NARSTO-1997-3

Narsto Strategic Execution Plan

Part 3: Science Plan

September 1997

Foreword

This third part of the NARSTO Strategic Execution Plan completes NARSTO's planning documentation for the period extending through 1998. In addition to this document, the complete ensemble of planning material available to date includes:

- *The NARSTO Research Strategy and Charter (November 1994);*
- *The NARSTO Strategic Execution Plan, Part 1: Introduction and Overview (NARSTO-1997-1, March 1997);*
- *The NARSTO Strategic Execution Plan, Part 2: Analysis and Assessment (NARSTO 1997-2, March 1997);*
- *The NARSTO Quality Systems Management Plan (July 1997).*

All of these documents are available in electronic form on the NARSTO Web site, under the URL <http://narsto.owt.com/Narsto/>.

The Strategic Execution Plan is intended to serve as a "living document," with the expectation that it will be updated periodically throughout NARSTO's lifetime. The current edition of this Plan was begun in November 1995 at NARSTO's General Meeting in San Antonio, Texas, where scientists in the Observations, Assessment, Modeling and Chemistry, Emissions, and Quality-Systems and Data-Management work groups provided and discussed basic planning input associated with each of these areas.

Initially it was intended that material from all workgroups would be published in a common volume, and that the plan for future research would be grounded solidly in a well-defined "inventory" of current activities. Because some NARSTO elements (such as the 1998 Assessment) required launch times much earlier than others, and because the research inventory did not materialize in a suitably comprehensive form, it was subsequently deemed more appropriate to divide the Plan into multiple parts and to alter the focus slightly so as to make it more suitable as a resource to scientists writing research proposals to NARSTO sponsoring organizations. Thus, in addition to a planning, communications, and monitoring tool for use by all NARSTO participants, this Plan is intended especially for scientists applying for financial support of ozone-related research, as a means to help channel their proposed efforts in a direction that is most beneficial to NARSTO's goals.

This Plan has emerged from a somewhat tortuous process, which has been complicated by NARSTO's transition from a nascent concept to a program that is now achieving some semblance of maturity. Although far from perfect, we feel that the current edition provides a suitable structure for its desired purposes, as well as a launching point for future and more comprehensive editions, the first of which is expected some time during 1999.

This report is available electronically in Adobe™ pdf format on the NARSTO Home Page, <http://narsto.owt.com/Narsto/>.

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SCIENCE-PLAN OBJECTIVES, CONTEXT, and GENERAL STRATEGY

1.1 Objectives and Context

As stated in Part 1 of this three-part Strategic Execution Plan,[1] the North American Research Strategy for Tropospheric Ozone (NARSTO) is a tri-national partnership, which addresses the following Primary Objective:

> *. . . to coordinate and enhance policy-relevant scientific research and assessment of tropospheric ozone behavior, with the central programmatic goal of determining workable, efficient, and effective strategies for local and regional ozone management.*

In essence, NARSTO is an “umbrella” effort, designed to enhance the collective efficiency and productivity of North American ozone research through an overall coordination and communication framework. Created in 1996 by joint action of 68 initial charter signatories, NARSTO was cast into a vigorous, complex, and largely uncoordinated environment of ongoing ozone-research activity — a situation demanding careful deployment of NARSTO resources to optimize scientific progress within the context of numerous practical constraints.

This third part of NARSTO’s Strategic Execution Plan addresses this deployment from a science perspective. Its objectives are:

1. *To provide a focussed science strategy, for the period 1997 through 1998, to deploy available NARSTO resources for optimal progress toward its Primary Objective.*

2. *To provide a more general and extended research plan, in the form of required research tasks, to guide efforts toward this goal over a more prolonged (roughly five-year) period.*

A major challenge of this plan is to strike a meaningful balance between reality and utopia, that is, to determine the accomplishments that are practically achievable within the limits of program resources, as opposed to those that are ultimately desirable. Two constraints are particularly important in this regard:

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[1]Parts 1 and 2 of this Strategic Execution Plan are available as downloadable resources on the NARSTO Home Page, <http://narsto.owt.com/Narsto/>.

1. The existing ensemble of North American research programs on tropospheric ozone is large and disjoint. Because of this it is inappropriate to expect immediate or complete assimilation into the NARSTO framework. The timing and nature of this assimilation, however, is a strong determinant of NARSTO's developing science strategy; this suggests strongly that a strategy for programmatic development, via progressive assimilation, should be incorporated as a component of this science plan.

2. NARSTO operates on voluntary contributions from its funding membership. As a consequence, research funding is variable, uncertain, and often difficult to allocate in a focused and specific manner. Through its science-planning function NARSTO's Science-Team complex is responsible for actively creating the scientific vision to guide the financial contribution process; but it also must operate reactively, on the basis of final funding decisions. Moreover NARSTO has, at best, only indirect control over most of the funding resources deployed for the North American ozone-research effort. The reality of this peculiar resource-allocation scheme will continue throughout NARSTO's duration.

It is important here to recognize that NARSTO's progress is motivated by two basic types of driving forces: 1) long-term forces, which are expressed by NARSTO's Primary Objective and the Science and Policy Questions stated in Part 1 of this plan; and 2) more immediate forces, some which reflect the long-term impetus, but others which develop periodically and tend to focus on more transient issues. In contrast to the long-term motivations, which are quite stable and predictable on the basis of needed scientific development, many of the shorter-term influences are somewhat variable, difficult to predict, and at times almost stochastic in nature.

Several of these short-term factors are currently in various stages of existence and are likely to have profound motivating effects on the NARSTO community by altering funding and research emphasis. A primary example of this is the promulgation (mid 1997) of the revised U.S. ambient air-quality standard for ozone, and the new fine-particle standard. The new ozone standard is expected to induce substantial expansion of U.S. ozone noncompliance areas, and forthcoming widespread recognition of this fact will undoubtedly promote extensive public debate of the tropospheric ozone issue. The fine-particle standard, if adopted, will result in extensive debate as well. Obvious linkages between ozone and fine particles will bring this debate directly into the NARSTO science community.

Another example of current importance is the expected mid-1997 completion of the Ozone Transport Analysis Group's (OTAG) modeling effort. Public airing of these results is likely to result in extensive debate, again increasing the profile of the tropospheric ozone issue. Assembled as an ad hoc effort to establish boundary conditions at state borders through massive application of a chemical transport model to the Eastern U.S., OTAG's strong regulatory implications may affect state-level planning appreciably and are likely to induce requests for new and/or revised NARSTO activity.

Numerous additional examples include forthcoming publication of the Canadian and NARSTO assessment reports, output from the Federal Advisory Committee Act (FACA) subcommittee on Ozone, Particulate Matter, and Regional Haze, and NAFTA-related output from such organizations as the Commission on Environmental Cooperation (CEC). In a final analysis it must be concluded that these are significant features of NARSTO's environment, and that NARSTO must maintain cognizance of short-term motivators, anticipate their outcomes, and position itself to respond effectively, appropriately, and productively to these issues. In so-doing, however, NARSTO must ensure also that such responses do not detract significantly from progress along the long-term track toward attainment of its Principal Objective. A general strategy for accomplishing these ends appears in the section immediately following.

This third and final Part of the Strategic Execution Plan is intended for direct and interactive use by NARSTO's Science Teams, its Science and Resource Planning Group, and its Executive Steering Committee, as well as by the scientific community in general. In reflection of the features noted above, It provides a short-term blueprint for immediate action as well as listings of those longer-term and future projects necessary for attainment of NARSTO's Principal Objective. Besides providing a keel and compass to guide and maintain NARSTO's course, *these longer-term project listings are specifically intended to provide guidance to scientists responding to various NARSTO-related research solicitations, or proposing new research through alternative funding channels.* Appearing in Subsections 2.3.2 Tasks of the following text, many of these topics are presented as potential group efforts, some which are partially underway and others which are yet to be initiated. Persons proposing new research projects to NARSTO funding organizations are strongly recommended to consult these sections and to use them to advantage for creating, aligning, and justifying their individual research proposals.

1.2 Science-Development Strategy

As noted in the preceding section, NARSTO's progressive interactions with ongoing ozone-research programs are necessarily an important determinant of NARSTO's science strategy. Productive and meaningful ties between existing programs and NARSTO require time to establish, and although the NARSTO "umbrella" concept has significant appeal on a general conceptual basis, the advantages to individual projects/programs of merging under NARSTO usually are less obvious to the leaders of such efforts. Legitimate questions in this regard are:

- What are the advantages, to an individual program, of merging into the NARSTO framework?
- Will NARSTO impose conditions that will, in any way, constrain the resources or productivity of a particular program?

From this it is self-evident that any decision to merge into NARSTO must be motivated by its attractiveness to the individual projects/programs, if the system is to succeed and operate to the mutual benefit of all parties involved.

In reflection of these features NARSTO's basic development strategy is to create and maintain an attractive substrate for the orderly accretion of additional projects and programs, building on itself while continually enhancing its attractiveness for future additions. This strategy is currently operational, as evidenced by the following developments:

- Incorporation of NARSTO as a basic element of EPA's 1996 research grant solicitation (1996).
- Development of NARSTO's 1998 Assessment, with inclusion of numerous scientific review papers funded by NARSTO sponsoring members (1996).
- Association of the NARSTO Canada-East program as a field-study component of NARSTO (1997).
- Association of the Southern California Ozone Study (SCOS/NARSTO) program as a field-study component of NARSTO (1997).
- Initiation of the NARSTO data-management archive and quality assurance program (DOE and NASA contributions, 1997).
- Incorporation of NARSTO as a basic element of EPA's 1997 research grant solicitation (1997).
- Incorporation of NARSTO as a basic element of DOE's 1997 research grant solicitation under the Atmospheric Chemistry Program (1997).
- Association of the multi-investigator Program for Research on Oxidants: Photochemistry Emissions (PROPHET) program with the NARSTO effort (1997).

This strategic approach is generally known as NARSTO's "accretion model." Designed to enhance manageable and orderly program growth as well as to provide increasingly positive motivations for further additions, this model is expected to remain in-force throughout NARSTO's lifetime.

1.3 Science-Planning Strategy

In view of the discussion presented above, it is crucial for NARSTO's science strategy to maintain a consistent tracking toward the long-term programmatic objective, while simultaneously responding to new driving forces efficiently and effectively as they materialize. In this regard, the strategy must anticipate, and to some extent influence, future activities in NARSTO's external environment. This, combined with the currently obscure nature of NARSTO's external environment and the need for orderly program development, leads to the following three guidelines for this document's preparation:

1. Because of current inabilities to predict short-term driving forces into the extended future, the strategic blueprint described in this plan will be limited to a two-year time horizon: 1997 through 1998.

2. In reflection of the desire for orderly development noted above, the context of this initial science plan will be not attempt to cover the totality of all ongoing and projected ozone research. Rather, it will be limited to those elements recommended by the Science Team and required to enhance our practical competence in ozone management which, in addition:

   - cut across multiple individual NARSTO efforts,

   or else, while not necessarily cross-cutting,

   - are important features which have been neglected in past and ongoing ozone studies.

The following sections set forth this Science Plan, focusing individually on modeling and chemistry, observations, and emissions research. These sections adhere to a common format which first describes individual component responsibilities, followed by statements of near-term and extended objectives.

Individual task descriptions are provided within the extended-objective subsections, and again are described using a common format which assigns a priority to each task and indicates relevant NARSTO Science and Policy Questions. The priority ranking indicates whether a task is currently absolutely essential in the progression toward fulfillment of NARSTO objectives (Rank 1) or is important, but not absolutely critical, at the present time (Rank 2). Lower rankings are not included here under the premise that this Plan, by design, does not include non-relevant tasks. The NARSTO Science and Policy Questions referenced in these subsections were first published in the 1994 NARSTO Research Strategy and Charter (1). These questions are reproduced in the Appendix for easy access by readers of this document.

2

STRATEGIC PLAN: OBSERVATIONS

2.1 Observations Component Responsibilities

NARSTO's Observations component is responsible for all aspects of ozone-related field measurements, including:

- design, conduct, and coordination of intensive field studies;
- establishment and overview of routine and semi-routine monitoring networks;
- development of analytical methods for field-study and monitoring-network measurements; and
- processing and analysis of observational information, including observations-based analysis.

2.2 Near-Term (1997-1998) Objectives of the Observations Component

In reflection of the above responsibilities and in view of the current state of scientific understanding, NARSTO's Observations Team has set the following objectives for the 1977 - 1998 period:

- To contribute observations-based expertise and information to the 1998 NARSTO Assessment process. These contributions will take the form of:
    - preparation and review of Critical Review Papers pertaining to network observations, field studies, and observational-based analysis; and
    - participation in the creation and review of the 1998 NARSTO Assessment Document.
- To initiate and conduct data ingest from the SOS, NARSTO—Northeast, and NARSTO—Canada-East field studies by the NARSTO Data Center in Oak Ridge, with the final goal of depositing these data for general distribution on the NARSTO/EOSDIS Distributed Active Archive Center at NASA Langley.
- To conduct the Southern California Ozone Study (SCOS/NARSTO) during summer 1997, and to forward the resulting data to the NARSTO Data Center for ingest.

- To initiate measurement operations of the PROPHET field study, and to commence associated NARSTO data-ingest arrangements and operations.

- To contribute observations-based expertise and information to preparation of white papers and other decision material leading to Executive Assembly decisions on NARSTO's relationship and response to the fine-particle issue.

- To evaluate the advantages, impediments, and possible pathways for harmonization of ozone-network measurements within the three NARSTO countries.

- To coordinate and conduct the joint planning necessary for a next-generation regional ozone field study.

