1) **RfP Title:** Volatile Organic Compounds (VOC) and Reactive Nitrogen Compounds: Budgets and Contributions to Transboundary Ozone Pollution

2) **RfP Number:** AC-00-06

3) **TIP:** Atmospheric Chemistry Technical Implementation Panel (AC TIP)

4) **INTRODUCTION AND DESCRIPTION OF RESEARCH PROJECT:** The Atmospheric Chemistry Technical Implementation Panel (AC TIP) represents one of ten priority research areas, each represented by a Technical Implementation Panel (TIP), identified under the American Chemistry Council's (the Council) Long-Range Research Initiative. The AC TIP identifies research needs for the chemical industry related to atmospheric chemistry, drafts RfPs, and sponsors research projects.

The project described below will enable the chemical industry to better understand the role of its emissions of ozone precursors in regional and global pollution, particularly as related to transboundary impacts of oxygenated hydrocarbons and other VOC byproducts of the chemical industry.

**Background**

Transboundary air pollution includes the phenomenon of primary pollution from one region affecting atmospheric ozone levels in another region. Transboundary air pollution is both a domestic and international issue as air quality regulations are modified and international protocols cause countries to evaluate their export of pollutants. When ozone precursors (e.g., nitrogen oxides or NO\textsubscript{x}, carbon monoxide or CO, VOCs) and ozone are transported by convection from the boundary layer in the atmosphere to the free troposphere (i.e., 2-12 km in mid-latitudes), these compounds can be transported over long distances. If ozone continues to form photochemically during transport, ozone concentrations in air masses may increase. The northeastern U.S. and maritime Canada are exit regions for ozone and ozone precursors, allowing pollution to travel east over the entire north Atlantic Ocean. Under certain meteorological conditions, North American emissions have been detected in the free troposphere in air samples from European research in Portugal, Ireland, and the United Kingdom.

The free troposphere (FT) over eastern North America and the north Atlantic Ocean has been probed experimentally by several aircraft missions with highly sensitive instrumentation for reactive nitrogen species, reactive hydrogen, ozone, CO, VOCs, and oxygenated intermediate species (OIS). Examples of aircraft missions that produced publicly available data sets include the Subsonic Assessment Ozone and Nitrous Oxides Experiment (SONEX), the Pollution in North Atlantic Air Traffic (POLNAT), the North Atlantic Regional Experiment (NARE), among others. Regional- and global-scale models have been applied to these observations to analyze aspects of ozone and reactive nitrogen chemistry. In some cases, "labeled" NO\textsubscript{x} and NO\textsubscript{y} have been used to attribute sources to lightning, aircraft, and surface pollution. However, no evaluations of observed OIS, reactive nitrogen species, or VOCs have been performed with models to determine the anthropogenic-natural partitioning of sources. The Council would like to enhance the value of existing data sets and model analyses by supporting model runs and diagnostics aimed at this important missing information.

Documented models with appropriate chemical mechanisms and constrained with publicly available data sets of atmospheric trace gas measurements in the FT are the desired tools for this research. Published simulations might form the basis of this research, with new work required for the requested diagnostics and analysis.

**Research Objectives**

The objective of this project is to account for aircraft and related observations of critical oxygenated species that influence ozone formation in the FT over eastern North America and the north Atlantic Ocean. These critical species include:
Ketones
Aldehydes
NOx
Organic nitrates
Total reactive nitrogen
Peroxides
Organic acids
Nitric acid
Ozone

A sufficiently evaluated large-scale 3-D chemical transport model capable of process analyses should be coupled to a detailed chemical mechanism appropriate for tracking the species of interest. The chemical mechanism should include tagged species for tracing sources of biogenic, anthropogenic, elevated point, and aircraft emissions of critical oxygenated species. The coupled models should be run in 4-D data assimilation mode using available meteorological data for the observation period of the aircraft mission so that comparisons can be made between the model predictions and the observations of these critical species during aircraft missions.

The AC TIP is particularly interested in observation data from the SONEX aircraft missions, which are available on the Internet at http://telsci.arc.nasa.gov/~sonex/. Other publicly available data sets, such as those from POLNAT and NARE, may also be used. The 3-D model-derived mass budgets for each species should then be obtained, partitioned as follows:

- Transport to the FT from surface biogenic sources;
- Transport to the FT from surface anthropogenic sources;
- Transport to the FT from elevated point sources;
- Transport away from the FT domain of concern;
- In situ chemical loss; and
- In situ chemical production from local sources (i.e., lightning, aircraft).

Based on the simulated budgets, tracers should be identified that can tag the origin of various air masses in the FT. In addition, the relative contribution to FT ozone formation from all sources should be diagnosed.

The respondent should describe the suitability of the transport, chemistry, and emissions sources to be used. Whenever possible, the ability of the model to explain different aircraft data sets should be analyzed. Process analysis algorithms should be developed to enable quantification of the necessary budgets. Finally, sensitivity of results to boundary conditions, convective parameterization assumptions, and chemical mechanism assumptions should be explored, and corresponding uncertainties quantified.

