

# DRAFT

## **Task Subgroups 1, 5, 7 and 9** Leader Jay Olaguer [epolaguer@dow.com](mailto:epolaguer@dow.com)

### **I. Short-Term Research Priorities for Regional Reactivity Assessment**

The following list consists of projects that can be conducted relatively inexpensively and quickly (i.e., within 6 months to 1 year), but which can deliver important results yielding guidance on how to further proceed in developing a reactivity-based strategy.

- A. Develop model criteria and appropriate scenarios for general reactivity assessment.
  - 1) Identify short-term criteria for evaluating adequacy of existing regional and urban models -e.g., based on EPA criteria or model/ measurement inter-comparisons (0.1 person-years).
  - 2) Identify existing model runs satisfying criteria that can be re-run to test the effects of compositional changes on ground-level ozone (0.1 person-years).
- B. Use existing models to evaluate the utility of a VOC exemption scheme.
  - 1) Analyze a hypothetical scenario using model runs identified in A-2 in which ethane is substituted for all VOC emissions in two distinct regions (e.g., California vs. OTAG). Note the resulting impacts on both the local and large-scale regional environments using appropriate metrics (peak, exposure-weighted, etc.). This will allow us to conclude whether or not significant ozone impacts can be obtained with large, though unrealistic, VOC composition changes (0.5 person-years).
  - 2) If the results of B-1 are significant, repeat the experiment with other compounds (e.g., methane, acetone, etc.) and compare resulting impacts. Note any correlation of results with predictions based on existing reactivity scales (0.3 person-years).
- C. Assess effects of large-scale reactivity-based substitutions on regional air quality using existing models.
  - 1) Use the model runs of B-1 and B-2 to determine the “zone of influence” of VOCs. This can be done by changing the VOC composition (but not total VOC mass) in individual urban airsheds (rather than in all urban airsheds simultaneously) in a regional model and noting where significant changes in ground-level ozone occur (0.6 person-years).

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- 2) Analyze the changes in the reactive nitrogen and radical budgets induced during the experiment of C-1 to see how sensitive these budgets are to both local and remote changes in VOC emissions. If significant regional changes in the reactive nitrogen budget occur, determine the change in both the “total residence time” and “ozone chain-length” of a typical reactive nitrogen atom (0.4 person-years).

## **II. Intermediate Research Priorities for Regional Reactivity Assessment**

The following list consists of projects which depend on the results of short-term research and which require about 1 year to complete.

- A. Use existing models to evaluate exemption standard.
  - 1) If results of I-B are significant, adopt plausible substitution scenarios corresponding to various VOC exemption options and appropriate metrics to determine the merits and demerits of each option using the model runs identified in I-A (1.0 person-years).
  - 2) Apply sensitivity and uncertainty analysis to evaluate the robustness of the results of II-A-1 (1.0 person-years).
- B. Assess effects of large-scale reactivity-based substitutions on regional air quality using existing models.
  - 1) Determine appropriate “reactivity metrics” for application to regional scale based on results of I-C (0.1 person-years).
  - 2) Evaluate regional reactivities of representative VOCs using the model runs identified in I-A (0.8 person-years).
  - 3) Compare heuristically expected benefits of substitution scenarios of II-A using the reactivity scale of B-1 and B-2 with actual simulated impacts (0.1 person-years).
- C. Develop model criteria for reactivity assessments.
  - 1) Revisit the 1987 model scenarios used in the 1995 SCAQMD SIP using the recently corrected mobile source (EMFAC2000) emissions inventories, and then simulate the O<sub>3</sub> response using emissions inventories for 1997. Modeling could be performed using a variety of models, such as the existing 1987 models and scenarios or new models and scenarios currently being developed for the 1997 SCOS. This study will be useful for assessing our confidence in the usefulness of models for evaluating the effects of reactivity-based substitution strategies, to inter-compare the capabilities of different models, and to set criteria for future model assessments (1.0 person-years).

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## III. Long-Term Research Priorities for Regional Reactivity Assessment

The following list consists of projects which depend on the results of short-term and intermediate research, or which require more than 1 year to complete.

- A. Develop appropriate scenarios for general reactivity assessment.
  - 1) Determine where (urban or rural) and when (spring or summer) exceedances of the 1-hour and 8-hour ozone standards can occur from monitor data (e.g., PAMS).
  - 2) Characterize the meteorological conditions both at the exceedance sites and in the surrounding large-scale environment using a) observations at ground level, b) rawinsonde, aircraft, and satellite data, and c) NMC analyses.
  - 3) Characterize the chemical composition and ozone precursor budgets of the atmosphere at the exceedance sites and in the surrounding large-scale environment using Observationally Based Models (OBMs).
  - 4) From previous results, determine the essential meteorological and chemical features associated with typical exceedances.
  - 5) Select exceedance scenarios with identified essential features.
- B. Develop model criteria for reactivity assessments.
  - 1) Determine the spatial extent and resolution required to model exceedance scenarios developed in III-A.
  - 2) Identify which chemical mechanisms have sufficient detail to account for inferred budgets of reactive nitrogen and hydrogen in exceedance scenarios.
  - 3) Determine appropriate level of representation of sub-grid scale transports.
  - 4) Determine appropriate treatment of boundary conditions.
- C. Use existing models to evaluate exemption standard.
  - 1) Using exceedance scenarios of III-A and a regional model satisfying III-B, analyze the local and large-scale impacts of substitution scenarios of II-A. Explain differences in results of II-A and III-C in terms of model processes.
  - 2) Use sensitivity and uncertainty analysis to evaluate robustness of results.

