. Thompson, J. C. Witte

Jet Propulsion Laboratory, Pasadena, California
M. J. Mahoney

National Center for Atmospheric Research, Boulder, Colorado
E. Atlas, Eric Apel, Elliot Atlas, Jack Calvert, Chris Cantrell, Stephen Donnelly, Frank Flocke, Alan Fried, Timothy Gilpin, Jim Greenberg, Alex Guenther, Sam Hall, B. Henry, Lee Klinger, Shane Mayor, Katie Purvis, Bian Ridley, Daniel Riemer, Sue Schauffer, Rick Shetter, James Walega, Andrew Weinheimer, Bryan Wert

National Research Council of Canada, Ottawa, Ontario, Canada
Thomas Biesenthal

National Institute for Environmental Studies
Shinjui Wakamatsu

National Institute of Standards and Technology, Boulder, Colorado
George Klouda
Rutgers University, New Brunswick, New Jersey
H. Lim, Barbara Turpin

South Dakota School of Mines and Technology, South Dakota
Patrick Zimmerman,

Southern Company, Birmingham, Alabama
John Jansen

State of North Carolina, Raleigh, North Carolina

State of Georgia, Atlanta, Georgia
Ron Methier*, Harold Reheis*, Susan Dauphinee

State University of New York, Old Westbury, New York
All Alaoule, Barbara Hillery, Jun Zheng

Tennessee Valley Authority, Muscle Shoals, Alabama

Texas A & M University, Lubbock, Texas
C. Boring, Don Collins, P. Dasgupta, Roberto Gasparini, Z. Genfa Purnendu, Stephanie Naumann, Gammon Nielsen, Karl Schulze

Texas Hazardous Waste Center
George Talbert

Texas Natural Resource Conservation Commission, Austin, Texas

University of Agricultural Sciences, Vienna, Austria
Gerhard Wotawa

University of Alabama in Huntsville, Alabama
Mohammed Ayoub, Robert Clymer, Noor Gillani, Richard McNider, Michael Newchurch, William B. Norris, Scott Podgorny, Tim Rushing, Aaron J. Song

University of California, Berkeley, California
Ronald Cohen, Rebecca Rosen, Ezra Wood, Paul Wooldridge, Joel Thornton, Rob Harley

University of California, Los Angeles, California
Bjorn Alicke, Jochen Stutz, Ralf Akermann
University of California, Riverside, California
Keith Coffee, Anne Johnson, Don Liu, Sylvia Pastor, Kimberly Prather, David Sodeman, Gail Tonneson, Ryan Wenzel, Sylvia Wood

University of California, San Diego, California
T. H. Mark, G. Michalski

University of Colorado, Boulder, Colorado
Alice Delia, Raymond Fall, S. Lee, Russell Monson

University of Delaware, Newark, Delaware
D. Phares, M. V. Johnson, Kevin Rhoads, Tony Wexler

University of Denver, Denver, Colorado
D. W. Gesler, B. G. Lefleur, J. Mullen, R. M. Reeves

University of Heidelberg, Heidelberg, Germany
Gerd Hoenninger, Ulrich Platt

University of Houston-Clear Lake, Houston Texas
James Lester, Ron Mills

University of Innsbruck, Innsbruck, Austria
Armin Hansel, Thomas Karl, Werner Lindinger, Armin Wisthaler

University of Maryland, College Park, Maryland
A. D. Frolov, R. D. Hudson, John Ondov

University of Miami at Miami, Florida
Charles Farmer, Hal Maring, Peter Milne, Giovanni Piedimonte, Daniel Riemer, Dennis Savoie, E. R. Stabenau, Rod Zika

University of Michigan, Ann Arbor, Michigan
Mary Ann Carroll, Dongyang He, Margaret Pippin, Sanford Sillman, Perry Samson, T. Thornberry, Maria Witmer-Rich

University of Minnesota, Minneapolis, Minnesota
Peter McMurry

University of Tennessee, Knoxville, Tennessee
Douglas Ryan, Thomas Miller

University of Texas, Austin, Texas
David Allen, Vickie Amidon, Dyanne Cortez, Teresa Howard, Matt Mangum, McDonald, Buller, Gary McGaughhey, Charles Mullins, Matt Russell, Paul Tanaka, Vincent Torres

University of Washington, Seattle, Washington
Y. Pang

URS Corporation, Austin, Texas
Walter Crow, Albert Hendler

U. S. Department of Commerce
  Cooperative Institute for Research, Boulder, Colorado
D. P. Hereid, Richard Marchbanks
U.S. Department of Energy

Brookhaven National Laboratory, Upton, New York

Federal Energy Technology Center, Germantown, Maryland
Thomas Feeley*

Lawrence Berkeley National Laboratory, Berkeley, California
Laura Gundel

Oak Ridge National Laboratory, Oak Ridge, Tennessee
Les Hook, Sigurd Christensen, Meng-Dawn Chen

Pacific Northwest Laboratory, Richland, Washington

U.S. Environmental Protection Agency

National Exposure Research Laboratory, Research Triangle Park, North Carolina

National Exposure Research Laboratory, Las Vegas, Nevada
Paul Solomon

National Health and Environmental Research Laboratory, Research Triangle Park, North Carolina
John Vandenburg*

National Risk Management Laboratory, Research Triangle Park, North Carolina
Chris Geron, Larry Jones*

National Center for Environmental Research, Washington, DC
Meetre, Daren Pashayan*, William Lofton, James Vidley

National Center for Environmental Assessment, Research Triangle Park, North Carolina
Les Grant*, Jay Garner

Office of Air Quality Planning and Standards, Durham, North Carolina
John Bachmann*, Dennis Mikel, Thomas Helms*, Michael Jones*, David Mobley*, Rich Scheffe*

USEPA – Region 4, Atlanta, Georgia
Winston Smith*, Allen Powell

USEPA – Region 6, Dallas Texas
Jim Yarbrough*, Robert Hanneschlager*
Washington State University, Pullman, Washington
Peng Yanbo, Brian Lamb, Brian Hopkins

Western Michigan University, Kalamazoo, Michigan
Steve Bertman, Wang Chun Chen, Mei Ma

York University, North York, Ontario, Canada
C. A. Stroud