Although the rationale and intent are obvious for most of the above items, the last deserves some additional comment. During the past several years a number of high-quality, regional field studies of ozone have been conducted, and currently the research community is analyzing the resulting data on both collective and individual bases. In addition, some geographically extensive modeling studies are currently in progress, which undoubtedly will result in new insights, further questions, and increased debate with regard to validity. Moreover, possible future adjustments to ozone standards and goals, as well as the possibility of merging fine-particle and ozone efforts, will result in significantly different reference frames for future studies.

The progression of these activities is likely to result in the demand for a future, possibly merged field study that is based on these recent findings and addresses a variety of additional questions, such as quantification of trans-state/province/estatio and trans-national border fluxes, regional representativeness of atmospheric-chemistry simulations, and ozone—fine-particle linkages. It is essential to draw from NARSTO's diverse base of experience and expertise to design such an effort; therefore, the Observations Team plans to coordinate a number of workshops to this end during 1998. Results from these planning efforts are intended to flow directly into the succeeding version of this Strategic Plan, which will be written sometime early in 1999.

2.3 Extended Observations Component Objectives

2.3.1 Priorities

The priorities of NARSTO's Observation component reflect three paramount programmatic needs. First, NARSTO is obligated to provide progressive, policy-relevant scientific assessments of the ozone problem as it is perceived to exist in North America. For this reason, the activities and schedules of Observations component must continue to support the needs and schedules of the Assessment Team, as it moves forward from its 1998 Assessment. Second, for NARSTO to succeed in the future, cooperation among the various stakeholders must be promoted. Joint scientific projects involving the individual research groups should be developed to provide integrated research teams capable of generating the most useful new information that is required to satisfy stakeholders needs. Finally, NARSTO's long-term vitality requires that NARSTO define ground-breaking new research opportunities, and secure the resources required to accomplish them.

Seven areas are of immediate concern in this regard:

1. **Data availability:** It is clear that data already on hand will likely provide the informational base to give near-term answers. All reliable data that are accessible should be gathered and made available for analysis, interpretation and assessment.

2. **Measurement Capability and Validity:** Considerable attention must be directed toward developing and validating measurement techniques. Many critical measurements cannot yet be made; the accuracy and reliability of others are open to question.

3. **Monitoring Network Design and Implementation:** Monitoring networks that are in operation or are to be deployed are of critical importance to future progress in managing air quality in North America. Hence, the definition and design of these networks demand immediate attention.

4. **Limited Field-Study Measurements:** There are several specialized, focused field studies of limited dimension that may be undertaken. These may be aimed at addressing specific issues dealing with atmospheric processes or emission inventories uncovered during previous field studies and their interpretation.

5. **Integrated Field-Study Measurements:** Resources must be available for the design of integrated field studies that may be contemplated under the auspices of the various regional programs. This includes super-regional and cross-boundary studies. Careful consideration must be given to defining the scientific questions that are to be addressed and additional resources required. This planning must begin now for studies that may occur several years in the future.

6. **Observation-Based Analyses:** Considerable effort should be focused on the development and validation of new observational-based methods for data

verification, interpretation and assessment. This must occur in close coordination with the design of supporting field studies.

7. **Multi-Pollutant Couplings and Associations:** Research programs and integrated assessments done to manage the ozone problem should be coupled to other atmospheric environmental concerns, such as inhalable particles and visibility impairment, which result from the same precursors and chemical transformations that cause excessive ozone levels.

These topics fall into four broad categories: <u>data collection and archiving</u>; <u>measurement technique development</u>; <u>field measurements</u>; and <u>observation based model development and verification</u>.

Recognition that individual atmospheric science deals with the processes common to all atmospheric concerns (item 7) and that they should not be artificially compartmentalized, should be common to all areas. In addition, in planning for new monitoring activities and future measurement campaigns, it should be recognized that the wish to obtain new observations in the atmosphere may stand in the way of providing reliable data. Too often the methodical processes involved in development of new measurement techniques in the laboratory, the testing of those techniques in the field, and adequate planning of measurement campaigns are short-circuited by the pressure to obtain field measurement data immediately. There are several factors that contribute to this: 1) the perception that the only major investments that are required are those to establish and to support monitoring networks and integrated field studies; 2) the failure to recognize that the limited capabilities of certain critical measurements greatly compromise the information to be extracted from those studies. Additional resources must simultaneously be spent in development, field testing and validation of new measurement and modeling tools and in the study of fundamental kinetic mechanisms and spectroscopic techniques in the laboratory. In the planning process there needs to be a detailed evaluation of how the lessons learned from previous studies (both in North America and abroad) have been addressed in the design of a new undertaking.

Finally, there may appear to be areas of overlap between the activities and tasks that are called for and described in this chapter and those described and called for in the chapters dealing with companion sections, “Modeling and Chemistry” and “Emissions”. This is a natural consequence of the crosscutting nature of the key problems in atmospheric sciences, particularly as they relate to the ozone problem. As these apparent areas of the overlap indicate, the approach to understanding and managing ozone must be cooperative and interdisciplinary. This section is intended to indicate the information, advice, and consent the Observations component must provide in each of the priority areas enumerated above to make the joint NARSTO collaboration a success.

The tasks itemized in the following subsection form the extended research activities selected to respond to these longer-term needs. As can be noted from Section 3.2, there is some overlap between these tasks and the shorter-term goals set forth for the Observations component. This is a natural consequence of the intended alignment of shorter-term and extended research objectives, and will reoccur periodically throughout the remainder of this Plan.

2.3.2 Tasks

Program Element O1: Data Bases

Description: Clearly, the most cost-effective means to gain insights concerning ozone and ozone-precursor trends and distribution is through the analysis and evaluation of existing data. The first step in this process is to develop an inventory of quality assured (i.e., retrospective QA/QC) data sets (in standard units and a standard data base format) that are available and accessible for O_3 and O_3-precursors. Eventually, the aim would be to archive certain of these data sets in a common format including a protocol to access the data. For the available data, estimates of its reliability and uncertainty (bias and precision) must be provided. Indeed as the understanding of measurement techniques increases the estimated reliability of the data sets may change. The system must allow for this new understanding and contain a protocol for data review. Since future data sets obtained through the NARSTO member institutions will be included in this archive, the design of new field measurement programs should give attention to data type and format requirements that are compatible with this archive. Likewise, attention should be given to develop *user friendly* sharing protocols. Finally, resources must be found to maintain this facility throughout the life of NARSTO.

Approach:

- Develop inventory of existing data sets that contain measurements of O_3 and O_3-precursors. Determine what data can be acquired with reasonable ease.

- Provide guidance for data formatting.

- Develop methods procedures for retrospective quality assurance and quality control of existing data.

- From the data available, provide up-to-date estimates of the reliability and uncertainty (bias and precision) in measurements.

Relationship to NARSTO Science and Policy Questions: Depending on the data base under consideration, this tasks supports NARSTO science and policy questions 1-2.1, 2.2, and 2.4.

Priority: 1

1. **Customer value:** Of general interest to all NARSTO stakeholders.

2. **Requirements by other NARSTO functions:** Required by Integration and Assessment, Modeling and Chemistry and Quality Systems and Data Management.

3. **Timing requirements:** Immediate and long-term.

Program Element O2: Instrumentation Improvement

O2A. Development of Techniques for Routine Measurements

Description: NARSTO must support air-quality monitoring. This includes development of new, and improvement of existing, air-quality monitoring instruments. The effective use of new measurement technologies will require that measurement and analysis strategies be devised to enhance and maximize information and utility of the existing and planned networks. It will be necessary to enhance the reliability, and increase the operational simplicity, of existing techniques so they can be more easily adapted to operational needs. Methods to calibrate instruments must be developed and calibration standards must be provided.

Monitoring requirements must address development of techniques that are complementary to, and matched with, existing and planned measurement platforms and sites. The design of the monitoring studies to use these resources must provide data that fulfill specific needs with formats can be readily and easily used. Methods for short turnaround/real-time data handling, visualization, and interpretation (see section on Observation Based Modeling) of monitoring network must be produced.

Given the difficulty of monitoring photochemical precursors and products, consideration should be given to establishment of a *demonstration* site to determine the operational feasibility of instruments. This demonstration site will provide a testbed for all measurements, data acquisition and control hardware, and data-archiving down-links prior to their implementation at network sites. In addition, the site will provide a convenient venue for training technical personnel in proper operation of research-grade instruments.

Approach:

- Form a NARSTO Monitoring Working Group to provide advise and guidance to the air-quality monitoring community. This Group will also work to generate a dedication to excellence by the monitoring network sponsors and a commitment to provide additional support as required to ensure rigorous, scientifically defensible measurements and measurement strategies by the air-quality monitoring community.

- Develop a white paper to address the capability of monitoring instruments and methods that are currently used to measure ozone precursors and photochemical byproducts. *The initial activity will be a workshop(s) to determine the capabilities of current instruments to properly measure NO, NO_x, NO_y, and speciated VOCs.*

- Evaluate methods to calibrate routine measurements and identify suppliers that can provide calibration standards.

- Continue intercomparisons of the techniques to measure NMHCs.

Relationship to NARSTO Science and Policy Questions: This tasks supports NARSTO science and policy questions 1-2.1, 2.2, 2.3 and 2.4.

Priority: 1 for evaluation, 1 or 2 for instrument development.

1. **Customer value:** This tasks supports NARSTO science and policy questions 1-2.1, 2.2, 2.3 and 2.4.

2. **Requirements by other NARSTO functions:** Required by Integration and Assessment and the monitoring component of Observations.

3. **Timing requirements:** Report providing a critique of capabilities of routine required for the 1998 NARSTO Assessment.

O2B: Development of New Measurement Techniques

Description: Improving management of the ozone problem will require additional information. Acquiring that information will involve new kinds of observations, increasing the size of observational databases, and/or improving the quality of existing observations. To do this, measurement technology must be improved. Improvement requires continued development and validation of measurement techniques that are already available or are under development in the laboratory. These developments are aimed at improving the sensitivity, specificity, and response times of instruments to measure the compounds of interest throughout the troposphere from the measurement platforms of choice.

The requirement for fast-response measurements opens exciting new possibilities for the development of fresh measurement strategies. These methods are needed to utilize the capabilities of aircraft platforms and permit the direct measurement of emission and deposition fluxes by eddy correlation. In this regard, many measurements, such as those currently used for the measurement of VOCs, are hampered by the lack of fast-response in-situ measurements of these compounds. Current instruments for organic precursors are typically insufficiently rapid to be competitive or complementary with the fast techniques used to measure O_3 and nitrogen oxide species. The task is difficult because of the large number of potentially interesting VOCs present in the atmosphere. However, innovative measurement techniques involving fast gas chromatography and/or ion-trap mass spectroscopy are emerging that may offer exciting new possibilities.

Further improvements can be achieved by the integration of the emerging technology with measurement platforms to produce inventive experimental systems. For example, fast-response instruments for NO, NO_2, NO_y, and CO mounted on a mobile platform that is located with a global positioning system (GPS) could be used to map concentrations. With observation-based analysis, these measurements may be used to identify the complex matrix of emission sources of the compounds that may exist in urban or industrial areas.

Approach:

- Carry out intercomparisons of the techniques to measure carbonyls including CH_2O.

- Assess the capability of currently available methods for the measurement of carbonyls (in addition to CH_2O).

- Carry out intercomparisons of the techniques, including new emerging chemical ionization techniques, to measure HNO_3.

- Participate in intercomparisons of techniques to measure odd-hydrogen (OH/HO_2) radicals including calibration procedures.

- Deploy, test and validate methods for profiling O_3, CO, H_2O and aerosols.

Relationship to NARSTO Science and Policy Questions: This tasks supports NARSTO science and policy questions 1-2.2 and 2.4.

Priority:1 for evaluation, 2 for development.

1. **Customer value:** This tasks supports NARSTO science and policy questions 1-2.2 and 2.4.

2. **Requirements by other NARSTO functions:** Required by Integration and Assessment.

3. **Timing requirements:** Report providing a critique of capabilities of routine measurements required for the 1998 NARSTO Assessment.

Program Element O3: Field Measurements

O3A: Monitoring

Description: The implications for air-quality monitoring of a revised air-quality standard for ozone and ozone precursors must be determined. These must recognize the similarities, differences, opportunities, and tradeoffs required to undertake adequate monitoring networks for exposure, regulatory/compliance, trans-boundary flow, and diagnostic monitoring of ozone and ozone-precursors. Once these criteria are in place the chemical and meteorological measurements appropriate to the needs of each network can be defined.

A concerted effort should be made to encourage cooperation among monitoring networks. Moreover, ozone monitoring networks should be able to assess the regional and super-regional dimension (as opposed to the local dimension) of ozone-related air-quality issues. If a regional network is established to monitor fine particulates and their precursor compounds, this network should be closely coordinated with a regional ozone/ozone-precursor network.

With regard to the regional aspects of current air-quality problems, over the last several years scientists have made considerable progress measuring fundamental, photochemically-active compounds such as nitrogen oxides and VOCs at the surface. However, it is clearly desirable and necessary to couple the surface measurements to vertical measurements of the most important species. Vertical measurements of ozone and aerosols along with their precursors are needed to determine the regional representativeness of observations. A systematic study coupling surface measurements with real-time vertical measurements (e.g., tethered balloon, lidar, and DIAL) should be undertaken to evaluate the vertical measurement approach. Such a study would promote the development of profiling techniques and enable better interpretation of data taken at surface sites.

Finally, it is generally recognized that the information germane to the ozone problem shares many common elements with other air-quality issues. Hence, monitoring ozone and its precursors should not be performed in isolation from other types of air-quality monitoring. Therefore, the first step toward coordinating monitoring activities is formulating a list of the air-quality networks, their aims, the location of network sites, and the instrumentation applied.

Approach:

- Create a NARSTO/PAMS/? Working Group to discuss the issues involved field studies that have very specific and limited purposes with monitoring network coordination. Representatives of the four NARSTO Science Teams, and representatives of the effects and alternate fuels communities, should be included in the Working Group to help evaluate network requirements.

