

Ad Hoc Task Force on VOC Reactivity

Minutes of Initial Meeting

May 14, 1998

The meeting was called to order by Robert Wendoll, who stated that the first order of business was to establish the initial steps for Task-Force action.

John Dege noted that we need to establish EPA's position on this topic, and then we need to formulate a concept paper to establish the basis for our downstream operations. It was emphasized that we need to set forth a list of the relevant research needs. Cyril Durrenburger suggested that we might want to develop one or more "issue papers" that define the primary considerations at hand. He also suggested that we consider commissioning several "critical review" papers, similar to those for the NARSTO Ozone Assessment, as a means of codifying salient scientific aspects. Gary Foley stated that we need to start thinking about focusing our scientific efforts, e.g., chamber studies, modeling efforts, . . ., in order to maximize relevance to the policy community: we need to reach closure on how to produce the most definitive information. He also recommended parallel, evolving, and communicative efforts between the scientific and policy communities.

There was a general discussion of how the science/policy interface should be handled. This arose at several points during the ensuing conversation. In particular it was asked whether NARSTO had any direct chain-of-command linkage to EPA's Office of Air and Radiation. Jake Hales said definitely no. Although OAQPS is a NARSTO signatory, NARSTO tries to be scrupulous in observing the line between policy-making, and performing policy relevant research. In observing this line NARSTO - in Jake's estimation - has been less effective than desirable to date in getting our research products conveyed to the policy community. Currently NARSTO is designed to make this linkage through a Liaison Team for Policy, a standing box on our organization chart. This has been relatively ineffective, however, and because of this NARSTO's Executive Steering Committee feels that in the future such liaisons need to be hard-wired into active, functioning groups. In view of this, Jake stressed the importance of having OAQPS staff take a strong and active role directly in this Reactivity Task Force.

Bob Avery stated that we need to plan a meeting to formulate a mission statement. Robert Wendoll agreed, saying that we need to establish a list of meaningful scientific objectives to go along with such a statement.

Howard Feldman stated that it is desirable to develop an assessment of the current state of the science associated with the reactivity issue: Is the scientific underpinning sufficiently "ripe" for policy application? If not, when will it be?

It was asked if this Task Force is to be considered a science group, a funding group, or both. If it's a funding group, what are the money sources? Basil Dimitriades responded that we need some time after this meeting to think this over; then we should reconvene to write a research plan.

Referring to the question of whether this effort should be incorporated as a part of NARSTO, Ed Edwards recommend that everyone here review NARSTO's structure and operational process. Jake Hales commented that the best way to do this is to visit the NARSTO Web site on <<http://narsto.oaw.com/Narsto/>>. Robert asked for a show of hands for those favoring incorporation into NARSTO. The response was ambivalent, mainly because of unfamiliarity of many of the attendees with NARSTO. There was a consensus that everyone should visit the Web site in the near future.

There were some questions regarding alternatives to NARSTO, such as a possible FACA committee or a dedicated EPA-coordinated arrangement. Jim Vickery responded that EPA definitely prefers the NARSTO route to a dedicated EPA option, for several reasons. First, NARSTO was established to promote public/private communications and offers an established resource base for operations of this sort. Secondly, EPA desires to operate on a multiorganizational, pooled resource basis with operations of this type, in order to encourage all interested parties to enter in the discussion process. FACA arrangements, on the other hand, are more suitable to short-term issues such as evaluating proposed standards and similar concerns.

Robert Wendoll then asked for a list of action items for this initial meeting. These items and their resolutions appear below:

1. Set date and place for our follow -on meeting: It was agreed that this meeting should be during the first week in September at RTP NC, at EPA's conference facilities. A pilot team will convene by conference call in early June to draft a mission strategy and design this meeting. This team will consist of Barbara Frances, Ed Edwards/Robert Wendoll, John Dege, John Schwind, James Neece, Cyril Durrenburger, Basil Dimitriades, and Ron Patterson (or Jake Hales).
2. Draft a Mission Strategy: This will be performed by the pilot team, as noted above.
3. Draft an agenda for the September meeting: Basil Dimitriades will do this.
4. Determine methods for communication: Jake suggested that, for the time-being, at least, the group use the NARSTO home page as a primary communication medium. He will set up a reactivity sub-page there for that purpose. There was also some question of how we communicate activities of this group to individuals not present at this meeting. Jake suggested that, as a first measure, we put an article describing our activities to-date in the NARSTO newsletter, the 1998 summer/fall issue of which will go

into press in early June. Robert Wendoll agreed to write this article and send it to Jake for inclusion in this issue.