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- D. Assess effects of large-scale reactivity-based substitutions on regional air quality using existing models.
- 1) Use the model and exceedance scenarios of III-C to evaluate regional reactivities of representative VOCs using the metrics of II-B .
  - 2) Compare heuristically expected benefits of substitution scenarios adopted in III-C using reactivity scales with actual simulated impacts.
  - 3) Apply uncertainty analysis by repeating D-1 and D-2 for a range of input parameters.
  - 4) Repeat D-1 and D-2 for an attainment scenario.

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**DRAFT**  
**Technical Elements**  
**Outlining Scope & Cost**  
**For Assessing Where To Consider Reactivity**  
**Task Subgroup 2**  
**Leader Dan Baker [dcbaker@equilon.com](mailto:dcbaker@equilon.com)**

- I. Analyze Existing Monitoring Data [**\$85K**]
  - A. Identify various data-driven formulation methodologies, indicators, OBMs, etc. (note limitations, independent evaluations, etc.), either stand alone, or when used more holistically in a conceptual model [**Short Term, \$5K – align work with CMA ARTG project**]
  - B. Collect existing studies that exploit these various methodologies [**Short Term, \$10K – align work with CMA ARTG project**]
  - C. Summarize results (extreme limitations, intermediate/uncertain) [**Short Term, \$5K – align work with CAM ARTG project**]
  - D. Critique existing studies (spatial/temporal scales and relevance to both local and transport issues, method inter-comparisons, vintage of data) [**Short Term, \$5K – align work with CMA ARTG project**]
  - E. Initiate new studies to fill holes, update, or address weaknesses (besides chemical indicators, consider physical indicators per actinic flux, cloud cover, others) [**Longer Term, \$40K – align work with CRC A-36**]
  - F. Collect monitoring data on the composition of the atmosphere, from past to present (i.e., particular interest in California reformulated fuels) [**Short Term, \$15K – align with possible studies in SCAQMD region**]
  - G. Analyze for compositional changes and ozone changes [**Short Term, \$10K**]
  - H. Update, if needed, the ROG composition used in smog chambers [**no additional cost**]
  
- II. Analyze Existing Modeling Results That Overlap With I. [**\$55K**]
  - A. Collect existing studies that used model output (versus monitoring data) to feed into various methods in I. – look at local sensitivities, where it makes sense to do so, use model to comment on global sensitivities [**Short Term, \$10K – couple with II B and C**]

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- B. Compare results from methods driven by monitoring data versus model output (base case modeling) **[see A]**
  - C. Critique existing studies (spatial/temporal scales – local vs. regional, 1 hr vs. 8 hr, duration simulated, vintage of modeling) **[see A]**
  - D. Initiate new studies to fill holes, update, or address weaknesses (use existing model output as input for I.) **[Longer Term, \$45K]**
- III. Analyze Existing Modeling To Map Proposed Control Strategy **[\$45K to \$155K – look for alignment with modeling task group]**
- A. Review SIP and other regulatory modeling **[Short Term with respect to already reviewed SIP submittals, \$5K – piggy-back on work with Dupont’s project. Longer Term with respect to latest SIP submittals, \$35K – broad enough topic to seek co-funding]**
  - B. Map proposed control strategy approach to attainment (consider importance of path to attainment, as well) **[Short Term, \$25 – align work with NARSTO reviews. Longer Term, \$60K – update where needed]**
  - C. Compare both mappings and contrast future attainment with results from I. **[Short Term, \$15K. Longer Term, \$15K – update with latest SIP submittals]**
- IV. Conduct Controlled Studies To Challenge/Verify Methodologies From I. **[\$100K]**
- A. Review smog chamber studies that included ambient air collection (consider the latest work planned for Mexico City) and make recommendations, including a designed study, for empirically validating methodology in I A. **[Short Term, \$25K]**
  - B. Conduct smog chamber study (piggy-back on, and incorporate any ideas in, planned field studies – CCOS2000, TX2000, etc.) **[Short Term if timing permits or Longer Term with future field studies, \$75K]**
  - C. Include chemical regimes representative of base case years and future attainment years **[attempt to design into the study at no additional cost]**

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*(Items V and VI are broader than the RRWG's charter. Some Task Group 2 members expressed a willingness to consider limited support of V if approached for co-funding; Task Group 2 would defer to the modeling Task Group to consider a similar position with respect to VI.)*

- V. Identify Additional Requirements For Analytical Techniques
  - A. Support emerging ambient data analytical techniques that advance value of methodologies from I.
  - B. Support efforts to make sophisticated analytical techniques more routine when this enhances the value of methodologies from I.
- VI. Support Modeling Studies – Efforts That Attempt to Reconcile/Unify Models & Observations
  - A. Support inserting suite of “probing techniques”<sup>1</sup> and methodologies from I. into modeling systems (automate II. A.)
  - B. Support comparison of “probing techniques” and methodologies from I. (across episodes, domains, chemical mechanisms, transport mechanisms, alternate control strategies)
  - C. Support development of model guidance for exercising “probing techniques” and methodologies from I. (extend model guidance to reactivity issues)

1. “probing techniques” include apportionment techniques (for emission sources, or for processes, or for reactions) and sensitivity techniques (local or global) – like Process Analysis, Direct Decoupled Method, others,

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# Atmospheric Availability and Environmental Fate Task Subgroup 3

Leader Jon Kurland [kurlanjj@ucarb.com](mailto:kurlanjj@ucarb.com)

### I. Short-Term Proposal - Workshop on Combining Environmental Fate and Air Quality Modeling

**Purpose:** To bring together researchers to educate us on the state of the science of environmental fate modeling and on incorporation of environmental fate (partitioning) into air quality models (emission and fate). A panel discussion following the presentations would help define the requirements for determining the importance of environmental fate as well as reactivity on ozone-forming potential of VOC. We could then take this knowledge and draft an RFP for a state-of-the-science report.