- This group will be expected to produce guidance describing:

  1). availability and capability of instrumentation for deployment in monitoring networks (see task O2A).

  2). design of deployment strategies that can be used to develop cooperative, appropriate and cost-effective exposure, regulatory/compliance and diagnostic networks for monitoring ozone and ozone-precursors;

  3). alternative observational approaches and strategies for non-overlapping functions of the various networks; and

  4). issues regarding joint or independent data archiving and management

  5). development of a comprehensive NARSTO monitoring plan that has broad support among all stakeholders.

- As a first step in this process, formulate a catalogue of North American air-quality networks, their aims, the location of network sites, and the instrumentation that is used for the monitoring activities.

The usefulness of such a catalogue is obvious to others as well. Currently, the Air Quality Subcommittee (AQS) of the Committee on Environment and Natural Resources (CENR) is developing a catalogue of air quality monitoring networks that are financed or mandated by the U.S. government. The networks under consideration are the networks for air quality and deposition monitoring that are operated under uniform standards and requirements and comprises permanent (i.e., those with no identified termination date) fixed stations. Monitoring networks would not include space-based satellite systems or temporary networks used in intensive field *campaigns or private sector networks not supported or required by the U.S. government. We recommend that the NARSTO catalogue be developed working in collaboration AQS/CENR.*

Relationship to NARSTO Science and Policy Questions: This tasks supports NARSTO science and policy questions 1-2.1 and 2.4.

Priority:1

1. **Customer value:** This tasks supports NARSTO science and policy questions 1-2.1 and 2.4 and those stakeholder invested with the responsible of addressing those issues.

2. **Requirements by other NARSTO functions:** Required by the Assessment Team and the routine measurements component of the Observations Team.

3. **Timing requirements:** Report providing a critique of network capabilities required for the 1998 NARSTO Assessment. Evaluation of monitoring activities could significantly impact those activities.

O3B: Focused Field Studies

Description: There is a need to undertake certain field studies that have very specific and limited purposes. The most important of these focused studies will involve the direct determination of ozone production rates. Additional such field studies will test whether current understanding can satisfactorily explain measured OH, H_2O_2, and HNO_3 concentrations in terms of the measurements of their known chemical production and loss processes. Studies also will be designed to fully determine the processes that control partitioning of the NOy reservoir and ascertain if there are additional atmospheric processes, including heterogeneous processes involving aerosols, that can convert more highly oxidized forms of NO_x (e.g., HNO_3 , particulate nitrate) to NO or NO_2. Other studies might be undertaken to confirm a specific an unexpected result obtained in the course of one of the comprehensive regional field campaigns.

Processes associated with meteorology and dynamics play a central role pollution chemistry. Measurements must be able to gauge these processes, and models must be able to simulate them adequately. Recent measurements indicate that turbulence-driven concentration fluctuations on time scales of tens of seconds can be large. In addition, they can be sufficiently variable from day to day to call into question the current averaging approaches for setting regulatory strategies. Meteorological and dynamical processes and their significance bear more careful investigation. These processes should be identified, and their understanding made the subject of carefully planned, focused field studies.

Approach:

- Direct measurement of ozone production rate. (i.e., k_1•[[NO][RO_2]), contrasted with simultaneous direct measurements of the photochemical stationary state (k_1•[RO_2][NO] + k_2•[O_3][NO] = j•[NO_2] and Lagrangian measurements of the evolution of the ozone distribution. The measurements should be made in several regions that possess unlike O_3-precursor compositions and different controlling physical parameters.

- Comparison of the measured production rates with those predicted by model simulations.

- Testing of current understanding regarding OH, H_2O_2, and HNO_3 from the measurements of their known chemical production and loss processes.

- Determination of the processes that control the partitioning of NOy reservoir.

- Determination of field studies that are need to accomplish other very specific and limited purposes.

Relationship to NARSTO Science and Policy Questions: This tasks supports NARSTO science and policy questions 1-2.2 and 2.3.

Priority: 2

1. **Customer value:** This tasks supports NARSTO science and policy questions 1-2.2 and 2.3 and those stakeholder invested with the responsible of addressing those issues. These studies would be used to fill gaps of critical information uncovered during the interpretation phases of the regional studies. These focused studies are limited in scope and could be undertaken at a fraction of the cost of a comprehensive regional study.

2. **Requirements by other NARSTO functions:** Required by and managed by the regional studies.

3. **Timing requirements:** Timing not critical since the data gathered by these studies and the interpretation of that information would not be available prior to the 1998 assessment.

Scheduling Requirements: Development of new studies should be coordinated with the interpretation of data from the regional studies to identify well defined “bit-sized” informational gaps. Planning and execution of the study will be led by the sponsoring regional program.

O3C: Comprehensive Field Studies

Description: Regional studies are the outgrowth of urban studies with the recognition that air quality problems are not urban alone, either in their solution or in their effects. In response to this, comprehensive regional studies have been undertaken. The recent themes of the regional studies have been:

- Developing a quantitative estimate of the role of vertical mixing in the redistribution of compounds between the boundary layer and the free troposphere.

- Obtaining a quantitative estimate of the exchange of ozone and ozone precursors between urban and rural areas.

- Determining the relative contribution of biogenic and anthropogenic NO_x and VOCs to O_3 formation in urban and rural areas in various areas of North America.

- Promoting the development of diagnostic observation-based models (OBMs) and prognostic emission-based models (EBMs).

In addition (and in a US context), the studies provide information that is useful for production and revision of state implementation plans (SIPs). Interpretations of results from recent field measurement campaigns (e.g., NARSTO—Northeast, NARSTO—Canada-East, and the Southern Oxidant Study) will be used to plan the focus and location of the next generation of those and other regional studies.

The next five years will probably see the need to undertake super regional studies. These may involve two or more regions in a particular country or studies that address the import and export of ozone and ozone precursors across international boundaries.

Approach:

- Review data taken through each regional program as well as existing data taken from state air quality and acid-rain research programs to guide future activities in each region.

- Assemble observations in an accessible data archive.

- Provide assistance in implementation and maintenance of PAMS-level sites in each region with the aim of future instrument development, demonstration, refinement, and instruction.

- Identify major field studies required to understand the factors that control ozone accumulation.

In addition, consideration should be paid to the utility and importance of international investigations. Two international studies that have been envisioned are:

- Midwestern and Eastern U.S., Ontario, Quebec, and Canadian Maritime Provinces: *Determine the factors that control the transport of ozone and ozone precursors across the Eastern United States and Southern Canada: from the Midwestern United States into the through the Ontario-Quebec Corridor in Canada into the Eastern U.S. and subsequently into the Maritime Provinces of Canada.*

- Mexico/Southwestern United States.
  Examine the impact of transborder transport of ozone and ozone precursors on the air quality of Mexico and the U.S. and the impact of economic expansion within Mexico upon its air quality and the air quality of the southern U.S.

Relationship to NARSTO Science and Policy Questions: This tasks supports NARSTO science and policy questions 1-2.2, 2.3 and 2.4.

Priority: 1, in terms of interpretation of the results from past studies; 2 in terms of design of new studies.

1. **Customer value:** This tasks supports NARSTO science and policy questions 1-2.2, 2.3 and 2.4 and those stakeholder invested with the responsibility of addressing those issues.

2. **Requirements by other NARSTO functions:** Data analysis and interpretation is required by the Assessment, Modeling and Chemistry and Quality Systems and Data Management Teams. Future planning is required for and managed by ongoing regional studies.

3. **Timing requirements:** Data reduction and interpretation being carried out by the ongoing regional studies should be encouraged since this will factor strongly into the deliberations of the Assessment Team of NARSTO. Timing of new studies not critical since the data gathered by these studies and the interpretation of that information would not be available prior to the 1998 assessment.

Program Element O4: Observational Based Modeling

Description: An important air-quality science goal is the further development and testing of a hierarchy of observation-based analyses and models, which use field observations and data to diagnostically address the science questions identified for NARSTO. Because of their potential applicability to management of a number of air-quality concerns, NARSTO must evaluate the various observation-based modeling approaches to ascertain their relative merit, to foster their improvement, and to determine their applicability to air-quality management issues.

Observation-based models (OBMs) use observed data to draw inferences about the processes that shape the state of the atmosphere. They are the conjugates of emission based models (EBMs), which predict the atmospheric state from detailed knowledge of the controlling processes themselves. When emission-based and observation-based approaches are used in conjunction, one can obtain an increased measure of the robustness of technical understanding.

OBMs have limitations. By their nature, OBMs are diagnostic, not prognostic. OBMs attempt, by selective use of databases, to emphasis the controlling influence of select processes. By applying the same selection criteria to the data base created by EBMs as to observational databases, the description of selected processes by these models can be evaluated. However, the veracity of the conclusions reached by OBMs will reflect uncertainties in the isolation of the controlling influence of single processes. For example, while attempting to focus on the control of emissions, the influence of chemical processing and meteorological influences such as dry and wet removal have to be taken into consideration. Incomplete understanding of the competing influences of a variety of chemical and physical processing make it difficult to evaluate the uncertainties of conclusions reached by OBMs.

Similarities and differences between conclusions reached by OBMs and EBMs should be evaluated. This testing can be initiated and exemplified by addressing key questions relevant to the ozone control strategy.

a) Evaluation of emissions.

Observational based modeling techniques such as inverse modeling or mass-balance approaches can be applied to estimate the relative contribution of emission-source classes (heavy industrial sources, automobiles, etc.) to the ozone-precursor burden in a given area. Furthermore, in a given area, OBMs can provide estimates of the relative amounts of ozone-precursor emissions, for example, the ratio of NO_x to CO or NO_x to VOC . In this way OBM analysis can be used to evaluate critical output of EBMs. Evaluation of emission databases, including identification of O_3-precursor sources and the relative emission of

O_3-precursors, is of critical importance for the development of appropriate control strategies based on EBMs.

b) Evaluation of ozone production efficiency.
OBMs that focus on the relationship of ozone to other photochemical oxidation products or to relatively inert anthropogenic tracers can be applied to approximate the ozone production efficiency of anthropogenic precursors. Examination of the corresponding relationships predicted by the EBMs is an important step in the evaluation of the chemical processing by the EBMs.

c) Evaluation of ozone-precursor effectiveness.
A critical and difficult model test addresses the isolation of critical parameters for the control of ozone. Presently it is a challenge to develop appropriate model tests to correctly answer the question if ozone production in a given area or region is hydrocarbon- or NO_x-limited. OBMs that look at the ratios of particular reaction products promise an approach to use observations to directly test this important question and thus to provide stringent tests for EBMs.

d) Determination of incremental reactivities.
The incremental reactivities of volatile organic compounds depend critically on ambient concentrations of the compounds. OBMs can help to determine the incremental reactivities that are characteristic of an area of interest. A knowledge of incremental reactivities for the VOCs can direct a targeted, cost-effective control of selected VOCs.

e) Evaluation of meteorological processes.
Observational based modeling techniques can be applied to estimate relative contributions of specific meteorological variables (e.g., mixing height) to ozone production and/or ozone-precursor dissemination (e.g., concentration of O_3-precursors). Examination of the corresponding relationships predicted by the EBMs is an important step in the evaluation of the meteorological processes simulated by the EBMs.

The development of OBMs must involve careful testing to ascertain how well they preform on different measurement data bases and how well they hold up when compared to predictions drawn from state-of-the-art emission based models for the same data. It is the responsibility of the NARSTO's Observations group to provide databases and analysis methods suitable for use in the development of OBMs.

Approach:

- Develop an inventory of observation-based analysis and models in use and under development.

- Identify existing observational data sets that might be used to evaluate OBM's and compare results of different observation-based analyses and more traditional emissions-based approaches.

- Using existing data, compare observation-based and emission-based approaches for consistency and precision. On the basis of these findings, develop basic protocol for integrating results of observation-based and emission-based approaches as a means of assessing the robustness of findings.

Recent regional studies (e.g., SOS, NARSTO-NE) have provided comprehensive high quality data sets required to address these questions and hence to speed the development of observation-based modeling and their comparison with EBMs.

Relationship to NARSTO Science and Policy Questions: This tasks supports NARSTO science and policy questions 1-2.2, 2.3, 2.4 and 2.5.

Priority: 1, in terms of evaluation of EBMs; 2 in terms of future development.

1. **Customer value:** This tasks supports NARSTO science and policy questions 1-2.2, 2.3, 2.4 and 2.5 and those stakeholders invested with the responsibility of addressing those issues.

2. **Requirements by other NARSTO functions:** Required by Integration and Assessment, and Modeling and Chemistry.

3. **Timing requirements:** Data reduction and interpretation being carried out by the ongoing regional studies should be encouraged since this will factor strongly into the deliberations of the Assessment Team. Timing of new studies is not critical since the data gathered by these studies and the interpretation of that information would not be available prior to the 1998 assessment.

Scheduling Requirements: To be determined by the needs of the regional study.

3

STRATEGIC PLAN: MODELING & CHEMISTRY

3.1 Modeling & Chemistry Component Responsibilities

As its name implies, NARSTO's Modeling and Chemistry (M&C) component is charged with two major classes of activity. First, it is responsible for the important task of developing, evaluating, applying, and disseminating advanced air-pollution and meteorological models, which are aimed at practical, decision-oriented evaluation of the ozone issue. Second, the M&C component is accountable for continued and efficient development of the fundamental atmospheric-chemistry knowledge that is necessary for advancing the utility and reliability of these models, as well as for enhancing our understanding of tropospheric ozone in general. In more specific terms, the M&C component focuses on the following activities:

- air-quality and meteorological model development,
- model applications research,
- model evaluation,
- laboratory studies of chemical reaction rates and basic reaction kinetics,
- chemical mechanism development.