5) SPECIAL REQUIREMENTS: A goal of the Long-Range Research Initiative is to share broadly the results of funded projects. Thus, results are expected to be submitted for publication in peer-reviewed journals and/or presented at scientific meetings, conferences, and/or symposia within six (6) months of completing the research. Otherwise, the Council will publicly release the Principal Investigator's final report. All proposals should include costs for preparing manuscripts for submission of results to peer-reviewed journals. Semi-annual status reports and annual financial reports are required for all funded research projects.

6) ELIGIBILITY: Proposals may be submitted by any domestic or foreign for-profit or non-profit organization, public or private, such as universities, colleges, hospitals, laboratories, or units of state and local governments.

7) PARTNERSHIP OPPORTUNITIES: The respondent is expected to have existing funding for related work from an institution other than the Council. This will enable the Council to efficiently leverage limited funds and create fruitful partnerships with other agencies, such as NASA, NOAA, and NSF.

8) FUNDS AVAILABLE/PROJECT DURATION: A single award will be issued for this project. Total cost for this project should be in the range of $50,000 - $75,000 per year. The project costs are expected to be commensurate with project scope. Investigators should include in their preliminary proposal funds necessary to participate in necessary travel and to complete the status reports and preparation of manuscripts for submission of results to peer-reviewed journals and/or scientific conferences. Publication would include making any model codes available to the public.
Projects are expected to begin immediately upon execution of a contract. The duration of the project is expected to be commensurate with the goals of the project. Two years is expected to be the maximum duration, but longer projects will be considered. Projects may require annual renewal.

9) REVIEW OF PROPOSALS: All proposals received in response to this RfP will be reviewed for completeness and responsiveness. Incomplete or non-responsive proposals will be returned to applicants without further review.

Proposals that are complete and responsive will be peer reviewed for scientific merit by scientists from outside of industry. Proposals that receive a rating of "Excellent" or "Very Good" for scientific merit will be forwarded to the Council’s AC TIP for further review and award recommendations. The AC TIP is composed of scientists from industry, government, and academia. The Council’s Strategic Science Team, which oversees TIP activities, will approve award recommendations.

10) REVIEW CRITERIA FOR SCIENTIFIC MERIT: The following criteria will be used by peer-reviewers to evaluate full proposals:

- Scientific merit
- Scientific feasibility
- Technical feasibility
- Reputation of institution/investigator
- Compatibility with known skills of investigator
- Management of QA, animal care/human subject ethical considerations

In addition to using the above criteria, the AC TIP will also consider the following criteria when evaluating full proposals for funding:

- Consistency with the TIP research plan
- Quality of proposed milestones/timeline
- Appropriateness of the budget
- Use of external collaborator/leveraging

11) PRELIMINARY PROPOSALS: Submission of preliminary proposals is required. Preliminary proposals must be received by the Council no later than April 6, 2001 and must be no longer than 5 pages in length. Preliminary proposals must be prepared using the Preliminary Project Proposal Form (Attachment A). Biographical information (no longer than two pages per person) about the Principal Investigator and all other key personnel, including subcontractors and consultants, should also be submitted.

One unbound original and ten (10) copies of the preliminary proposal should be sent to the address indicated under submission of full proposals.

Preliminary proposals will be evaluated for scientific merit, relevance to the AC TIP’s research plan, and cost-effectiveness by members of the AC TIP. Investigators will receive a letter by April 20, 2001 either encouraging or discouraging submission of a full proposal.

12) AWARD CRITERIA: The criteria that will be used in making awards include: receipt of a sufficient number of proposals of adequate scientific merit, as determined by peer review; high technical merit; relevance of proposals to the priorities outlined; availability of funds; and program balance.

13) SUBMISSION OF FULL PROPOSALS: Full proposals must be received by the Council no later than June 15, 2001 and must be no longer than 8 pages in length, not including appendices and attachments. All proposals must be prepared using (or mimicking) the Full Project Proposal Form (Attachment B). Curricula Vitae for the Principal Investigator and all other key personnel, including subcontractors and consultants, should also be submitted. One unbound original and ten (10) copies of the proposal should be sent to the following address:

Cheryl Morton
American Chemistry Council
1300 Wilson Blvd.
Arlington, VA 22209
The proposal must be signed by an individual who is authorized to sign on behalf of and bind your organization to the proposed rates (including indirect costs). The Council must be notified if there is a change in the proposed key personnel and/or Principal Investigator. In the event of any such change in key personnel and/or the Principal Investigator, the Council reserves the right to modify the agreement.

Summary of Timeline for Proposal Submission, Review & Award

<table>
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<tr>
<th>Event</th>
<th>Timing</th>
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<tr>
<td>Preliminary proposal due to the Council</td>
<td>Deadline of April 6, 2001</td>
</tr>
<tr>
<td>Preliminary proposal reviews sent to</td>
<td>April 20, 2001</td>
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<tr>
<td>investigators</td>
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<tr>
<td>Full proposals due to the Council</td>
<td>Deadline of June 15, 2001</td>
</tr>
<tr>
<td>Award Notification</td>
<td>Approximately July 27, 2001</td>
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14) PROPOSAL PROCEDURES: Each applicant will receive a copy of the Full Project Proposal Evaluation Form (Attachment C) and Final Project Proposal Selection Form (Attachment D). Successful applicants will receive an award letter from the Council on approximately July 27, 2001.