#### **Description:**

Duration: One and a half days to 2 days

Date: June 6-7 or September

Place: Near EPA in North Carolina, Charlotte, Raleigh-Durham

Sponsorship: RRWG

Organization: RRWG Subgroup 3 with assistance from CMA

Participants: The usual RRWG members, invited experts on environmental fate and air quality modeling from the US, Canada and Europe.

Funding: ~\$20,000, from RRWG members and CMA panels

Use of funds:

Travel funds (and honoraria) for scientists who are authorities in either environmental fate or air quality modeling (preferably with environmental fate modules).

Conference room, coffee, etc.

Selection of funded scientists: RRWG in consultation with an ad hoc CARB-industry-academic VOC group in California and others.

#### **Advantages:**

Broad participation and cross-fertilization. Not “one man’s opinion.”

CMA (and others) have experience in doing this.

It substitutes for advertising for pre-proposals. We can expect potential contractors to participate.

We will be able to make a better decision on what to do and can better judge proposals. The subgroup members either don’t have the expertise or are constrained by being potential contractors.

A panel discussion at the end of the workshop would help set a path forward for a state-of-the science report and/or developing RFPs for specific projects.

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**Disadvantages:**

- It's an ambitious project to carry out in a short time and requires effort on our part.
- We may not get all the people we want together at one time.
- We would be spending money on other than a project.

**Path forward:** Get consensus on the concept

- Set up an organizing committee.
- Identify key individuals or groups necessary for success.
- Obtain funding commitment
- Round up key participants and locate facilities
- Confirm "GO" and announce the meeting.

**Potential Funding:**

Dunn-Edwards Corporation  
CMA Panels  
SDA  
CSMA

**Leveraging:**

There are ongoing discussions with an ad hoc industry-academic-regulator coalition that was brought together with the cooperation of the California Air Resources Board (ARB) to discuss environmental fate and its impact on ozone formation. They have exceptional expertise in environmental fate modeling. Tom McKone was enthusiastic about getting together with atmospheric modelers. Don Mackay will be on sabbatical at U. California at Davis so he will be available as well. California EPA personnel from outside the ARB with experience in environmental fate modeling have participated. They can help with a workshop.

## II. Long Term Research Objectives

- 1) To determine the importance of transport to and from water, soil, sediment (and other "compartments" such as vegetation and urban films that may serve as sources and "sinks") and transformations therein on tropospheric ozone-forming-potential.
- 2) To determine the importance of transport to and from indoor sinks and transformations therein on indoor concentrations and on emissions to outdoor air of indoor emissions.
- 3) Obtaining the physico-chemical parameters needed to obtain equilibria between compartments and assess the effects of variable conditions on rate and final equilibria.

**Background**

Christensen, Keen and Kurland ("Atmospheric Availability as a Component of the Tropospheric Ozone-Forming Potential of Volatile Organic Compounds" presented at the

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US/German Ozone and Fine Particle Workshop) have shown that the Mackay Level III EQC model predicts that some biodegradable hydrophilic semi-volatile compounds react mainly in soil and water even if emitted to air. Having done this screening test we need to do more detailed modeling for a "real" atmosphere to see if the issue is truly important.

### Tests of the Model

The first test would be a screening test case with "landscape" resembling an area in the US with exceedance of the ozone NAAQS and fast, nearly irreversible transport to water and/or soil. Use a mixing height of 500 meters. Consider the fate of ground-level emission of a VOC with  $k_{OH}$  of  $1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ sec}^{-1}$  and the partition coefficients and transport properties describing the case above. Consider the same case with the same VOC having no transport to water or soil, but yielding VOC2, with the above properties. Add to the model interaction with aerosol particles with fairly "sticky" parameters.

- 1) If significant loss by transport is observed in the screening test then we should
  - A. Repeat the modeling with "best guess" estimates of partition and transport constants for a range of semi-volatile compounds.
  - B. Obtain, estimate, or contract for research to determine the fundamental physico-chemical constants for the equilibria of the VOC.

### Aerosols

The role of aerosols in deposition has received considerable attention (more than any other fate other than oxidation), but much has yet to be learned, especially for hydrophilic compounds. Considerable work is underway in many laboratories. The emphasis has been on persistent organic pollutants (POPs) which are hydrophobic (PAHs, PCBs), but the scope is expanding. Our niche may be to study aerosols with the conditions (particle concentration, water droplet concentration, OH concentration, photoperiod) under which ozone control is most important.

Repeat the work of Cautreels and Van Cauwenberghe cited in the EPA policy statement in 1989 [G.T. Helms (1989). Definition of VOC: Rationale. Memorandum from USEPA Office of Air Quality planning and Standards. Research triangle Park, NC] using other aerosol and/or polar VOC, not hydrocarbons, to see if there are significant differences in partitioning.

### Indoor Air

Historically indoor air quality has been mainly concerned with the toxicity of HAPS. Indoor formation of ozone has received relatively little attention. The contribution of indoor releases to overall ozone formation may be small overall, but large fractions of many consumer products are used indoors.