3.2 Near-Term (1997-1998) Objectives of the Modeling & Chemistry Component

In reflection of the above responsibilities and in view of the current state of scientific understanding, NARSTO's Modeling and Chemistry Team has set the following objectives for the 1977 - 1998 period:

- To contribute modeling- and chemistry-based expertise and information to the 1998 NARSTO Assessment process. These contributions will take the form of:
    - preparation and review of Critical Review Papers pertaining to model development, model application, meteorological process characterization, and atmospheric chemistry; and
    - participation in the creation and review of the 1998 NARSTO Assessment Document.

- To complete a test version of Models-3 (Models-3 Framework and the Community Multi-scale Air Quality (CMAQ) model) in summer 1997 and "beta" test the system with a select group of users over the summer and early fall.

- To release and distribute an operational version of the Models 3 system in May 1998, with the purpose of providing an advanced model to the air-quality community for SIP planning in conjunction with new ambient air-quality standards.

- To develop advanced model-evaluation tests and test procedures including documentation, to better diagnose model performance.

- To develop advanced model sensitivity analyses and procedures, to better understand model predictions and to better characterize model uncertainty.

- To apply the advanced model evaluation methods to the operations version of Models-2CMAQ and initiate a model evaluation or evaluations including other models from the international NARSTO community, using data collected by the SOS, NARSTO--Northeast and NARSTO--Canada-East field studies.

- To support the EPA FACA process. This includes participation in the technical workgroups, performing modeling studies and conducting model development to examine approaches of estimates of Areas of Influence (AOI's), now being defined as a step in the future regulatory process, and studies related to tracking progress of control actions.

- To participate in the joint planning for a next-generation regional ozone field study.

3.3 Extended Modeling & Chemistry Component Objectives

3.3.1 Priorities

Extended Modeling and Chemistry priorities include five broad activity categories, which are itemized sequentially below.

1. **Synthesis of Completed and Current Modeling Work:** Results of completed modeling studies will provide a source of information for near-term answers. Continued synthesis of these efforts is necessary to draw out the most important implications and highlight the most robust answers. A synthesis will also clarify where we are now and help suggest where we should be going next. Available studies need to be made accessible for compilation, analysis, interpretation and assessment.

2. **Model Studies:** An important means of developing an understanding of emission-based models and of our composite understanding of photochemistry is through modeling studies designed to provide insights into the functioning of the models and insights into the functioning of the photochemical system.

   Model Sensitivity and Uncertainty Studies
   Considerable, continued attention must be directed towards model sensitivity and uncertainty studies. Such studies are needed to provide up-to-date insights into the functioning of the models and to highlight key uncertainties related to process parameterizations and interactions, in order to help develop recommendations for further model research and development.

   Studies Oriented Towards Key Science Questions
   Clearly, part of the information base for an assessment needs to come from specific studies that are keyed to the major science questions put forth by NARSTO. Specialized, focused modeling studies, especially those performed in conjunction with field study data, serve an important role in this regard.

3. **Model Evaluation:** Model evaluation, focusing on comparisons of model predictions against observational data sets, provides a vital information base to develop judgments about the state of our current modeling science. Progress is needed in model-evaluation techniques, testing, and interpretation. It is necessary to significantly enhance the diagnostic probing possible through testing against measurements and build this into new evaluation protocols.

   Individual Model Evaluation
   Efforts should be placed on focused, in-depth evaluations of individual models to break new ground and to enhance our abilities to probe the emission-based models. Specialized efforts on individual models will provide an information base on performance and issues that relate to all models, fostering overall advancement of the emission-based models and understanding.

   Cross-Model Evaluation
   Resources need to be made available for a diagnostic, comparative cross-model evaluation of the new multi-scale models that are or will shortly be available. An important means to develop an understanding of the state of our modeling science is to define and carry out an objective and highly diagnostic model evaluation of several models. A cross-model evaluation fosters the development of a scientific consensus regarding judgments and interpretations of the strengths and weaknesses of the emission-based

models. Careful planning, coordination, and resource allocation will be required, especially if several models are to be involved.

4. **Process Development:** Model and process-evaluation studies have already pointed out areas requiring new or updated process-level information, and resulting efforts are currently underway on a number of projects. It is important that resources be effectively targeted and that new information is taken into account on a periodic basis. Research priorities have been updated to provide a list of top-priority process-oriented research projects that need to be funded to provide the basis for the next round of model improvements (parameterizations of processes and model system development) in 3-5 years. Key areas are meteorology, gas-phase chemistry and fine-scale processes.

5. **NARSTO Planning Studies:** Modeling can help to suggest critical new measurements that would significantly improve model evaluation capabilities or would help to test scientific hypotheses. Modeling studies can also aid the planning and design of super regional studies. In addition, testing the capabilities of observational based modeling can benefit greatly from interaction with the emission-based models. This planning must begin now for studies that may be several years in the future.

3.3.2 Tasks

3.3.2.1 *Chemistry*

Program Element M&C-1: Development of an Improved Isoprene Chemistry Mechanism Using Existing Kinetic/Mechanistic Data and Smog Chamber Data

Description: Isoprene is a highly reactive volatile organic compound that is emitted by vegetation in substantial amounts and may contribute significantly to ozone formation in some regions of the country. Because of its potentially large contribution, and the fact that it is essentially a noncontrollable source, it is important to describe isoprene photochemistry as accurately as possible. Work under this element will overcome identified weaknesses in our treatment of isoprene chemistry in current air-quality chemical mechanisms, and significantly reduce the uncertainty in the modeling of isoprene oxidation. A detailed isoprene mechanism, as well as a condensed version, will be developed and evaluated as a starting point. A mechanism with an appropriate level of detail will then be included into the general chemistry mechanism used in the air-quality models.

Relationship to NARSTO Science and Policy Questions: This work contributes directly to Science Question 1 because it will significantly improve our knowledge of atmospheric chemistry. It supports Science Question 2 by utilizing laboratory studies to reveal some fundamental processes involved in ozone production; Question 3 by helping to assess the role of natural sources on ozone accumulation; and Question 4 by reducing the uncertainty in model predictions of ozone for regions that are affected by biogenic chemistry.

Priority: 1. The photochemistry of isoprene has been identified as a persistent and significant uncertainty that needs to be reduced to better understand regional photochemistry.

Scheduling Requirements: The completion of this task in 1996 is critical in order to allow time for the improved mechanism to be incorporated into the air-quality models, and used for model sensitivity and application runs during 1997. Results from these runs will support the 1998 Assessment

Program Element M&C-2: Development of an Improved Mechanism for the Monoterpenes Using Existing (though Limited) Kinetic/Mechanistic and Smog Chamber Data

Description: Monoterpenes, a class of volatile hydrocarbons with moderate-to-high reactivity, are emitted in large quantities from vegetation and may play a major role in ozone formation and decay. However, few monoterpene reaction products have been identified and even fewer have been quantified, resulting in their exclusion from or extreme simplification in chemical mechanisms. Under this element, existing kinetic and smog chamber data for selected monoterpene compounds will be used to develop an improved description of monoterpene reactions in the atmosphere, which will then be incorporated into existing chemical mechanisms used in air quality models.

Relationship to NARSTO Science and Policy Questions: Contributes directly to Science Question 1 because it is a significant research development. It supports Science Question 2 by utilizing laboratory studies to reveal fundamental photochemical processes that produce ozone; Question 3 by helping to assess the role of natural sources on ozone accumulation; and Question 4 by reducing the uncertainty in model predictions of ozone for regions that are affected by biogenic chemistry.

Priority: 1. The role of monoterpenes in local ozone production is a major source of uncertainty that needs to be addressed in order to increase our confidence in the models' ability to correctly predict ozone production.

Scheduling Requirements: A completed mechanism for monoterpenes should be available in 1996 to allow time for it to be incorporated into the air quality models, and used during 1997 for model sensitivity runs to support the 1998 Assessment.

Program Element M&C-3: Obtain Smog Chamber Data for Testing Chemical Oxidant Mechanisms for Ethanol, MTBE and ETBE

Description: The introduction of reformulated gasolines and other alternative motor vehicle fuels will reduce aromatic hydrocarbon emission inventories but will increase emissions of other volatile hydrocarbon species. By altering the chemical production and cycling of other pollutants, there is some uncertainty about the degree to which this strategy will reduce ozone, and how it will affect the concentrations of other air pollutants. In order to understand the ramifications of using these fuels, we need detailed knowledge of the atmospheric chemistry of oxygenated organics, such as methanol, ethanol, formaldehyde, methyl t-butyl ether (MTBE) and ethyl t-butyl ether (ETBE). Under this element, smog chamber simulations will be performed to help identify the products and their subsequent reactions resulting from the oxidation of ethanol, MTBE, and ETBE. This information will be used to evaluate current photochemical mechanisms for their accuracy in predicting the potential impact of these alternative fuels on atmospheric production of ozone.

Relationship to NARSTO Science and Policy Questions: This research contributes to Science Question 1 because the use of alternative fuels may alter how the ozone problem is managed. It supports Science Question 2 by using laboratory studies to further elucidate fundamental ozone production processes and Science Question 4 by reducing uncertainty in how the model handles atmospheric chemistry.

Priority: 2. This research should be completed before making a final assessment of the role of reformulated fuels on ozone control.

Scheduling Requirements: Enough studies must be completed in 1997 in order to be incorporated into the 1998 Assessment Report. Continuing smog chamber studies in 1998 will further enhance our database for supporting recommendations on the benefits and disadvantages of alternative fuels.

Program Element M&C-4: Obtain Smog Chamber Data at Low Concentrations and Low VOC/NOx Ratios to Determine if Existing Mechanisms Yield Accurate Predictions in This Regime

Description: One problem with existing smog chamber databases that are used to develop and evaluate current chemical mechanisms is that the experiments were carried out at high reactant concentrations of VOCs and NOx, and high VOC/NOx ratios. However, evidence suggests that these mechanisms, which were adjusted to fit the high VOC/NOx conditions, may in fact underpredict ozone formation at low VOC/NOx ratios. As a result, existing AQSMs may be underpredicting the amount of VOC control needed to achieve the O3 NAAQS and underestimating the utility of NOx control. Research under this task will develop new smog chamber data sets at VOC and NOx conditions that are more representative of the real atmosphere. These simulations will be documented following standard model-evaluation protocols, added to the existing smog chamber database, and made available to all for use in evaluating new and existing chemical mechanisms.

Relationship to NARSTO Science and Policy Questions: This research will contribute to Science Question 1 because it is a significant contribution to the experimental research databases, and to Science Question 3 by helping the models to better define the relative contributions of VOCs and NOx to ozone formation. It contributes to Science Question 4 by increasing our confidence that the chemical mechanisms are accurately predicting ozone concentrations at realistic atmospheric conditions.

Priority: 1. The availability of these more realistic databases will help reduce the uncertainty that is still present in air quality chemical mechanisms.

Scheduling Requirements: A large database of chamber runs is needed to evaluate the mechanisms for the 1997 model simulations. However, these runs do not necessarily all have to be completed by 1997; additional chamber runs may be continuously supplied.

Program Element M&C-5: Develop an Improved Mechanism for the Reaction of Alkenes with O_3 and OH Radicals

Description: Alkenes are highly reactive in the atmosphere. Although the reaction mechanism of ethene is relatively well understood, the reactions, products, and further reactions of intermediates are highly uncertain for the higher alkenes, and thus their implementation in the model-based chemical parameterizations is questionable. Smog chamber research is needed to help identify the products of these longer-chain alkene reactions. These experimental measurements will be used to develop an improved description of alkene chemistry which can be incorporated into existing chemical mechanisms. This will improve the reliability of the ozone concentrations predicted by air-quality models.

Relationship to NARSTO Science and Analysis Questions: A better understanding of alkene chemistry is an important research development which will contribute to Science Question 1. It will improve the accuracy of predictions from chemical mechanisms which will reduce the associated uncertainties, contributing to Science Question 4. It will support Science Question 2 by improving our understanding of some fundamental reactions involved in ozone production.

Priority: 1. The photochemistry of long-chain alkenes has long been cited as an uncertain component in chemistry models.

Scheduling Requirements: A portion of this task must be completed in 1996 so that the improved chemical mechanism can be used in the model simulations needed for the 1998 Assessment. Work should continue to improve the mechanism and its interaction with the model beyond 1997.

Program Element M&C-6: Improve the Chemical Mechanisms for Anthropogenic VOCs Using Existing Data

Description: Current chemical mechanisms are unable to represent all of the individual VOC species which participate in atmospheric photochemistry and ozone production. Instead, they lump individual VOCs into fewer, broad categories, using numerous approximations and assumptions, all of which cause varying degrees of error in the final concentrations. In addition, our knowledge of VOC reactions and products has increased immensely since these original mechanisms were formulated, but the mechanisms are unable to represent these advancements. This research will develop new methods for representing our current knowledge on the complex photochemistry in the atmosphere by formulating a new, innovative mechanism that can account for the formation and decay of every VOC that contributes to oxidant formation in the atmosphere. The mechanism and its integration into the model will utilize advanced program structures and algorithms so that air-quality simulation models can efficiently perform the simulations much faster than current models. This improved chemical mechanism will be rigorously evaluated using standard protocols and incorporated into the air quality models.

Relationship to NARSTO Science and Policy Questions: The resulting improved mechanism will be a significant research development, contributing directly to Science Question 1. It will also contribute to Science Question 4 by improving the connection between our scientific understanding of ozone formation and our ability to duplicate it in an air quality model.

Priority: 1. There are so many inherent sources of error resulting from assumptions made in the current chemical mechanisms that they must be improved before we can expect them to do an accurate job of representing chemistry in the real atmosphere.