The meeting concluded at 1:40 pm.

**PRESENTATION SUMMARIES FROM EPA REACTIVITY WORKSHOP
May, 1990**

(Drafted by Bill Johnson)

Session I Summary of Questions and Discussions

Current EPA Regulatory Viewpoint on Reactivity

Bill Johnson, Ozone Policy and Strategies Group, EPA

Mr. Johnson was asked how to get a copy of Rule 66 and vapor pressure cutoffs. He responded that inquiries on this rule, now referred to as Rule 442, can be made through Los Angeles County (i.e., South Coast Air Quality Management District). Mr. Johnson was also asked about obtaining a list of the 14 pending petitions. Mr. Johnson said that he will make this list available.

William Carter (University of California) commented that this workshop group should look at other scales in addition to the maximum incremental reactivity (MIR) scale. He added that for compounds with low vapor pressure, the equilibrium vapor pressure should be considered.

Robert Hamilton (Amway Corporation) asked about the mole versus mass based reactivity and what the advantage would be if the standards are weight based. Mr. Johnson commented that reactivity comparisons made on the mole basis would be more scientifically sound. The regulation of emissions is still done on a weight-basis. A question was asked concerning the basis for exempting compounds and what goal was trying to be accomplished. Mr. Johnson responded that the goal is ozone reduction, but that other collateral effects are being considered as well.

Brian Keen (Union Carbide) commented about the wide range of compound concentrations and reactivities, and about the pit falls of using bright line cutoffs. Mr. Johnson responded by stating that this is one of the issues he hopes will be discussed at this workshop. At the present time, bright line cutoffs work well from a regulatory perspective. Mr. Keen also commented on the problem of the uncertainty of the information.

Current EPA Research Viewpoint on Reactivity

Basil Dimitriadis, National Exposure Research Laboratory, EPA

Alan Hansen (EPRI) asked about the difference between relative versus absolute reactivity. He stated that the question of gram-based versus mole-based reactivity isn't important unless the reactivity is absolute. Dr. Dimitriadis responded by stating that the problem depends on how the data is used. The differences between cases depends on the applications or how the material is used. For example, comparing paint solvents with ethane on a per-gram basis is affected by the problem; but intercomparing solvents on a per-gallon basis is not. John Festa (American Forest and Paper Association) asked if Dr. Dimitriadis had stated that there was no basis for excluding any VOC. Dr. Dimitriadis responded that he was referring to an exclusion from the inventory requirements. Another question was asked about the distinction made between VOCs and non-VOCs. Dr. Dimitriadis and William Carter (University of California)

clarified this issue. The distinction is a legal or regulatory one; EPA has defined compounds as being VOCs or non-VOCs and this information is provided by means of a table.

Dr. Carter also commented that there are several issues that will drive the science. The first issue is what type of policy is going to be used. If the policy continues to be the exemption policy, then the question is whether ethane is the appropriate dividing line and, if not, what substance should be used. One area of research is to determine what is the best dividing line or bright line. The second issue, once the bright line has been determined, is to determine where other compounds fall relative to the bright line. Dr. Carter commented that the most appropriate comparison is on a mass basis, because this is how the VOCs are emitted. Dr. Dimitriades responded by stating that the question of which basis to use is one that needs further discussion.

Dave Morgott (Eastman Kodak Company) asked if MOIR has been considered over MIR as the basis for a reactivity scale. Dr. Carter commented that exemption decisions were based on a number of reactivity scales (e.g. EBIR or MOIR) and not on just the MIR scale. Dr. Dimitriades commented that the discussion on the reactivity scales is still an open one. Jake Hales (ENVAIR) suggested that this workshop group try to develop a good definition for the term reactivity.

California's Hydrocarbon Reactivity Program

Randy Pasek, California Air Resources Board

Cari Roque (Naval Aviation Depot) asked if California was integrating their research with those from other states. She continued by asking if there would be a shift from air pollution to water pollution when changing over to material using water-based chemistry. Dr. Pasek responded by stating that they are seeking opportunities to share studies. He also stated that California doesn't plan to shift from air to water pollution. An addition, a comment was made concerning the need to recognize instances where multimedia consideration must be made.

Bernie Zysman (Occidental Chemical Corporation) asked about other research facilities doing work on MIR. William Carter (University of California) stated that he was not aware of others doing reactivity research, except Harvey Jeffries's group (University of North Carolina). Mr. Zysman add that he would like to see more research and development to clarify Dr. Carter's work.