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There are then two question. How much is released to the indoor atmosphere, and how much is released to the outdoors? Down-the-drain factors considers the first question. Transport to and from “sinks” and the exchange rate determine the answer to the second. For compounds strongly adsorbed on indoor materials, identifying their fate other than participation in ozone formation chemistry will be the challenge..

A first step could be to review studies of releases to indoor air and existing models for such releases to see if a general estimation method can be developed for down-the-drain factors for consumer products that would simplify utilization of these factors in regulatory activity.

### **Relevance**

This work is relevant to getting proper emissions inventories and ozone-forming potentials (reactivities). Ozone-forming potential is a matter of reaction rate (e.g.,  $k_{OH}$ ) and of availability (v.p.,  $K_H$ ,  $K_{OW}$  other indices). This work will also be a preliminary first step to help improve the understanding of, and to evaluate the scientific plausibility and framework for, other related issues, such as the potential for down-the-drain and low-vapor-pressure adjustments, and the oxidation of biogenic and aromatic compounds.

The work will aid in assessing personal exposure to VOC.

**Strategy** - The work must lead to a scientifically sound and practical scheme for incorporating fate and transport into policy decision-making, such as prioritization of control measures and a reactivity-based substitution program. Consistency with current EPA protocols (such as fate and transport models of persistent pollutants from other programs or Models-3 airshed model) may be desirable to obtain acceptance. The science should be peer-reviewed to gain credence with regulators and environmentalists.

**Evaluating Emissions Suitable for  
Reactivity-based Controls  
Task Subgroup 4  
Leader Dave Morgott dmorgott@kodak.com**

**Summary**

At first glance, the development of a research strategy to examine the VOC emissions categories suitable for reactivity-based controls appears to be a relatively straightforward task. Three well conceived and precisely described projects were outlined in the RRWG Research Plan finalized in June 1999 (see below). In addition, mobile, biogenic and stationary source emissions data can be readily obtained for counties throughout the United States by consulting the CHIEF (Clearinghouse for Inventories and Emissions Factors) database and accessing the most recent information. VOC speciation profiles are likewise available through the FIRE (Factor Information Retrieval) and FREDS (Flexible Regional Emissions Data System) databases maintained by the EPA. Even the well acknowledged and often cited problems with emissions data base can be somewhat controlled by incorporating a sensitivity analysis into a research strategy that evaluates each source type in light of potential errors in the emissions database.

Despite the apparent ease of conducting research on reactivity-based emissions control, however, it is recommended that research on this topic be postponed until further information is obtained from the projects outlined by subgroup 1. The primary reasons for this recommendation stem from i) the need for a better theoretical understanding of the actual impact of reactivity-based substitutions using more realistic regional and urban airshed models (see subgroup 1 proposal); ii) uncertainties in the definition of reactivity and the type of reactivity scale that will ultimately yield the greatest benefit to the environment; iii) the need to proceed in logical and reasoned manner with a research subtopic that can have such strong policy-related ramifications.

As noted in their proposal, the short-term research priorities outlined by subgroup 1 have been specifically designed to yield guidance on the future development and use of a reactivity-based control strategy. Until the results of this research have been obtained and properly evaluated, it is both prudent and appropriate to postpone the initiation of the three projects described below. Once information is obtained that demonstrates the feasibility of using reactivity based substitutions to limit tropospheric ozone formation, RFPs should be developed and distributed to all interested parties.

**Project Descriptions**

The RRWG Research Plan describes three specific projects that can be completed separately or in combined fashion. The specific aim of these projects centers on an assessment of the amount and type of VOC emissions suitable for reactivity-based controls. The three projects as outlined in the Research Plan include:

(a) An examination of existing emissions processing systems to obtain information on the relative importance of each major source classification (mobile area,

non-mobile area, minor point source, major point source and biogenics) in contributing to the total inventory in terms of both total mass and reactivity. This should be done to as great a degree of speciation as is possible with the current emissions databases and processing systems.

(b) An examination of existing emissions processing systems to obtain information on the relative importance of each source type within the source classifications, in contributing to the total inventory for that classification in terms of both total mass and reactivity. Again, this should be done to as great a degree of speciation as is possible with current databases and processing systems.

(c) A determination of the practicality of a reactivity-based VOC policy by evaluating enforceability and ability to measure or track compositional information, and the amenability of the source to substitutions.

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**Completion of Adaptation of the Sparse Matrix Operator Kernel  
Emission Processor for Use in Modeling the Effects of Chemical  
Compound Reactivity on Air Quality**

**Task Subgroup 8**

**Leader Basil Dimitriadis [dimitriadis.basil@epamail.epa.gov](mailto:dimitriadis.basil@epamail.epa.gov)**

**Request for Proposals**

**Purpose**

The purpose of this Request for Proposals is to invite technical and cost proposals for the completion of the implementation of the Sparse Matrix Operator Kernel Emission (SMOKE) processor and its associated SMOKE Tool within the Models-3 air quality modeling framework.

**Period of Performance**

The period of performance for the proposed contract(s) shall be ten months from the initiation date of the contract(s).