Scheduling Requirements: A preliminary version of a new mechanism should be available halfway through 1997 so that it can be used in the model simulations used for the 1998 assessment. Work should continue to improve the mechanism and its interaction with the model beyond 1998.

Program Element M&C-7: Expand the VOC Chemistry in Existing Mechanisms so the Mechanisms Can be Used for Diagnostics of Current Air-Quality Model Predictions

Description: Because of computer constraints, it is impossible to model all the numerous individual organic reactants and products that participate in ozone formation. Because of this, existing mechanisms employ numerous approximations and "lump" organic species into general classes of compounds which are then applied to the air-quality models. However, the model predictions of these lumped species do not directly relate to observations of individual VOC species. Research under this element will start with current mechanisms and "unlump" some of the more important VOCs, thus developing a more detailed representation of these species within a standard, existing chemical mechanism. These modified mechanisms will be applied with the air-quality models so that the predictions of these models can be compared directly with air-quality data. These predictions are an integral component of assessing how well the models represent ozone photochemistry in the real atmosphere. This task will proceed concurrently with Element 6, resulting in two different, detailed approaches for describing atmospheric chemistry in the AQSMs, which can then be compared and contrasted.

Relationship to NARSTO Science and Policy Questions: This element contributes directly to Science Question 4 because it will improve our confidence in model-predicted changes in ozone concentrations and help reduce one of the uncertainties in predicted ozone formation by allowing more direct comparisons between field measurements and model predictions.

Priority: 2. This task is necessary for allowing us to more rigorously compare field measurements with model predictions. This ranking is based solely on its short-term support. If it is not completed in the short term, its ranking will drop significantly.

Scheduling Requirements: The mechanisms with more detailed VOC descriptions must be incorporated into the modeling runs performed during 1997.

Program Element M&C-8: Conduct an Intercomparison of Existing Chemical Mechanisms Within AQSMs to Determine the Effect of Mechanism Uncertainty on Model Predictions

Description: Research under this element will help to identify how different existing chemical mechanisms, with their different formulations, assumptions, and characteristics, affect the uncertainties associated with model predictions. This work will help to provide guidance on where efforts should be focussed to obtain data which will improve these ill-defined aspects of the mechanism that are introducing the most uncertainties into the model predictions.

Relationship to NARSTO Science and Policy Questions: This work will support Science Question 4 by identifying some critical uncertainties in current models for assessing ozone production resulting from the atmospheric chemical mechanisms.

Priority: 2. While not as critical for the assessment as some of the other near-term tasks, performing these tests will help to quality-assure the chemical mechanisms and provide confidence that the mechanisms are performing in a competent manner.

Scheduling Requirements: Some intercomparisons should be in early 1997 to allow alteration (if necessary) the chemical mechanism used in the modeling simulations performed in 1997. Since mechanisms will continue to be modified, this task could also continue on into 1998.

3.3.2.2 *Meteorology*

Program Element M&C-9: Develop Approaches to Maximize the Use of Current Information and New, Satellite-Derived Information for Use in 4-Dimensional Data Assimilation (4DDA)

Description: 4DDA can be used to high advantage for maximizing the fidelity of simulated meteorological fields through their constraint in conjunction with observational data (nudging). Past work in data assimilation has centered on the use of twelve-hour rawinsonde data at the synoptic scale (winds, temperatures, pressure and humidity). With higher frequency observations, nudging coefficients need to be increased. This can lead to nudging waves in the system which need to be controlled. Also, current, previously unused data exist which can help reduce uncertainty in surface processes that control rates of dispersion. GOES visible data can provide solar insolation data into model surface-energy budgets, and long-wave cloud effects can be included from satellite data. Additionally, NEXRAD radars can provide regional coverage and composite radar products so that rainfall rates can be assimilated. This program element will bring to fruition new 4DDA techniques to reduce the uncertainty in the calculation of meteorological fields used to drive the chemical-transport models.

Relationship to NARSTO Science and Policy Questions: Contributes directly to Science Question 1 by improving our ability to represent meteorology important to air pollution. Supports Science Questions 2 and 3 by reducing meteorological uncertainty in model analyses for these questions.

Priority: 1. This work represents a critical element in the efforts to reduce uncertainty in the predictions of prognostic meteorological models for air quality. It will provide a critical underpinning for improving our ability to model seasons.

Scheduling Requirements: A phase of this work must be completed in 1997 to be available in time to aid the interpretation of the preliminary results of the cross-model evaluation that will be coming out in 1998. Work should continue to improve the meteorological information and its interaction with the air-quality model beyond 1998.

Program Element M&C-10: Develop Recommendations on How Best to Use 4DDA with Special Study Data and at the Different Spatial Scales Required for Combined Regional/Urban Air Quality Modeling

Description: During field programs special observations are often made which can be used to improve the fidelity of the meteorological simulations. However, there is insufficient theoretical guidance on how this information (usually at small scales and high frequencies) should be assimilated. This program element will investigate how assimilation of these special-study data should be carried out, using existing special study data. For example, boundary layer profilers are often deployed. How is the atmospheric energy (temporal and spatial spectra) in the model altered by assimilation of winds from these profilers? The profilers also can infer boundary layer depths. Should these be directly assimilated or should the root parameters controlling the PBL depths (heat flux, upper layer vertical velocities, or upper layer stability) be nudged. The goal is to test assimilation strategies to provide near term guidance on appropriate data assimilation techniques. Such guidance will be important to model evaluation and assessments of how best to reduce meteorological uncertainty stemming from the primitive equation meteorological models.

Relationship to NARSTO Science and Policy Questions: Contributes directly to Science Question 1 by improving our ability to represent meteorology important to air pollution. Supports Science Questions 2 and 3 by improving our ability to evaluate meteorological models, reducing uncertainty in model analyses for these questions.

Priority: 1. This work will contribute significantly to the evaluation of prognostic meteorological models and efforts to understand their sources of uncertainty.

Scheduling Requirements: This work needs to begin in 1996 or 1997 to achieve measurable progress prior to intensive meteorological evaluation using the Nashville '95 and the NARSTO-NE '95 and '96 data.

Program Element M&C-11: Incorporate New Soil Moisture, Surface Heat Flux Parameterizations into Meteorological and Chemical Models in a Systems-Integrated Manner

Description: This program element will improve model parameterizations of surface heat and moisture fluxes, and thereby improve the modeling of atmospheric boundary-layer (ABL) growth and processes. Also, by employing an integrated approach to meteorological and chemical surface fluxes, improvements in accuracy and consistency of dry-deposition simulations will be realized. Modeling of soil moisture and vegetative transpiration is very important for realistic simulation of surface fluxes and ABL processes over varying land-use and moisture conditions. The dependence of stomatal resistance on soil moisture is a key factor determining the partitioning of surface energy into latent and sensible heat as well as rates of chemical dry deposition. Soil moisture initialization and dynamic adjustment through data assimilation may be important parts of this effort. The goal of this work is to improve modeling of surface-flux and ABL processes which are important for air-quality simulation. Also, this work will significantly improve dry-deposition modeling by benefiting from more sophisticated parameterizations of stomatal processes in the transpiration model. Dry deposition is an important sink for many air pollutants and their precursors. Evaluation of modeling techniques through comparison to field-study measurements of both meteorological and chemical surface fluxes will be a part of the program.

Relationship to NARSTO Science and Policy Questions: Contributes to Science Question 1 by improving our ability to represent processes critical to boundary layer development, which is critical to air pollution. Supports Science Questions 2 and 3 by reducing uncertainty in the boundary layer and surface loss representations in the model analyses for these questions.

Priority: 1. Boundary layer processes are central to air-quality predictions at the surface. They are in need of improvement and their contribution to the uncertainty of air-quality predictions needs to be assessed. This work will also provide a critical underpinning for improving our ability to model seasonal time periods.

Program Element M&C-12: Update Parameterizations of Photolysis Fields and Provide Methods to Reduce Uncertainties in the Photolysis Rates Employed by Air-Quality Models

Description: This program element will improve the regional scale calculation of actinic flux fields in 4-dimensions (space and time) leading to better estimates of photolysis rates. Key factors influencing actinic flux include clouds, ozone column, surface albedo, and aerosol loadings. Clouds fields have the most important impact on actinic radiation and are notoriously difficult to model. Therefore, the use of satellite information to derive 4-dimensional cloud fields will be a great improvement over modeled or ground observed cloud data. Ozone column data can be acquired from TOMS satellite observations. Seasonal high resolution surface albedo estimates from land use information and/or direct satellite measurements will also improve actinic-flux simulations, particularly near the ground where most of the air quality chemistry is occurring. Satellite data may also be valuable for deducing aerosol loading in the lower troposphere which can greatly affect low level actinic flux. The goal is to reduce the uncertainty of direct photolysis processes in the photochemical system.

Relationship to NARSTO Science and Policy Questions: Contributes to Science Question 1 by improving our ability to represent a basic forcing function for photochemical production. Supports Science Questions 2 and 3 by reducing uncertainty in rates of chemical production in model analyses for these questions.

Priority: 1. Errors in photolysis directly result in errors in computed photochemical production. Current approaches are woefully out of date and inadequate. This work will provide a critical underpinning for improving air-quality modeling competence.

Scheduling Requirements: A phase of this work must be completed in 1996 to be incorporated in time for models to be included in the evaluation scheduled for calendar 1997. The work can continue throughout.

Program Element M&C-13: Incorporate Stratospheric Influences Into the Regional Air-Quality Models

Description: Regional modeling has typically either neglected stratospheric ozone or simply provided climatological upper- to mid-tropospheric ozone as a fixed boundary condition. The infusion of stratospheric ozone into the troposphere is highly variable in time and space with perhaps the predominant input occurring during tropopause folding events. While strong folding events are more likely to occur during the winter and spring, the summer especially at higher latitudes can also provide enough frontal activity to produce modest folding events. Once a fold has developed, other processes such as deep convective mixing or descent over surface high-pressure areas are capable of transporting this ozone to the lower troposphere. There is also the possibility that deep tropospheric convection carried out over extended periods could gradually entrain tropopause and lower-stratosphere air in much the same way that dry boundary-layer thermals entrain air out of a capping inversion. This program element will critically examine these processes, using existing special-study data as well as a climatological examination of ozonesonde data, to provide a near-term understanding of the contribution of the stratosphere to the summertime tropospheric ozone budget. If needed, this work also will suggest first-order parameterizations for regional-scale models. Stratospheric ozone may affect the control-strategy responses in the regional models, creating a source of uncertainty for current models, because this additional ozone serves as a further source of both ozone and radicals driving the photochemistry.

Relationship to NARSTO Science and Policy Questions: Supports Science Questions 2 and 3 by reducing uncertainty in the estimation of background conditions affecting pollutant levels and photochemical production rates. Reduces uncertainty for Science Question 4 by providing better estimates of the "uncontrolled" sources of ozone affecting regional levels.

Priority: 2. The uncertainty introduced by the neglect of stratospheric influences needs to be defined, yet inhouse resources may be able to cover the task.

Scheduling Requirements: Elements of this work need to be accomplished in time to coordinate with the first interpretation phase of the cross-model evaluation in 1998.

Program Element M&C-14: Incorporate Newly Available PBL Schemes in Prognostic Meteorological Models and Compare Their Properties

Description: This program element will lead to the improvement of the modeling of PBL processes, including growth of the PBL and turbulent mixing within the PBL, which are critical elements of realistic air quality modeling. New and innovative PBL schemes, including non-local closure, will be applied in a consistent manner to both meteorology and atmospheric-chemistry models. Meteorological models will be evaluated through comparison to existing models and to field data. The objective is to improve boundary layer modeling for the air quality applications. Therefore, realistic treatment of the turbulent mixing of both meteorological and chemical parameters is necessary. The emphasis on chemical dispersion requires capability to simulate sources within or above the PBL as well as at ground-level. The techniques resulting from this program must be sufficiently simple to provide the computationally efficiency required by multiscale meteorology and atmospheric chemistry modeling systems.

Relationship to NARSTO Science and Policy Questions: Contributes to Science Question 1 by improving our ability to represent processes critical to boundary layer mixing away from the surface, which is critical to air pollution. Supports Science Questions 2 and 3 by reducing uncertainty in the representation of vertical mixing at the surface in the model analyses for these questions.

Priority: 1. Boundary-layer processes are central to air-quality predictions at the surface and possible advances in their parameterization need to be made available as quickly as possible because this is a poorly understood area of uncertainty.

Scheduling Requirements: This project should begin immediately to reap the greatest benefits for near-term model evaluation work. Research should continue beyond 1998 to improve the meteorological parameterizations and their interaction with the air-quality models.

3.3.2.3 *Fine-Scale Processes*

Program Element M&C-15: Develop an Advanced Plume-in-Grid capability for Regional and Urban Air-Quality Models for Incorporation into Eulerian Chemical Transport Models

Description: This program element will develop and test a module for incorporation into Eulerian chemical transport models, in addition to relevant parameterizations and decision rules to compute the sub-grid chemistry of multiple, selected large NO_X

plumes until transfer to the main model grid. A Lagrangian reactive plume characterization will serve as the basis of the plume-in-grid approach. The goal of this work is to overcome identified weakness in current plume-in-grid treatments. Large NO_X plumes are a very important feature of regional photochemistry and they are believed to have an important impact on urban chemistry and the assessment of management options.

Relationship to NARSTO Science and Policy Questions: Contributes directly to our ability to answer Science Questions 2 and 3. Supports Science Questions 1 and will enhance our ability to answer Science Question 4.

Priority: 1. The desired ability to adequately characterize chemical impacts of large NO_X plumes has been identified as an important uncertainty in understanding regional and urban photochemistry.

Scheduling Requirements: Critical to complete initial phases of the work in 1997 to allow time for incorporation into the models, testing and completion of model sensitivity runs during 1997 and 1998 to provide information for the NARSTO assessment.