15) TYPE OF AWARD: The form of award under the Long-Range Research Initiative is a contract between the American Chemistry Council and the research institution.

16) INQUIRIES: The American Chemistry Council’s web site (http://www.americanchemistry.com) contains general information about the Health and Environmental Effects Research Initiative. Questions regarding this RfP should be directed to Allison Benjamin, American Chemistry Council Consultant TIP Staff Executive, at (703) 934-3814 or AllisonBenjamin@ICFConsulting.com.
ATTACHMENT A

Preliminary Project Proposal Form

American Chemistry Council RfP No:

Project Title:

Research Institution/Department:

Principal Investigator/Title:

Preliminary Research Plan:
   a. Key Objectives

       b. Thoughts on Research Approach/Hypotheses

       c. Preliminary Ideas on Research Design/Methods

Preliminary Milestones and Timelines:

Preliminary Estimate of TOTAL Costs (Direct + Indirect):

Collaborators:
Prior Relevant Studies by Investigator/Institution:

QA/Animal Care/Human Subject Review Statement:

Safety/Environmental Considerations Statement

Additional Comments:

Principal Investigator: ______________________________ Date: ___________
ATTACHMENT B

Guidelines for Full Project Proposal

The Full Project Proposal should include sufficient information to allow evaluation of the project, independent of any other document. Guidelines for completing key portions of this document follow:

Research Plan:

a. Key Objectives: List the major objectives, being as specific as possible in describing what the proposed research is intended to accomplish.

b. Research Approach/Hypotheses: State the hypotheses to be tested, sketching the background leading to the present proposal. Critically evaluate the existing knowledge and specifically identify the gaps that the project is intended to fill. State concisely the importance and health relevance of the research by relating the specific aims to the major objectives listed above.

Major Milestones and Timelines:

Identify the key project activities and major milestones, providing a sequence and timeline for each. Use of a Gantt Chart format is recommended, if appropriate. Some of the major milestones should identify manuscripts or final reports as deliverables. The timeline should include activities in out-years if the project is a multi-year effort.

Resources:

Provide a detailed budget for personnel, supplies, equipment, contracted services, travel, etc. If the project has an external collaborator (as listed in the next section), identify the amount of funding provided. All costs related to institution overhead and indirects, sub-contracted services, such as assay analyses, pathology reports, etc. should be included. Costs for preparing reports and publications should be included.

Collaborators:

Identify any external individuals on the project, their key responsibilities, and the organization with which they are affiliated.

QA/Review Process for Animal Care, Human Subjects and Environmental Protection:

Provide the following information, as applicable:

A. Describe the Quality Assurance organization, if any, in your institution. Discuss the Quality Assurance measures taken to ensure the integrity of the data obtained in the proposed activities.

B. Describe the institution’s review process to identify and address ethical issues related to animal care or human subjects as well as those for environmental protection. If your project involves animal care, please describe the institution’s processes to guard the welfare of the animal(s) and adhere to all relevant laws and rules. If your project involves human subjects, please describe the institution’s processes for human subjects research approvals. Please note that if your project involves human subjects research (as defined in 45 C.F.R. 46.102(f)), the Council will require a copy of an approved Institutional Review Board package after the award is made and before research on human subjects begins.
ATTACHMENT C

Full Project Proposal Evaluation Form

American Chemistry Council RfP No.:

Project Title:

Comments on the scientific merit and feasibility of Full Project Proposal:

Overall Assessment of Proposal:
? Unsatisfactory (1) Satisfactory (2) ? Good (3) ? Very Good (4) ? Excellent (5)

Reviewer: ___________________________________           Date:  __________
Title:  ______________________________________
Institution: ____________________________________

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**Final Project Proposal Selection Form**

American Chemistry Council RfP No:

<table>
<thead>
<tr>
<th>Project Title:</th>
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Research Institution/Department:

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<th>Principal Investigator/Title:</th>
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<tr>
<th>Scientific Merit:</th>
<th>? High</th>
<th>? Medium</th>
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<tr>
<td>Scientific feasibility:</td>
<td>? High</td>
<td>? Medium</td>
<td>? Low</td>
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<tr>
<td>Consistency with TIP research plan:</td>
<td>? High</td>
<td>? Medium</td>
<td>? Low</td>
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<tr>
<td>Reputation of institution/investigator:</td>
<td>? High</td>
<td>? Medium</td>
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<td>? High</td>
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<td>? High</td>
<td>? Medium</td>
<td>? Low</td>
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<tr>
<td>Responsiveness to TIP inputs:</td>
<td>? High</td>
<td>? Medium</td>
<td>? Low</td>
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<td>(two-step process only)</td>
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Gate decision and rationale:

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<tr>
<th>? Award Contract</th>
<th>? Reject</th>
<th>? Hold</th>
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</table>

Other gatekeeper comments:

TIP chair: __________________ Date: __________________

SST Approval: __________________ Date: __________________