**Background**

During the past two years, there have been several requests from industry to U.S. EPA asking for exemption of specific organic chemical compounds from ozone precursor air quality regulations on the grounds that the specific chemicals have negligible reactivity in the atmosphere. However, it was found that the tools for evaluating compound-specific reactivity in the overall context of realistic atmospheric chemistry were lacking. It was not possible to scientifically investigate the degree of effect that the absence or addition of a compound in the spectrum of volatile organic compounds might have on ozone formation. Such an analysis requires thorough state-of-the-art air quality modeling and detailed information about the spectrum of emitted chemicals. The conclusion was that the U. S. EPA's Third Generation Air Quality Modeling framework (Models-3), with its Eulerian grid multi-pollutant (e.g. "one-atmosphere" approach) Community Multi scale Air Quality (CMAQ) model was the best available tool to address the problem. Models-3 is a flexible multi-platform modeling framework which accommodates multiple spatial and temporal scales, and can potentially incorporate any chemical compound for which there are emission data. However, given the knowledge and modeling capability, it is also necessary to provide the compound-specific emission information in a temporally and spatially allocated form usable by CMAQ. Most existing emission data processors, including the current processor in Models-3 (the Models-3 Emission Processor and Projection System, or MEPPS), can handle only the standard or "criteria" pollutants which are directly addressed by rules defining ambient concentration limits. These processors receive volatile organic compounds (VOC) as composite values reported in emission inventories, and "speciate" the VOC data by applying relatively simplified "lumped species" parameterizations such as Carbon Bond 4 to group discrete compounds into a relatively small number of categories. The lumped species mechanism are also defined in Models-3 for CMAQ by Chemistry Mechanism portion of the Model-3 Science

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Manager module. Lumped species mechanisms are used because of chemistry knowledge limitations, and because of the computational limitations of processors such as MEPPS, which operate sequentially upon emission inventory data and create large temporary files requiring tens of gigabytes of storage space. In part because of this problem, a decision was made to work toward adapting and installing the Sparse Matrix Operator Kernel Emission (SMOKE) emission data processor.

The SMOKE is an air quality emission data processor designed to take advantage of the speed and efficiency of using combinations of sparse matrix arrays to iteratively process large emission data sets for use in analyses of alternative emission scenarios and regional air quality modeling. A prototype of SMOKE was originally developed by the North Carolina Supercomputing Center (NCSC) under a cooperative research agreement with the U.S. Environmental Protection Agency, National Exposure Research Laboratory, Atmospheric Modeling Division. The original intent was that SMOKE would operate as a module within a framework such as Models-3. SMOKE was designed to use the internal file format of the Models-3 system, NetCDF with an input/output applications programming interface (I/O API) designed to accommodate atmospheric modeling. For resource reasons, the development of Models-3 proceeded without SMOKE, which remained at the prototype stage. However, it became clear that a sequential emission data processor such as MEPPS, was not adequate for rapid and efficient iterative processing of many combinations of compounds and sources, as is needed for evaluation of compound reactivity. The amount of processing required with MEPPS would overwhelm the computer performance and file storage capacity available. Consequently, EPA funded NCSC during 1998 and 1999 to begin work on updating and adapting SMOKE to operate within the Models-3 framework. It was clear that resources would not allow a complete implementation, therefore the focus was first on updating the basic functionality of SMOKE to operate within Models-3, with emphasis on those features needed to accommodate reactivity analysis, such as accommodating any specific emitted compound. A key design decision was that SMOKE (which is programmed using Fortran 90) will use dynamic allocation within the Models-3 framework to avoid the constant recompilation necessary every time a new spatial grid, or chemical mechanism or case (time period) is selected. This requires at least limited implementation of dynamic allocation in the Models-3 framework, initially limited to grid selection. In addition, because SMOKE does not contain the ability to create Geographic Information System (GIS) coverages, or to quality control and format its own input files it was necessary to begin development of a tool, called SMOKE Tool to serve these functions in Models-3. This work was accomplished for U.S. EPA under contract by Science Applications International, Inc. Typically, much of the time involved in processing emission data is in the preparation and quality control of the input files. Without a SMOKE Tool facility, the files would have to be prepared manually and much of the performance advantage of SMOKE could be lost. As with SMOKE, it was recognized that the initial work would not be sufficient to complete SMOKE Tool. The initial effort for SMOKE Tool was focused on the ability to create the basic input files required by SMOKE.

On November 19, 1999, a partial initial version of SMOKE (Ver. 1.0) was delivered to U.S. EPA. This version of SMOKE has the following attributes germane to reactivity analyses:

- SMOKE is able to accept emission data for any emitted chemical compound. The compounds emitted are defined in the input file header supplied through SMOKE Tool.
- SMOKE is able to accept files (“packets”) created by SMOKE Tool, which define source type and/or geographically specific controls for defined chemical compounds. This allows a wide variety of potential situations and strategies to be applied to emission data in SMOKE, and then passed to CMAQ for modeling of resultant atmospheric concentrations.
- SMOKE is able to either speciate VOC compounds to defined compound groups (lumped species approach), spatially and temporally allocate them, and pass the data to CMAQ; or pass compound-specific data through without the speciation step.
- Iterative changes, for example in potential reactivity controls defined in a packet file, can be applied by SMOKE without changing any other input data. This allows for rapid turn-around and analysis. Analysis can take advantage of the visualization tools contained in the Models-3 framework.

A full description of the current Models-3 framework, including MEPPS and CMAQ may be found on the world wide web at: <http://www.epa.gov/asmdnerl/> under Models-3. For more information on SMOKE Tool call 919-541-0821 or e-mail to [benjey@hpcc.epa.gov](mailto:benjey@hpcc.epa.gov). A description of SMOKE Models-3 compatible Version 1.0 and of the NetCDF I/O API format is available at: [http://envpro.ncsc.org/EDSS/edss\\_register/](http://envpro.ncsc.org/EDSS/edss_register/).