3.3.2.4 *Model Evaluation*

Program Element M&C-16: Characterize Meteorology's Effect on Chemistry from the Perspective of a Coupled System, Including Incorporation of Newly Available Process Descriptions and Accounting for Behavior Related to Control Strategy Projections

Description: This program element will apply sensitivity analysis to identify meteorological variables having a major impact on the emission/concentration sensitivity relationships. The goal is to identify those meteorological variables that may cause the greatest uncertainty in the prediction of the effect of a management strategy. The focus is on prognostic meteorological models, with their dynamic interactions. This program element also will assess the effects of more scientifically advanced descriptions of processes, such as planetary boundary layer (PBL) processes, including growth of the PBL and turbulent mixing processes within the PBL, on key elements of air-quality model predictions. New and innovative process parameterizations (e.g., PBL schemes, including non-local closure) will be applied in a consistent manner to both meteorology and atmospheric-chemistry models, so that both models have matching parameterizations. The goal is to assess the impact, on air-quality predictions, of the newer descriptions. This work will provide important information needed to guide meteorological research to those areas that can best reduce the air quality prediction uncertainties and to assess the robustness and quality of air quality model predictions.

Relationship to NARSTO Science and Policy Questions: Contributes directly to our ability to answer Science Questions 2 and 4. Supports Science Questions 3 by developing information to interpret and reduce uncertainty in model answers.

Priority: 1. Meteorology is a key input to the air-quality models. The uncertainty in this input can have direct impact on model prediction uncertainty. Timing is critical for the 1998 deadlines and to effectively guide meteorological research planning.

Scheduling Requirements: Critical for a phase of work to be completed in early 1997 to allow time for synthesis and review and incorporation into the Assessment. Work should continue beyond 1998.

Program Element M&C-17: Conduct Comparisons of the Predictions of Different Prognostic Meteorological and Chemical-Transport Models for the Same Geographic Domains, Spatial Scales, and Time Periods

Description: This program element will bring to fruition ongoing model comparison studies that are assessing the predictions of a set of models applied to the same simulation periods across more than one geographic region. The goal is to compare different models, either meteorological or chemical, using consistent inputs. The objective is to bring recent studies and/or work in progress to a point of completion so that results can be summarized in a timely manner for inclusion in the work-in-progress reviews for the 1998 NARSTO Assessment. There are interesting comparative studies underway, such as the CREME Project, that can provide up-to-date information on the modeling tools now being used in different geographic locations. Cross-comparison of models will provide insight into the state of our modeling knowledge.

Relationship to NARSTO Science and Policy Questions: Contributes directly to Science Question 4 by defining the overall level of skill modeling systems possess. Supports Science Questions 2 by developing a comparative description of the system-level performance of modeling systems, by use of similar inputs.

Priority: 1. Ongoing work needs to be brought to fruition as quickly as possible for possible inclusion in the NARSTO assessment papers.

Scheduling Requirements: This work needs to be active in 1996 and 1997, and results completed and interpreted in 1997 for inclusion in the syntheses for the 1998 NARSTO assessment. Work should continue beyond 1997.

Program Element M&C-18: Develop a Diagnostically Oriented Model-Evaluation Protocol for the Chemical-Transport Model, Backed By Process Analysis Software in the Air-Quality Models

Description: This program element will investigate and develop a set of model-evaluation tests that are designed to probe the fidelity of photochemical-process simulations through theory-based construction of state-variable combinations. The tests are to be designed to probe the functioning of the model as a system for comparison to the functioning of the real world as a system. They will augment more typical model-evaluation comparisons. As part of their development, the interpretability of the newly constructed tests will be assessed through process analysis that quantifies sources of photochemical production and mass balance of species concentrations. The goal is to identify those diagnostic tests that characterize system behavior important to extrapolation to new chemical situations and describe how model behavior in such tests translates into biases or uncertainties regarding extrapolation to new conditions. Tests sensitive to extrapolation behavior are also needed. The best data sets available to implement the new tests are also to be identified. The goal is to test key, basic photochemical process and rate formulations in the model to augment the more traditional history-matching. Because of complex and competing interactions of the photochemical system, the state variables result from multiple interactions and do not represent well the functioning of the system. The reliability of the model as a predictive tool depends on the fidelity of its representation of the major photochemical processes. This fidelity is not adequately tested through state-variable comparisons.

Relationship to NARSTO Science and Policy Questions: Supports Science Questions 2, 3, and 4 by defining tests to probe the modeled processes important to model answers for these questions. Supports Science Question 1 by developing tests aimed at assessing our ability to represent the processes well in the models.

Priority: 1. A new protocol that addresses process representations in air-quality models is critical to development of better, more substantive scientific insights into the strengths and weaknesses of the air-quality models.

Scheduling Requirements: This work is critical and must begin immediately to be completed and reviewed in early calendar 1998 to guide the new model evaluation.

Program Element M&C-19: Complete, Collect and Compile Model-Evaluation Results That Have Occurred Since the Work Referenced in the NAS Report and Include an International Perspective

Description: This program element will compile recent model evaluation results completed in the late 1980's and the 1990's. This program element calls attention to the high-priority need to complete ongoing model-evaluation studies, and to compile consistent and comparable summaries to prepare a synthesis of major results. The intent is to provide up-to-date information on the modeling tools now being used in different geographic locations. Of additional interest is a synthesis that recognizes the important compilation of recent comparisons, based principally on history matching of state variables, and provide a backdrop for the newer, more diagnostic, process-oriented testing that will be undertaken in future NARSTO efforts.

Relationship to NARSTO Science and Policy Questions: Contributes directly to Science Questions 1 and 4 by helping to define the overall level of skill a modeling system possesses.

Priority: 1. Completed work needs to be collected and synthesized as quickly as possible for possible inclusion in the NARSTO assessment papers.

Scheduling Requirements: This work should begin in 1996 for completion in 1997 for inclusion into the synthesis work of the 1998 NARSTO assessment.

Program Element M&C-20: Conduct Model Sensitivity- and Uncertainty-Analysis Studies with Reference to the Compositional Validity and Appropriate Structuring of the Models for Application to Photochemical Issues

Description: This program element will provide data for characterizing the effects on model-based air-quality predictions resulting from individual process descriptions within the model (i.e., which processes are included or excluded or which are overly simplified or use mathematical approximations). The goal is to provide guidance on how to model the photochemical system, and to identify those aspects of uncertainty that are caused by the scientific basis of the model, as opposed to those imposed purely by computational constraints.

Relationship to NARSTO Science and Policy Questions: Contributes directly to Science Questions 1 and 4 by helping to define the how the level of skill a modeling system possesses is influenced by its design and resolution.

Priority: 2. The construction of a model and its resolution is an important, hidden source of uncertainty to its air quality predictions that can mask true chemical and physical sources of uncertainty. This uncertainty needs to be resolved as part of the model evaluation interpretation process.

Scheduling Requirements: Elements of this work need to be accomplished in time to coordinate with the first interpretation phase of the model evaluation in 1998. Work should continue beyond 1998 to further develop improved model assessments.

Program Element M&C-21: Conduct the Initial Phase of a NARSTO Model Evaluation or cross-model evaluation, Including Peer Review of the Interpretations

Description: This program element will focus on the implementation of the new, diagnostic model evaluation protocol (M&C-18) in a cross-model evaluation of the new modeling systems that might be recommended for regulatory and applications modeling at the end of the century, using the best data bases. The intent is for all modeling systems to be included, for the evaluation protocol to be applied as consistently as possible across all of the models, and to have science teams with knowledge of each modeling system contributing substantively to the interpretation of the test results. The goal is to provide a more process-oriented interpretive examination and characterization of model behavior prior to the rounds of model applications envisioned at the end of the century and to provide an initial diagnostic interpretation of the state of our modeling in as short a time frame as possible. History matches of state variables have been found to be inadequate diagnostics model behavior, leaving an unacceptable degree of uncertainty in the interpretation of model evaluation results. The goal of the independent, scientific peer review is to ensure as objective a model evaluation and interpretation as possible and to provide a thorough scientific review of the process and results. An independent scientific review panel is essential to the overall credibility of the model-evaluation process, given its intended diagnostic nature and the need to involve scientists familiar with each model.

Relationship to NARSTO Science and Policy Questions: Contributes to Science Questions 2, 3, and 4 by assessing the performance of models, with a new emphasis on modeled processes. Contributes to Science Question 1 by providing an assessment of our ability to represent the key processes in the models.

Priority: 1. A cross-model evaluation that is more diagnostic than any past model evaluation is critical to the assessment of the modeling tools and modeling science that is being asked of NARSTO. A first phase of such an evaluation needs to occur in time for the first NARSTO assessment.

Scheduling Requirements: The model evaluation needs to commence as soon as possible to allow a year to provide preliminary results and have them reviewed and refined for the NARSTO assessment. Ideally the evaluation should begin in 1997.

3.3.2.5 *Model Application*

Program Element: M&C-22: Organize and Compile Photochemical Modeling Study Results that have Occurred Since the Work Referenced in the NAS Report. Commission Principal Participants of the Major Studies to Help in this Effort

Description: In this program element, an individual or individuals will compile and critically review the range of urban and regional modeling studies that have been conducted both before (a few) and after (somewhat more) the NAS report. A key component of this task is to compare and contrast the results, identifying major differences in the studies' execution and results. Principal scientists involved in the various studies might be commissioned to help in this effort.

Relationship to NARSTO Science and Policy Questions: This relatively low cost item is directly related to NARSTO Science Questions 1, 2, 3, 4 and 6, providing a current, comprehensive snapshot of our current scientific understanding of modeling results related to ozone formation and control, and the available modeling tools.

Priority: 1. There has been very little done since the NAS report to conduct an extensive evaluation of the various modeling results. This is critical since most of the modeling studies at the regional scale have been conducted since the NAS report. There is a need to assess the consistency of the recent studies with the NAS findings, and identify the current issues. Also, the NAS report was only suggestive of the need for NO_x control. This question should be revisited.

Scheduling Requirements: This project should begin immediately to reap the greatest benefits in guiding application and other NARSTO projects.

Program Element: M&C-23: Conduct Model Analyses and Model Sensitivity and Uncertainty Tests Directed Towards the NARSTO Analyses and Assessment Questions with Particular Reference to Development of an Understanding of the Photochemical System, its Scales, and Model Predictive Ability

Description: The exercise of different models in a coordinated fashion and report of the results is important to critical examination of model predictions and model attributes. Critical examination is important to scientific acceptance of various models for scientific and policy application, and for developing a foundation for interpretation of future results. A major goal of coordinated model analyses is a better assessment of the confidence one can place in various modeling results. Sensitivity and uncertainty analysis have proven invaluable to both air-quality modeling and other fields to provide a quantitative understanding of how a complex system responds to inputs and parameters. Further, it is used to identify the key parameters in complex systems, be it the atmosphere of other physicochemical systems. A third use is in model intercomparison. For example if all models included, as part of their formulation, simultaneous calculation of not only the concentration, but the sensitivities of those concentrations to parameters, a very detailed cross-comparison of models would be possible. This goes well beyond just comparing concentration predictions over a usually limited range of emissions, boundary conditions, and initial condition inputs. In this program, sensitivity and uncertainty analyses will be performed using comprehensive air-quality models and formal sensitivity and uncertainty techniques. This work would provide quantitative uncertainty assessments for model applications, indicating the capability of those models to make photochemical predictions.

Relationship to NARSTO Science and Policy Questions: This research is directly related to NARSTO Science Questions 1, 2, 3, and 4. Given the dual policy and scientific direction of NARSTO, this provides foundations for further interpretation of past and future modeling results. In addition, the uncertainty-analysis techniques developed will be immediately applicable to other environmental models.

Priority: 1. There are currently a number of models being exercised for policy and scientific analysis. However, there has been no coordinated exercise and forum for investigating the differences in those models. Sensitivity and uncertainty analysis has been identified as being a critical need in determining model response, for use in model evaluation and for assessing which parameters are most critical to our ability to better understand atmospheric pollutant dynamics and the effects of controls. The results of this project would have widespread use.

Scheduling Requirements: This project should begin immediately to reap the greatest benefits in guiding NARSTO projects and to develop the techniques in a timely fashion. Given its potential use in model evaluation, it would be appropriate if the techniques were developed and employed for planned, major model evaluation studies.

Program Element: M&C-24: Conduct Studies to Define the Attributes of a Successful Air-Quality Model Application Including Comparisons and Contrasts Between Science and Regulatory-Directed Modeling Efforts

Description: At present, there are a variety of modeling studies that have been conducted, or are underway. Some of them are definitely policy-focused (e.g. OTAG), while others have a scientific focus (e.g. studies by NOAA and universities). It is often viewed that there are definite contrasts between those two classes of studies, as was evidenced in the NAS report. In that report, many of the modeling results were taken from scientifically-directed studies, even though a large majority of the modeling is performed for policy development (e.g. SIPs). Thus, while the science studies may have less immediate use for air-quality management, they can have a longer-term impact for successful policy development and decision making. In this project, the types of modeling projects are to be investigated and contrasted to help identify attributes of successful model applications in support of decision making and air-quality management. As a specific example, there is currently concern over how grid-based models treat emissions from power plants and other large, sub-grid sources. Few studies have dealt with this question. A potential project could investigate how different representations of point-source emissions effect air-quality modeling results, and the impact on related control strategies.

Relationship to NARSTO Science and Policy Questions: One of the key questions in NARSTO is how models are used in the development of effective air-quality management programs. A key question here is what makes a modeling study have long-term value, and the basis behind good policy decisions. This project directly addresses Science Questions 1, 2, 3 and 4.