Bob Kozak (Atlantic Biomass Conversions, Inc.) asked if CARB was considering in-use vehicle speciation testing for possible upgrading of smog check equipment. Dr. Pasek stated that these types of measurements are not being done on a routine basis, but there is a need for this type of information. Mr. Kozak also asked if tropospheric ozone production work might interfere with any stratospheric ozone depletion work being done by CARB. Dr. Pasek stated that they have taken this into account by considering the effects compounds might have on stratospheric ozone and global warming, as well as its toxicity.

VOC Reactivity - Beyond Ozone

Alan Hansen, EPRI

Dave Golden (SRI/Stanford) stated that no one knows the chemical mechanism of the SO₂ to sulfuric acid reaction. There is a lot of the chemistry in the models that may not be correct, but care must be taken when jumping to the complexity of the model. Mr. Hansen agreed with these comments.

Jake Hales (ENVAIR) asked about the counter-intuitive findings that result when you increase NO_x , the nitrate aerosol decreases. He asked if there was a mechanistic explanation for this occurrence. Mr. Hansen responded that he didn't know the mechanistic reason why this occurred. Ted Russell (Georgia Institute of Technology) commented that since you're decreasing NO_2 , you're increasing the OH radical pool. This allows for faster oxidation of VOCs, the ozone concentration increases, and, with more ozone, there is more OH. The presence of more ozone also causes faster nighttime conversion of NO_2 to nitric acid.

Session II Summary of Questions and Discussions

Comparison of POCP and MIR Scales

Richard Derwent, Meteorological Office, United Kingdom

Eduardo Olaguer (Dow Chemical Corporation) commented on moving from an urban MIR scale to a regional POCP scale, because the MIR scale underestimates the reactivity of the medium reactive compounds. Dr. Derwent responded by stating that the best benefit is from a high reactive to a low reactive. He stated that the MIR scale underestimates the impact of controlling the middle reactive compounds. Mr. Olaguer asked what happens if meteorological conditions are taken into account, especially where there is fast vertical transport such as in thunderstorms and how would this effect reactivity. Dr. Derwent stated that this has not been considered, because ozone is not produced in thunderstorms.

Donna Carvalho (Pennzoil) asked if Dr. Derwent had made any assumptions about the reactivity of C-13 or greater compounds. Dr. Derwent responded that he had not. These compound were not included in his calculations, because they are not included in the emission inventory.

Dr. Derwent was asked about why formaldehyde was not photolyzed. He responded that whether or not to photolyze formaldehyde is not a user's choice, but is determined by the hydroxyl radical concentration.

Session III Summary of Questions and Discussions

Dunn-Edwards Proposed NARSTO Research on Ozone Formation Potential of VOC Emissions from Architectural Coatings

Edward Edwards, Dunn-Edwards Corporation

Jeff Gaffney (Argonne National Laboratory) commented that by investigating low NO_x chemistry, a great deal can be learned about regional scale reactivity. He also commented that on a regional scale, consideration must be given to the formation of species other than ozone, such as organic peroxides and the conversion of SO_2 to sulfate. These species have impacts on other environmental concerns such as regional haze.

Harvey Jeffries (University of North Carolina) commented on the importance of reactivity in low NO_x conditions. In low NO_x environments, the VOCs determine the fate of the NO_x ; the loss of NO_x limits the formation of ozone. These effects can cause increases in ozone

downwind of urban areas. As illustrated by an SAI study, changes in solvent content from a more reactive solvent based on toluene to a less reactive solvent based on paraffins can cause increases in ozone concentrations in a downwind NO_x-limited environment. Dr. Jeffries concluded by stating that some of Dr. Edwards' concerns are legitimate and the issues of nitrate yields and nitrate formation in these mechanisms are important pieces of information.

William Carter (University of California) commented about his chamber study that was used to evaluate the isoprene mechanism. The changes made to the model were based on better fundamental chemistry, but the predictive capability of the model was not evaluated. Dr. Carter continued by stating that the current regional models are not designed to handle organic reactions under low NO_x conditions, with the exception of the RADM mechanism. He stated that the data have not been adequate to evaluate these models and to gather the necessary data would require the use of advanced analytical equipment to analyze for other species.

Edward Edwards (Dunn-Edwards Corporation) added a comment about the need to do full circle analysis: model, chamber, and ambient air.