### **Scope of Work**

Although much has been accomplished, a substantial amount of work remains to be completed before SMOKE and SMOKE Tool are capable of routine use for reactivity analysis or for emission data processing in general. Because the needs of reactivity analysis specifically and emission data preparation in general are not mutually exclusive, some of the remaining work will necessarily benefit both applications. All of the work described below shall be prepared for, and be consistent with, the Models-3 implementation on the Sun UNIX computing platform. All work shall be consistent with the overall design of the Models-3 system. Changes and version tracking shall be accomplished with the Concurrent Versions System (CVS). The Contractor(s) shall accomplish the following tasks under the proposed contract(s):

1. The Contractor(s) shall modify the SMOKE and Models-3 framework design as necessary to accommodate the following tasks. The SMOKE design shall maintain SMOKE’s ability, operating from Models-3 Study Planner, to access and use data objects defined by the User in the Models-3 Science Manager; to share data with Models-3 components using the NetCDF I/O API format; and the ability to rapidly manipulate temporally, spatially, or by emission

source category all emission data imported and provided via the SMOKE Tool.

2. The Models-3 Science Manager module, which includes the modeling definitions of chemical mechanisms, shall be modified to allow the user to specify the addition or deletion of any chemical compounds or compound (or user-defined groups of compounds or compounds) present in the source-compound (species) profiles. Given specification of the addition or deletion of chemical compounds or compounds in Science Manager, the SMOKE Tool shall be modified to accept the change in compound specification from Science Manger and apply it to user selected groups of source categories, and/or user-specified geographic areas. The specification of compounds shall be available generically (without regard to a particular lumped species chemical mechanism), and in conjunction with established chemical mechanisms defined in MEPPS Tool (Carbon Bond 4, RADM2, and SAPRC). In addition, the Science Manger and SMOKE Tool shall allow the user to introduce a new chemical compound, not contained in the existing chemical mechanisms, along with its emission data, and pass it to SMOKE for processing.

3. SMOKE uses source-category-specific compound profile files and source category and geographic cross-reference files provided by SMOKE Tool. Consequently SMOKE shall be modified in conjunction with Science Manager and SMOKE Tool to accept and apply the modified source-compound profile, and geographic application cross-reference files from SMOKE Tool. In addition, the ability of SMOKE and SMOKE Tools to use additive controls in addition to multiplicative controls shall be completed.

4. The ability of SMOKE and SMOKE Tool to specify and apply Primary Control Equipment Codes (PCEC) in the control packets and in SMOKE shall be completed.

4. The library of compound profiles by source category type in SMOKE Tool (SCC) shall be updated to reflect the most current information. SMOKE and SMOKE Tool shall be modified to allow the user to specify emission categories by North American Industrial Codes (NAIC) and the old Standard Industrial Codes (SIC) in addition to the SCC's already used by the system. These codes will be supplied to the Contractor(s) by U.S. EPA.

5. The compound name length, currently limited to 16 characters in SMOKE, shall be extended to use the 80 characters allowed by the I/O API library, and SMOKE shall be modified to output multiple files when more than 120 variables are used. The I/O API library is currently limited to 120 variables. These changes reflect the increased length of chemical compound names and the increased number of chemical compounds as variables.

6. SMOKE's ability to accept hourly emission data shall be extended to accept hourly continuous emission monitoring data from SMOKE Tool. This will provide more accurate and current emission data for analysis.

7. Because SMOKE includes plume rise calculations, SMOKE output shall replace the current Emission Chemistry Interface Processor (ECIP) within Models-3. This will require

coordination with the EPA developers of CMAQ and ECIP.

8. In order to allow tracking of the contribution of all or specific pollutant compounds from specific sources through SMOKE, SMOKE Tool shall be modified to provide the necessary input file to SMOKE for the ACTrack and PCTrack subroutines.

9. The Models-3 grid object shall be made selectable (from Models-3 Science Manager) by SMOKE. This change must be in coordination with the change of Models-3 to dynamic allocation (the SMOKE design assumes dynamic allocation).

10. The current SMOKE plan definition within Models-3 Study Planner shall be modified to allow the emission processing studies and plans (e.g., temporalization, gridding, speciation, biogenic, and mobile sources) to link to the merge capability, within the same SMOKE study in Study Planner. This will avoid the need for the user to move between studies defined within Models-3 Study Planner in completing a SMOKE processing sequence.

11. The SMOKE Tool shall be modified to complete transfer and incorporation of existing emission data Quality Control functions from MEPPS and the Inventory Data Analyzer. These functions include but are not limited to import and quality control of user supplied annual, daily, and hourly emission inventory data (including continuous emission monitoring data), import and quality control of temporal and speciation (compound) profile data. These functions are necessary to ensure the reliability of emission data processed by SMOKE.

12. Computer code modifications shall each be tested (unit tested) as changes are made, and all modifications shall be tested together in the context of Models-3 (system test) prior to submission of the deliverables.

### **Deliverables and Reporting Requirements**

1. The Contractor(s) shall submit quarterly (calendar quarters) progress reports to the Project Officer, which summarize the overall progress, and shall describe each task or logical segment of work on which effort was expended during the quarter. Any problems, technical or administrative, that have developed shall be listed and shall continue to be listed until resolved. Memoranda summarizing meetings, and the events of any related travel by the Contractor shall be appended to the applicable quarterly report. Each quarterly report shall be submitted on or before the fifteenth (15<sup>th</sup>) day of the month following the end of the reporting quarter.