Priority: 2. This project can be used to help structure future air-quality management modeling studies, identifying the attributes of successful studies in both the scientific and policy efforts. Given the large resources currently being devoted to regulatory modeling, it will be beneficial to guide such studies to increase their lasting contributions.

Scheduling Requirements: This project should begin immediately to reap the greatest benefits in guiding application projects, as well as to develop the appropriate techniques in a timely fashion.

4

EMISSIONS

4.1 Emission Component Responsibilities

NARSTO's Emission component is responsible for developing, applying, and disseminating quantitative knowledge on all aspects of natural and anthropogenic pollutant emissions relevant to tropospheric ozone formation. In specific terms, the Emissions component is charged with the following activities:

- development of emission models,
- analysis of emission processes and activities,
- performance of anthropogenic and natural emission field studies,
- performance of emission projections
- performance of analyses with respect to control-policy implications

4.2 Near-Term (1997-1998) Objectives of the Emission Component

In reflection of the above responsibilities and in view of the current state of scientific understanding, NARSTO's Emission Team has set the following objectives for the 1977 - 1998 period:

- To contribute emission-based expertise and information to the 1998 NARSTO Assessment process. These contributions will take the form of:

    - preparation, coordination, and review of Critical Review Papers pertaining to characterization of natural and anthropogenic emissions relevant to ozone formation; and
    - participation in the creation and review of the 1998 NARSTO Assessment Document.

- To continue and complete work in progress on emission measurement, quality-checking and uncertainty-analysis of existing emission inventories, and improvement of emission models.

4.3 Extended Emission Component Objectives

4.3.1 Priorities

An important feature of NARSTO's research strategy and its current priorities resides in the fact that ambient ozone is largely a secondary pollutant, which must be regulated indirectly through control of its precursor emissions. Because of this, and also because pollutant emissions are an essential and primary input to ozone-simulation models, a quantitative understanding of pollutant emissions is critical to cost-effective ozone management. Unfortunately, many of today's inventory estimates are based on limited test data, engineering analyses, and invalidated emission-factor models, and thus are highly uncertain. Much more evaluation with real-world measurements is needed to bring such uncertainties within limits commensurate with effective ozone management.

Several projects to quantify mobile source emissions are currently in progress. These studies suggest that current emission-factor/activity models underestimate nonmethane organic compounds (NMOC) and carbon monoxide (CO) emissions. In addition to mobile sources, key areas needing increased quantification include emissions from solvent usage, oil and gas industries, and other stationary area sources. These are exceptionally are difficult to characterize because of the large number and variety of emissions. In addition, difficulties in measuring NO_x have led to unacceptable uncertainty levels in associated estimates of emissions from high-temperature point sources such as electric utilities and smelter industries. Finally, biogenic NMOC and NO_x emission estimates— and their current uncertainty levels — are receiving considerable attention because of their perceived contribution to rural, and in some areas, urban ozone problems.

As a consequence of the above features, the emission component priorities have been selected to fall into the four general categories as follows:

1. **General development and improvement of emission estimates:** This category addresses the development of emission estimates for use in air-quality models and emission-control strategies that are:

    - reasonably complete and accurate,
    - resolved in time and space, and
    - chemically speciated.

2. **Development of mechanistic understanding of emission processes.**

3. **Application of independent techniques to assess the accuracy of emission estimates.**

4. **Estimation of future emissions.**

4.3.2 Tasks

Program Element E 1: On-Road Mobile Source Emissions

Description: The goals of this element are:

- to develop timely estimates of on-road mobile source emissions which are reasonably complete and accurate, possess the needed time and space resolution, and have the needed chemical speciation; and

- to develop on-road mobile source emission models that have capacity to provide emission factors and activities of vehicles in various operating modes.

Mobile source emission inventories of large areas are estimated by multiplying an emission factor from an emission-factor prediction model by an activity factor from a travel-demand model. The earlier emission-factor models were found in several studies to underpredict the emission factor for non-methane hydrocarbons (NMOC) and CO by factors of three or more. The travel-demand models now in use were developed for other purposes, and some questions have been raised as to their application to mobile-source emission estimations. Some investigators feel that the emission-factor models do not adequately represent situations such as "high or gross emitters", evaporative losses, in-use fleet, and "off-cycle" driving modes. Studies are underway such as tunnel studies, remote-sensing roadside studies, portable dynamometer roadside studies, high-emitter studies, and off-cycle driving studies to provide needed data for updating these models. Other studies are underway to investigate other approaches for emission-factor and activity models. In addition, the situation has become much more complicated with the introduction of new fuels and vehicle technologies in response to regulations being implemented in Canada, Mexico, and the United States.

Major Subtasks:

- Survey mobile-source emission-inventory approaches and determine if the ongoing work of one area can be applied to other geographic areas. *(near term)*

- Evaluate the uncertainty of mobile-source emission inventories with present and future techniques with an integrated assessment of data sets used in developing emission and activity factors. Use this information to help set further research priorities. *(ongoing)*

- Establish a framework for a research-grade mobile-source emission model that provides estimates of emissions with temporal and spatial resolution. The model will need independent emission-factor and activity modules for various aspects of vehicle operation. Develop and test the approach for general use.

- Improve existing remote-sensing (RSD) modules for hydrocarbon and NO_x emissions. Test these improved RSDs in a variety of driving situations. Couple RSD to long-path ambient air measuring systems with air-movement measurements through tracer releases for emission-factor determination. *(ongoing)*

- Develop emission-factor techniques for areas of high "gross-emitter" fleets, coupling RSDs with portable dynamometers, and determine the cost of effective pollution reducing repairs. *(ongoing)*

- Develop modal emission factors for automobiles and light-duty trucks with improved travel-demand models. The models must provide estimates of vehicle activities for each modal emission factor. *(near term)*

- Develop modal emission factors for medium- and heavy-duty trucks and buses, both in laboratory tests and under on-road conditions. NO_x and NMOC emissions from medium-duty trucks such as delivery trucks in urban areas with a severe ozone problem need to be studied immediately so that their input to the emission inventories can be determined. The emissions from heavy-duty trucks operating in these same urban areas must also be studied. The emission factors must include temporal and spatial resolution and a variety of vehicle operating conditions. *(near term)*

- Evaluate the real-world effects of traffic controls on reducing emissions for incorporation into emission estimation models. *(long term)*

- Evaluate the existing chemical speciation data and measurement techniques and determine how well they produce emissions from in-use vehicles operating in various modes. Where needed, develop new techniques to provide data where gaps exist. *(near term)*

Relationship to NARSTO Science and Policy Questions: This task group will attempt to address the NARSTO policy oriented questions from a somewhat different perspective. It is recognized by many that substantially new ways of preparing strategic plans are need that account for the quality of information available, and account explicitly for socioeconomic dimensions of environmental protection. By evaluating the tools that will permit moving in this direction, the process of thinking about ozone management in new ways should be accelerated.

Priority: 2. This ranking is based on high customer value, long term, critical relevance to NARSTO science and assessment questions, present-day modest needs by other NARSTO functions, and somewhat flexible timing relative to other elements for the l998 assessment.

Scheduling Requirements: Timing for products from this group would be desirable to insure inputs into the l998 assessment. However, the timing is less stringent than the other elements needed to produce a high quality, substantive assessment.

Program Element E 2: Non-road Mobile Source Emissions

Description: The goal of this element is to develop new stationary area-source and point-source models or methodologies that are capable of estimating emissions from all significant sources.

The emission estimates for many stationary sources are currently of questionable quality. This includes such industries as those using solvents and the oil and gas industry. The traditional "top-down" approach uses surrogate data for activity levels, along with default spatial and temporal allocation factors and emission factors to estimate emissions. This approach relies on information which may be out of date, of unknown accuracy, and never assessed by independent measurements. Reports of emissions by major point sources may contain day-specific activity levels, but are often based on average emission factors. Better temporal, spatial, and chemical resolution of emissions, as well as knowledge of emissions for "even days" are also needed.

Major Subtasks:

- Evaluate uncertainties of non-road source emission estimates with an integrated assessment of data sets used in developing emission and activity factors. Use this information to set priorities for the different source categories. Pleasure water crafts and lawn and garden equipment should be high priorities since the preliminary data suggest they may be the biggest non-road contributors. *(near term)*

- Develop improved methodologies or models for non-road source emission measurements and estimates. The models will need independent emission factors and activity modules for various aspects of emissions. *(near term)*

- Develop measurement methods for measuring non-road mobile source emissions including exhaust, evaporation, and emissions from fuel spills. *(ongoing)*

- Develop modal emission factors with temporal, spatial, and chemical resolution activity data for high priority source categories. *(long term)*

Relationship to NARSTO Science and Policy Questions: This research contributes directly to the Science Questions 2, 3, 4, 5, and 6. The strongest input is to Question 4 on developing emission management strategies and the strengths and limitations of current scientific methods and tools for assessing ozone issues and Question 3 the contributions to VOCs, No_x, and CO accumulation. Questions 5 and 6 on control strategies are also important. Source research is also included in Question 2.

Priority: 1. The role of non-road emissions has been overlooked but is now recognized as an important contribution to the precursors of ozone formation. A reasonable measurement approach and inventory of these emissions is very important; these are needed immediately.

Scheduling Requirements: Research on several aspects of non-road mobile source emissions is now underway. However, because of the large diversity in the types of sources, several years are required before work on some systems can begin. The small engine, including marine uses, is well underway and some emission factors have been developed.

Program Element E3: Emission Inventories from Stationary Area and Point Sources

Description: The goal of this element is to develop timely estimates of non-road mobile source emissions that are reasonably complete and accurate, having the needed time and space resolution and having the needed chemical speciation. Develop models that are capable of estimating emissions from a wide variety of non-road engines, fuel evaporation, and fuel spills during refueling.

Non-road mobile sources include a large number categories of engine uses including construction equipment, agriculture equipment, airport operations, locomotives, marine vessels, pleasure water crafts, and lawn and garden equipment. Recent studies have indicated that these source may contribute one fourth of the emissions in some areas. However, major uncertainties of these data exist and the studies are far from complete. The accuracy and emissions factors for these emission estimates must be improved. This includes exhaust emissions, evaporative emissions, and fuel losses during refueling.

Major Subtasks:

- Development of Improved Statistical Methods for Emission Estimations. Specific areas of concern include: 1) identification of the distribution of the data and the appropriate methods of combining these data with parameters having other distributions; 2) treatment of data which is recorded as being below the level of quantification or below the detection limit or which does not meet proprietary data disclosure standards; and 3) determination of the minimum number of measurements required for regression analysis. *(near term)*

- Assimilation of Compliance Data: The Federal regulations require that owners or operators of all major source in the U.S. obtain permits. The regulations also requires that permitted facilities submit emission data to prove they are in compliance with all requirements upon which they are paying the appropriate emissions fees. In addition, the proposed Enhanced Monitoring rules of the US EPA will require all sources which emit 30% or more of the amount which constitutes a major source to monitor continuously their emissions. The goal of this task is to develop a framework which will permit incorporation of these data into the national emissions inventory. The implementation of the Enhanced Monitoring rule is schedule for November 1995. *(near term)*

- Incorporation of Unaccounted and New Sources: Recent reviews have indicated that there are a large number of emission sources not included in the emissions inventories. The goal of this task is to identify such sources and estimate their emissions. The program is envisioned as a continuing one that will track new or changing sources. *(ongoing)*

- Establishment of Criteria for the Development of Emission Factors: Establish comprehensive guideline which can be used for the development of emission factors. The guideline will incorporate experimental design, quality assurance, and data criteria from which one can judge the validity of the emission factors. *(near term)*

- Enhancement of Stationary Area-Source Data Inventory: Identify and implement alternate and surrogate sources of data which can be used for stationary area source emission inventory development. Such data sources can include such diverse sources as trade organizations, market surveys, point of sales, and local fuel distribution systems. *(near term)*

- Conduct of Stationary Area-Source Data Surveys: The goal of this task is to conduct surveys for those sources where data is not directly available. The data from the surveys will be analyzed and incorporated in models to permit evaluation under differing economic conditions. *(ongoing)*

- Development of Semi-Mechanistic Emission Models: Develop semi-mechanistic emission models for a range of industries. This approach to emission factor determination is required to account for and anticipate technological improvements, changes of work practices, and economics. The models should be dynamic and flexible. They should incorporate an understanding of mechanisms that are important in determining emission factors. The methodologies should be applied to about 10 industries per year. *(ongoing)*

Relationship to NARSTO Science and Policy Questions: The emission inventories from stationary and point sources is very important to Science and Policy Questions 2, 3, 4, 5, and 6. As with the other sources emissions areas, this area has the strongest input to Questions 3 and 4. Questions 5 and 6 are directly involved with inventories; both point and area sources are major contributories.

Priority: 1. The stationary sources are one of the keys to the input to the ozone formation and good inventories are needed for predictions and control strategies.

Scheduling Requirements: Inventories are an important area of the overall ozone program and must continue to be updated; therefore, this work should continue for the entire NARSTO program.

Program Element E 4: Biogenic and Natural Emissions

Description: The goals of this element are 1) to develop natural source emission models that are capable of estimating NMOC emissions over seasonal cycles of foliage development which are spatially resolved to reflect plant distributions and agricultural activities and 2) to develop models of soil NO_x emission due to natural processes and agricultural operations.

Emissions of biogenic NMOC may constitute an important factor in ozone formation in many areas. Uncertainties in biogenic NMOC emission inventories are associated with a variety of factors such as plant species, phenology, meteorology, stress effects, and seasonal effects that can cause both dramatic short-term and long-term changes in emission rates. In addition, microbial decomposition of waste products may be a significant source of oxygenated NMOC. This latter effect, however, has not been examined in any acceptable detail. Summertime NO_x emission rates from fertilized agricultural fields may exceed anthropogenic NO_x emissions in some Midwestern states; however, the uncertainties of these estimates is roughly a factor of three. An improved understanding of biogenic NO_x emissions is needed, because much of North America is though to be NO_x limited for ozone formation.