CMA Research Initiatives

Jonathan Kurland, Union Carbide Corporation

Following Dr. Kurland's presentation, William Carter (University of California) discussed the different factors that affect reactivity and the ways to evaluate whether a model can adequately predict them all. In systems with VOC reacting in the presence of excess nitrous acid and where the nitrous acid is forming all of the OH radicals, the amount of ozone or NO formed is very sensitive to how fast the VOC reacts and the NO is converted to NO₂. There is almost no sensitivity to radical initiation inhibition effects. This provides a way of testing that aspect of the model independent of the other uncertainties. This method could potentially be used for very low volatility compounds that cannot be done practically in environmental chambers. Dr. Carter commented on his new program with the California Air Resources Board to develop more generally applicable methods of measuring reactivity to replace the more expensive chamber experiments.

CSMA Position on the Importance of Relative Reactivity

Doug Fratz, Chemical Specialties Manufacturers Association

Harvey Jeffries (University of North Carolina) commented that the ozone formation in an urban area cannot be determined by multiplying an inventory by the MIR; a whole airshed model has to be used. He reiterated that nearly half of the ozone is produced by low reactivity chemicals. Mr. Fratz responded by stating that they found very good agreement between the MIR rated inventory approach and the urban airshed model approach. Both approaches predicted very small amounts of ozone formed considering the VOC controls targeted. William Carter (University of California) commented that he agreed with the way Mr. Fratz had used the MIR to look at how to prioritize controls and not to look at what caused ozone formation.

Reactivity Concerns

Phil Ostrowski, Occidental Chemical Corporation

John Festa (American Forest and Paper Association) commented that the branch of EPA administering TRI requires the air program to declare a chemical as a negligibly reactive VOC

before it can be removed from TRI. Mr. Ostrowski responded that maybe there would be a rethinking of the TRI exemption in the new policy.

Bob Avery (Eastman Chemical Company) commented that the cutoff for exemptions should be raised in the short term, rather than lowered, in order to get more useful chemicals in the 'tool box.' Mr. Ostrowski expressed his concern that this approach may end up impacting air quality in a negative way. Mr. Avery continued by stating that there may be some local adverse impacts, but overall, the substitution of low reactivity compounds would be directionally correct, and, overall, an improvement.

Categorization of Low Reactivity Compounds

John Owens, 3M Company

William Carter (University of California) commented that there are procedures to estimate upper limits of reactivity that could be used to establish the cutoff.

Harvey Jeffries (University of North Carolina) stated that, although compounds with a low kOH must be looked at closely, he is not calling for compounds with lifetimes on the order of months or years being studied in the smog chamber.

Richard Derwent (Meteorological Office, United Kingdom) stated that this is not so simple for theoretical studies. When working on CFC replacements, they looked at long-lived VOCs. It is important to have information about the degradation products and to consider the by-products from the production of these low reactive VOCs. This will require more than just a theoretical study, because there are a whole range of other problems. Mr. Owens responded by stating that 3M does sponsor these studies of degradation products and does a life cycle analysis of byproducts and products.

Impact of a Molar Ethane Standard on the Number and Type of VOC-Exemptible Compounds: Practical and Environmental Implications

Daniel Pourreau, ARCO Chemical Company

Harvey Jeffries (University of North Carolina) proposed a deferred control system of five years with possible renewal based on further analysis. Dr. Pourreau responded by stating that industry would be reluctant to use an alternative that might not be available in the future. He proposed that the new reactivity-based policy revisit the exemptions, but he thinks the exemptions granted now for the low-reactivity materials would still benefit under a reactivity based policy. Dr. Jeffries continued by commenting that it would be necessary to inventory the exempt products. He stated that it is necessary to know where and when and in what quantities the VOCs are emitted to know the impact on the environment. Dr. Pourreau stated that, although they are trying to replace highly reactive compounds to reduce ozone, there are practical limitations on how they can do this.

Jim Berry (Berry Environmental) commented on a specific slide referring to 37% solids from water-based solvents. He stated that for the comparison to be appropriate, the water must be removed. Dr. Pourreau stated that the information was in pounds/ VOC and pounds/solids and, therefore, water was not an issue. The weight percent solids was included as an illustration to show that the non-water coating applies more solids per application.

Session IV Summary of Questions and Discussions

Computing Volatile Organic Compound Reactivities with a 3-D AQM Zion Wang, University of North Carolina at Chapel Hill

Jake Hales (ENVAIR) commented that there are many choices: use kOH, use sensitivity coefficient, use MIR or MOIR, etc or use 3-D models over EKMA. It needs to be remembered that MIR isn't all that simple; even with the one-dimensional EKMA model, many parameters need to be specified such as the different ways to titrate the NO_x, how peak ozone is used in the numerator of the equation, and what domain is used. Dr. Hales concluded by soliciting comments from the 3-D modelers.