2. The Contractor(s) shall submit to the Project Officer, brief monthly letter reports describing current issues, their status, and proposed resolutions. The letter reports shall be submitted by the close of the last business day of each month by postal service, electronic mail, or telefax

3. The Contractor(s) shall submit to the Project Officer (a) memoranda(um) specifying

proposed modifications to the design of SMOKE, SMOKE Tool, and Models-3 to accommodate any changes required to implement the above tasks, in accordance with Task 1. The memoranda(um) shall be submitted 45 calendar days after the effective date of the contract(s). The Project Officer will respond with any comments within 14 calendar days of receipt of the memoranda(um), and The Contractor(s) will make any required changes within 14 calendar days of receipt.

4. The Contractor(s) shall demonstrate the implementation of the above tasks in SMOKE, SMOKE Tool, and Models-3 eight calendar months after the beginning of the contract(s). The demonstration shall be held at a site mutually agreed upon by the Contractor(s) and the Project Officer.

5. The Contractor(s) shall submit (a) draft final report(s) nine calendar months after the beginning of the contract(s) in Word Perfect format. The report shall document the implementation of all of the above tasks in SMOKE, SMOKE Tool, and Models-3 - including testing procedures and results. Because of the need to re-create the revised SMOKE on other than a test Models-3 database, the report shall include specific instructions on how to install SMOKE within Models-3 and how to create SMOKE studies and plans within a Models-3 Study Planner interface. Revised uncompiled source code shall be provided as an appendix.

6. The Contractor(s) shall submit (a) final report(s) ten calendar months after the beginning of the contract(s) in Word Perfect format. The report shall document the implementation of all of the above tasks in SMOKE, SMOKE Tool, and Models-3, including revisions reflecting comments on the draft final report. The final revised uncompiled source code shall be provided as an appendix.

### **Proposal Evaluation Criteria**

The successful Contractor(s) shall submit proposals that demonstrate their capabilities in the following areas:

1. The availability and use of experienced personnel knowledgeable in object oriented programming, air quality modeling, and emission data modeling and processing. The personnel shall be experienced in the use of Fortran 90, C++, and SAS programming languages.

2. The availability and use of personnel experienced and knowledgeable concerning the design and functioning of Models-3, SMOKE, and SMOKE Tool. This is important because the proposed work builds on recent previous work.

3. The availability of Sun Unix computing platforms and storage devices adequate to develop and test SMOKE and SMOKE Tool in the context of the Models-3 framework. The

minimum hardware and software requirements for Models3 and SMOKE are given in the above referenced world wide web pages.

4. Demonstrated history of institutional achievement in the area of air quality modeling, emission processing, and object-oriented software design and implementation.

### **Cost Estimate**

Based on 2500 hours of high-level software design and programming expertise at \$80/hr (fully loaded)

\$200,000

# DRAFT

## Survey and Compile Existing Chamber Databases

### Task Subgroup 10

Leader P.A. Makar ([paul.makar@ec.gc.ca](mailto:paul.makar@ec.gc.ca))

Request for Proposals

### Executive Summary:

**Smog chamber experiments, in which pollutant gases found in the ambient atmosphere are combined and allowed to react under controlled laboratory conditions, are invaluable aids in understanding atmospheric chemistry and essential for the evaluation of the reaction mechanisms used in regional and urban pollution models. The chambers are operated by a variety of researchers in several countries, each chamber having its own set of laboratory techniques and procedures for record keeping. Not all of the data are currently publicly available. Some of the data have not been released, due to a lack of funding to complete quality control and quality assurance procedures on the raw measurements.**

**This proposal is for a short (4 month) scoping study, which will compile a catalogue of all of the experiments which have been performed in smog chamber studies to date, and which will provide information regarding the availability and readiness of the data for outside use. The primary purpose of the catalogue will be to identify experiments, which are currently available for inclusion into a common database, and to determine the level of effort required to create this database. The database would be a resource available to laboratories wishing to perform future chamber experiments, and regional modelers wishing to evaluate reaction mechanisms. The details for this call for proposals follow.**

#### 1. Background

This Request for Proposals (RFP) addresses proposed short term project 2.4.1 of the Research Plan of the Reactivity Research Working Group: Survey and compile summary of existing chamber data that can be used to evaluate reactivity and models that calculate effects of VOCs on air quality.

The EPA had funded projects in the early 90's to document the UCR, UNC, and CSIRO chamber data base, which resulted in a comprehensive documentation of the UCR data base up to 1993, and progress towards documentation of the UNC and CSIRO data bases. UCR researchers are committed to releasing updates to their database as a part of the work plan of ongoing programs. An Environment Canada project to place UNC and SAPRC chamber data into a common format for use with SMVGEAR was completed in May of 1999; evaluation and tests of the system are to be completed by March of 2000.

There is a large database of existing environmental chamber data that is relevant to evaluating reactivity and chemical mechanisms that predict reactivity. Full advantage may not have been taken of the existing low NO<sub>x</sub> database from Graham Johnson's

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chamber at CSIRO or the TVA chamber. A survey of the existing database would result in more effective use of the funding available for reactivity-relevant environmental chamber research.