Major Subtasks:

- Fundamental Investigations: To continue progress on this task, studies are needed that begin in the laboratory to understand the mechanistic basis for emissions; that extend into controlled plant chambers to look at environmental response of emissions to such factors as temperature, solar radiation, and moisture stress; that continue in the real environment to examine seasonal variations of emissions; and, then attempt above forest canopies to verify the leaf-level derived emission factors using ambient measurements. Historically, emission factor estimates have been limited to isoprene and monoterpenes. Additional measurements of oxygenated hydrocarbons need to occur and should be coordinated with the Measurement Team as the technology for making these difficult measurements continues to improve. In addition, advice from the Modeling Team is needed to understand what oxygenated compounds may be important for air quality analysis. Components within the emission model that need improvement and testing include emission factors (particularly for oaks and oxygenated compounds in general), land use characterization, and environmental effects. *(ongoing)*

- Biogenic and Natural NO_x Emissions**:** Field and laboratory studies are needed to estimate NO_x emissions from soils and from lightning. The area most needing attention appears to be NO_x emissions from fertilized soils. In particular, a comprehensive study using ambient and chamber measurements is needed to verify the emission fluxes that are currently being estimated within the air quality models. The emission models need additional work with improved emission factors (based on more chamber measurements), emission algorithms that account for mechanistic processes such as soil nutrient levels, temperature, and soil moisture, and land use characterization to include soil type distribution and fertilizer application rates. The role of lightning as a source of natural NO_x to the troposphere should also be considered. *(ongoing)*

- Other Natural NMOC Emissions: Screening studies are required to assess the importance of NMOC emissions from disturbed vegetation such as lawn mowing, timber and crop harvesting, and biomass burning, microbial decomposition, and geogenic sources. Emission models are to be developed and evaluated for those sources determined to be significant. *(ongoing)*

- Long-Term Changes in Natural Emissions: Changes in climate or land use may have a significant effect on natural NMOC and NOx emissions. Research is needed to assess potential changes and their impact on emissions. *(ongoing)*

- Testing Biogenic Source Models: Current biogenic emission models extrapolate leaf level VOC or small scale NOx measurements to landscapes of several hundred square kilometers or more (e.g. county level). In order to test validity of such extrapolations, simultaneous measured emission factors and surface fluxes at scales ranging from 6 cm^2 to over 2500 km^2 were made. Techniques employed include environmentally controlled leaf cuvette enclosures, branch or whole-tree chambers, canopy micrometeorological flux measurements, and mixed layer and atmospheric box model calculations. This is performed over diurnal and seasonal cycles to see if biogenic emissions measured at large scale levels compare with leaf level extrapolations used in models such as BEIS and BEIS2. Meteorological and ecological variables are measured and incorporated into these studies of model validation. *(ongoing)*

Relationship to NARSTO Science and Policy Questions: Biogenic and other types of natural emissions are major concerns to NARSTO. As with the mobile and stationary sources, Questions 3 and 4 are very important. Question 2 is also important, with Question 6 less so. Control of many of these natural sources is generally impractical; thus Question 5 is of little significance here.

Priority: 1. Since only a few established inventories currently exist and the magnitude of the input from some of the natural sources may be very important to the overall burden of the ozone precursors, the work in this area must continue.

Scheduling Requirements: As with stationary-emission research this area of natural emissions should continue as long as NARSTO is active.

Program Element E 5: Independent Assessment of Emission Inventories

Description: The goal of this element is to corroborate emission inventories with independent estimates of emissions and evaluate the effectiveness of reformulated gasoline, enhanced inspection and maintenance, RSD measurements, and other control programs to verify emissions model estimates.

Large uncertainties often exist in emission inventories. Ambient air measurements are needed to confirm the levels of ozone precursors in these inventories. Approaches for independent assessments of emission inventories include: 1) Tunnel studies and other roadway measurements; 2) spatial and temporal comparisons of ambient and emission inventories of $NMOC/NO_x$ and CO/NO_x ratios; 3) comparison of long-term trends in ambient air pollution levels and concentration ratios with emission inventory trends; and 4) tracer and flux measurements. Previous studies have focused on on-road mobile sources and biogenic sources with little attention to non-road mobile sources. However, the latest non-road emission estimates have major uncertainties and these uncertainties will be translated to uncertainties in the overall inventories. The introduction of reformulated gasolines and the implementation of enhanced inspection and maintenance programs provide unique opportunities to observe and measure cause and effect relationships between emissions and atmospheric concentrations of pollutants.

Major Subtasks:

- Analyze Existing Data: Analyze the existing data to assess current emission inventories in urban areas of North America. Compare a variety of approaches, including tunnel and remote sensing studies, ambient pollutants concentration ratio comparisons, and receptor modeling. *(near term)*

- Evaluate and Improve Assessment Techniques

- Field Studies: Conduct field studies before and after implementation of major control programs in different areas of North America in order to compare the observed effects on air quality with emission inventory projections. *(near term)* Also design and execute field studies to evaluate the accuracy of stationary source NMOC emission inventories. Possible approaches include receptor modeling, "tracers of opportunity," upwind downwind measurements, and other techniques that rely on ambient data. Test the approach in one city then after testing and validation, expand to other cities with different source characteristics. *(near term)*

- Tunnel Studies: Conduct periodic tunnel, street canyon, and other special roadway studies to reconcile mobile source emission inventories and to track progress. *(long term)*

- Uncertainty Analysis: Analyze the results from the above studies to set priorities for further work to reduce the most important uncertainties in emission inventories. *(long term)*

- Upgrade Measurement Systems: Upgrade the hydrocarbon and NOx channels for the RSDs and other roadway measuring systems. Continue to validate the RSDs under a variety of vehicle operating conditions. *(near term)*

- Whole Gasoline Inventories: Determine the sources of the large amounts of the uninventoried whole gasoline found in ambient air. *(near term)*

Relationship to NARSTO Science and Policy Questions: The research under this element is very important to Questions 5 and 6. This element also has an impact on Questions 2, 3, and 4.

Priority: 1. Several components of this element are very important to the overall NARSTO program.

Scheduling Requirements: Several of the subtasks in this element are currently ongoing and should be continued until completed. Other subtasks, such as tunnel studies, should be scheduled when sites and funding are available. Other studies that are coupled to and funded by other programs, such as the use of remote sensing for mobile source inventories and emission-factor work, should be scheduled as planned by the funding groups.

Program Element E 6: Emission Projections

Description: The goal of this element is to project the effects of future activity and alternative controls on emission estimates.

The US EPA's Economic Growth Analysis System (EGAS) projects region economic growth for each of the 30 current multi-state ozone nonattainment areas in the United States. The EGAS uses macroeconomic forecasts as a basis for developing the regional economic growth forecasts. The MultiProjections System (MPS) is another US EPA product that adjusts baseline emission inventories for emission controls and for growth in the regional economy forecasted by EGAS. Both of these systems need to be maintained.

Major Subtasks:

- Develop regional economic models for ozone nonattainment areas, including maintenance and annual forecasts. *(ongoing)*

- Maintain existing US EPA forecasting capability for stationary sources. *(ongoing)*

- Develop emission control reduction factors for alternative emissions control systems and keep the file updated as new technologies are developed. *(ongoing)*

- Develop emission control technology degradation factors for alternative technologies. *(ongoing)*

- Develop interfaces for integrating emissions projection models into the MODELS-3 modeling system. *(ongoing)*

Relationship to NARSTO Science and Policy Questions: This element deals with the effects of future activity and alternative controls on emission estimates, and therefore has direct input to Questions 4, 5, and 6.

Priority: 1. All the major subtasks in this element are currently ongoing The important of these subtasks to NARSTO are obvious.

Scheduling Requirements: As stated above, all the major subtasks in this element are ongoing and therefore the scheduling is governed by the programs funding these tasks.

References

1. NARSTO *Research Strategy and Charter*. November, 1994 (Available in electronic form on the NARSTO Web site <http://narsto.owt.com/Narsto/>)

Appendix

Summary of NARSTO Science and Policy Questions

NARSTO Science Questions

1. **How can we determine the current trends in ozone concentrations and exposures on local and regional scales in North America?**

   1.1 What measurements, monitoring networks, and analyses are needed to establish ozone trends and exposures?

   1.2 What measurements, monitoring networks, and analyses are needed to establish regional and local precursor trends in North America?

   1.3 What refinements and developments are needed in instrumental methods to enable routine monitoring of ozone, its precursors, and meteorological parameters?

   1.4 What are the uncertainties associated with these measurements, networks, and analyses?

   1.5 How can the monitoring data be archived so that they are easily accessed and incorporated into analytical tests of ozone distribution and trends?

   1.6 Can the effects of meteorological variability on the trends of ozone and its precursors be distinguished from the effects of precursor emissions on these trends?

2. **How can we better understand, further identify, isolate, and explain the fundamental physical, chemical, and meteorological processes responsible for ozone accumulation on local and regional scales in North America?**

   2.1 What intensive field studies are needed to extend knowledge about these processes? Where should these be conducted?

   2.2 What laboratory studies are required to increase understanding of the gas-phase and heterogeneous chemical processes?

   2.3 How can the data associated with these measurements be archived so that they are easily accessed and incorporated into analytical tests of our understanding and the processes that control ozone accumulation?

   2.4 What modeling and diagnostic data analyses are needed to further understanding of these processes?

2.5 What refinements and developments are needed in instrumental methods to enable measurement of key chemical species, such as precursors, radical intermediates, and VOC-oxidation products?

2.6 How can we enhance and further build upon the existing science infrastructure in North America for performing tropospheric ozone research?

3. How can we incorporate and use the evolving scientific understanding of relevant processes in diagnostic and prognostic tools (methods and models) for explaining observed phenomena and estimating impacts of future perturbations of independent variables, such as emissions and meteorology?

3.1 Can we establish quantitative methods for estimating uncertainty levels associated with these methods and models?

3.2 How do we use the estimates from the methods and models in conjunction with socioeconomic analysis tools for impact assessments?

4. How do we evaluate and periodically assess the relative contributions VOC's and NO~ , and their controls, to ozone accumulation on local and regional scales in North America?

4.1 Is the production of ozone limited by the availability of VOC's or NO~?

4.2 Does this limitation change from day to day for a given area or region, or from area to area on a given day, based on changes in meteorology and emissions?

4.3 What data are required, and what precision and accuracy are needed to evaluate and apply diagnostic and predictive methods and models for ozone assessment and control strategies?

4 4 What portion of ozone near the surface can be attributed to natural intrusion from the stratosphere? Does this change with meteorology, location, and season?

4.5 Can we quantify the contribution of urban areas to rural and region concentrations, and conversely, can we quantify the rural/regional photochemical impact on particular urban areas?

4.6 Can we determine the emission fluxes of key ozone precursors through field studies or other measurement programs, and reconcile ambient measurements with emission-inventory estimates of fluxes?

4.7 What portion of the ozone precursors are from natural (biogenic) sources and how will these emissions change with meteorological variability, land-use, and climate-change perturbations? What are the biological factors controlling the rates of VOC and NO~ emissions?

5. What technologies and approaches are most cost-effective in achieving and maintaining ozone-precursor reductions and in reducing ozone concentrations and exposures?

NARSTO Policy Questions

1. For a given area, how do we determine whether an ozone problem exists, and how can we determine its severity?

1.1 What is the best way to characterize the nature of the problem? Are the forms of existing air-quality standards appropriate metrics to apply for this purpose?

1.2 Under potential alternative forms of an ambient air-quality standard for ozone (both acute episodic and chronic longer term type standards) will the perception of an ozone problem change? In what ways?

2. For an area considered to have an ozone problem, what portion of the problem is essentially irreducible (based on such factors as natural emissions of ozone precursors and stratospheric influx of ozone) and what portion of the ozone problem is potentially controllable (based on anthropogenic precursor emissions to the troposphere)?

2.1 For that portion that is potentially controllable, what part of the problem is due to locally generated ozone and precursors, and what part is due to sources outside of the area (regional transport)?

2.2 What are the principal anthropogenic sources of precursors and what options are available for their control?

3. Do we have evidence that existing control measures are having an impact?

3.1 Can we verify that existing emission-control programs for precursors have influenced ambient ozone concentrations? What demonstration will be made to establish the effectiveness of these programs for ozone control? How do the demonstrated changes in ozone compare to the anticipated changes?

3.2 Can we verify that existing source emission-control programs have decreased ambient concentrations of ozone precursors (VOC, NO~ and carbon monoxide)? What demonstration will be made to establish the effectiveness of these control programs on precursors? How do the demonstrated changes in precursors compare to the anticipated changes?

4. What are optimal approaches for reducing current and future high ozone concentrations for a given area considered to have an ozone problem?

4.1 What are the current predictions, and heir associated uncertainties, of existing policies on ozone and other related pollutants?

4.2 Will adequate scientific understanding that links the causes and distribution of ozone pollution, particularly with regard to model predictions and emission inventories, be available on the timetable of the US Clean Air Act amendments?

4.3 What are the risks and cost-benefit implications associated with these emission-control approaches? What is the technical, economic, social, and political feasibility of reducing tropospheric ozone?

4.4 What periodic assessments leading to "mid-course" adjustments in control programs are indicated, and when should these assessments be performed?

4.5 Will potential forms of ambient air-quality standards for ozone require a change or redirection of emission-control strategies? Should nontraditional air-quality management approaches be considered?

5. What is the magnitude and impact of transnational-boundary transport of ozone and its precursors?

6. How can the relevant science and scientific uncertainties be communicated meaningfully to the air-quality management and policy communities? How can tropospheric ozone science be translated into actionable knowledge (changes in activity patterns) by the public?