### 2. Scope of Work for Research

The survey should include the following information:

- A. Create a chamber experiment catalogue. For each chamber facility surveyed:
  - (a) A list of the experiments performed in the chamber. Each entry of this list should include:
    - i. The experiment name.
    - ii. The chamber name.
    - iii. The chamber operator/contact person name (who to contact for queries about the data).
    - iv. A one-line (80 character) precis description of the experiment.
    - v. A list of the names of all species for which initial conditions are known in the given experiment (including estimates/best guesses of the chamber operator). This list should be fully speciated, that is, any initial conditions expressed as total concentrations of a mixture in the chamber operator's original data should be stated in terms of the component compounds of the mixture.
    - vi. A list of the names of all species for which measurements were made in the given experiment.
    - vii. A "Number of primary hydrocarbons designator", "1" for single-hydrocarbon (aside from background hydrocarbons in the initial conditions) experiments, "2" for two-species experiments, etc. Mixtures of thirty species would be given a "30".
    - viii. A "Name of primary hydrocarbon(s)" designator. A 40 character name of either the hydrocarbon (if the experiment is a single hydrocarbon experiment), both hydrocarbons (if two hydrocarbons were present in the same experiment, aside from background initial values) or the mixture name (if greater than two hydrocarbons were present as initial conditions in the experiment, aside from background initial values).
    - ix. A "State of the Data" designator. The following classification scheme is to be used:
      1. Chamber operator is willing to have data incorporated into a publicly available database, concentration measurements have been qa/qc'd, wall conditions have been estimated by the chamber operator, boundary conditions (light intensity as a function of wavelength, temperature, pressure, water vapour concentration) as a function of time are qa/qc'd and available. Chamber operator feels that the data are of suitable quality and usefulness for comparison to model simulations.
      2. As in 1., but the operator feels that some aspects of the data may inhibit its usefulness for comparison to models. Nevertheless, comparisons with models may be useful, provided the limitations of

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- the data record are acknowledged. A one-line (80 character) description of these limitations should be provided in a second file.
3. As in 1., but operator prefers to retain control over distribution of the data. Instructions on how to contact the operator should be provided in a separate file.
  4. As in 1, but the datafiles have not been qa/qc'd. The chamber operator feels that this data would be of potential use for model simulations, and is not likely to contain serious deficiencies preventing its use, but qa/qc operations must be completed prior to use.
- (b) A description of the chamber operator's current (dated) best estimate of wall conditions, including boundary conditions such as wall reactions, and initial concentrations for species (if believed to be the same for all experiments). This should be provided in a set of separate supplementary files, one for each chamber, and should include: all chamber reactions believed to be relevant, their reaction rates, and any default initial values to be used as initial conditions for instances in which an experiment-specific value has not been provided by the operator. These files will form an appendix to the main body of the report.
- (c) Two tables, the first of which assigns a unique 3 character name to the measurement devices used in the experiments taking place in the chamber, and a second table which lists experiments in the first column, and species in the first row, with 3 letter device names in the appropriate locations to indicate which devices were used in which experiments in the measurements of the given species.
- (d) For experiments in the chamber identified as class "3" (A-a-viii, above), a separate file which includes the experiment names, operator names and contact information (mail, email, phone, fax) for the experiments in a given chamber for which data distribution is operator controlled.
- (e) For experiments in the chamber identified as class "4" (A-a-viii, above), a brief (2 page) scoping document discussing the work that would be required to make the data available for a public archive should be provided. This should include the time in person years required to complete data qa/qc, the cost of materials, and expected deliverables). For work of this nature which is already ongoing, the scope of this work (i.e. sufficient to make the data available?), the expected delivery date, and the contact information for those providing the funding should be listed.
- B. Describe the work required to convert the available data into a single database utilizing a common format. Note that some of this work (UNC/SAPRC chambers) may have already been completed. A two page scoping document should be provided for each chamber considered.
- C. The chambers to be included in the above catalogue are:  
 The UNC chambers of H. Jeffries  
 The SAPRC chambers of W.P.L. Carter  
 The CSIRO chamber  
 The TVA chamber

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The EPA chamber

The Europhore chamber [K.H. Becker – note that their laboratory sharing structure probably will make most of the data “3”, but a list of the experimenters and their contact addresses would be invaluable for negotiating use of the data via collaborations].

The Canadian chambers at York University, and at AES Downsview.

### 3. Milestones

The main outcome of this RFP is to be a document describing the experiments that have been completed in smog chambers to date. The document will be a publicly available (via NARSTO website) resource for those wishing to use chamber data for simulation purposes, and to plan future chamber experiments. The document should be available in Word, Wordperfect and pdf formats, and the data tables should be available in Excel, Lotus 1-2-3, and text file formats.

Milestone 1: Initial contact with holders of the data completed, agreements made for providing information

Milestone 2: All relevant information collected by the contractor.

Milestone 3: Data organized in the format suggested above.

Milestone 4: Documents created.

Milestone 5: Documents revised following feedback from funding agency, final versions prepared.

Milestone 6: Scoping document for conversion of data into common database created.

### 4. Deliverables

1. Covering document including an introduction describing the project, the work done to achieve each of the above milestones, a description of the data catalogue, and operator contact information (as per 2. A-a-viii)
2. Appendices to 4.1, including the data catalogue in the formats given above.
3. Scoping document(s) for work required to place all of the above data into a single common database.

### 5. Cost Estimates

An initial estimate of the project is a 1 person, 4 month contract, at \$30K US. This may lead into further contracts depending on the outcome of section 4.3, and available funding.

### 6. Rationale

There is a need to make the data measured in chambers more publicly accessible, in order to promote its use in the wider scientific community. These data are a valuable resource, since they constitute the best available means of characterizing atmospheric chemistry and comparing to simulations. However, the multitude of data sources, formats employed by different operators, and the need to use chamber-specific software for each database hampers their easy use by the scientific community. As a first stage towards a common public database, a catalogue describing the experiments performed to date and their availability to the community at large is required. Once this is established, further work to build the database should follow.