Ted Russell (Georgia Institute of Technology) commented that many of these are policy questions. It needs to be asked: what is the metric for the policy makers. Once that decision is made, then the modelers can react. There is a need to get away from boundary conditions and initial conditions and to look at how these emissions are added. When looking at the impact of change in fuel composition, the emissions change needs to be linked to the fuel. For a solvent, the solvent emission distribution used would be different. It is necessary to normalize the results to a mixture of compounds and different people might have different ideas on this normalization process. It will also be necessary to compare the 3-D models results to the box model results.

Gary Whitten (Systems Applications International, Inc.) agreed with Dr. Russell's comments about policy. A policy decision is needed. Currently, xylene and ethane are treated equally, but clearly they are not. He commented that there needs to be a methodology for trading solvents with lower reactivities. He proposed a 4-tier reactivity scheme in place of the 1-tier scheme currently in place. Compounds in the highest tier (e.g. xylene) would be counted twice as much; lower reactive compounds would be counted half as much. This would encourage switching from solvents like xylene to paraffins and would be beneficial even if the alternative was still somewhat reactive. In this way, industry can be a big credit for making the switch and for making improvements in the reactivity in the atmosphere. Dr. Russell responded to this proposal by stating that more bright lines don't help, especially there aren't huge gaps in the reactivity spectrum where these different classes would divide. Dr. Russell believes that this is defeating the purpose of reactivity and he would prefer the policy to be driven by the best science.

William Carter (University of California) agreed that the policy will drive the approach. He continued by stating that there are two main ways of looking at policy: (1) reactivity scale which is generalized and (2) assessment or specific substitution scenario where replacement should be handled in detail with a detailed model. There is also a need for a generalized scale to be used for prioritizing, but the reactivity scale poses different modeling problems in trying to answer the question: what is the optimum scale to use. The scale would need to be representative of the criteria and to represent a distribution of conditions (set of scenarios). Lastly, Dr. Carter is not convinced that an EKMA model is not adequate for the purposes of developing a scale.

Chris Walcek (State University of NY at Albany) commented that, because the scale can't be made to be a simple one, this doesn't mean that it is impossible to have a scale. The scale won't be simple and there will be a great deal of controversy about its development. Dr.

Carter added that it is important to have a standardized protocol for the scale; it is important not to vary the metrics.

Barbara Francis (CMA) commented that the CMA hasn't developed positions on yesterday's or today's discussions and those positions expressed here are not the consensus positions. She continued by saying that CMA is committed to a large industrial research program.

Temperature Dependence of Ozone Chemiluminescent Reactions with Organics: Potential Screening Method for VOC Reactivities

Jeffrey Gaffney, Argonne National Laboratory

Chris Walcek (State University of NY at Albany) asked about the cost of the chemiluminescence system. Dr. Gaffney stated that the system costs between \$6,000 and \$7,000 which is cheaper than the NO_x system and it could also be used to look at reduced sulfur gases. *VOC Receptor Modeling as an Aid to Evaluating the Effect of Reactivity Changes on Ozone Formation*

Donna Kenski, US Environmental Protection Agency

Alan Hansen (EPRI) asked about the reconstruction of the emissions mix at the monitoring stations and the complicating factor of emissions in between the monitoring sites. Ms. Kenski responded by stating that the model a very simple, screening-level model and does not include any reinforcement or deposition. Mr. Hansen continued by asking about the lack of impact from refineries being an artifact of the location of intermediate sources. Ms. Kenski answered that they tried to account for this issue with the trajectory, and by comparing the upwind trajectories.

Computational Studies of Oxidant Reactions of Volatile Organic Compounds Relevant to the Formation of Tropospheric Ozone

David Dixon, Pacific NW National Laboratory

Eduardo Olaguer (Dow Chemical Company) asked all the presenters if neural network techniques had been applied. Dr. Dixon responded that he wasn't sure, but that the work is continuing.

It was asked if Dr. Dixon was going to look at the reaction between the hydroxyl radical and NO₂ and he answered affirmatively. Dave Golden (SRI) commented that the potential energy surfaces for the hydroxyl radical and NO₂ reaction are inaccurate. There are two groups that have estimated this, the IUPAC estimate is wrong and the JPL estimate is correct. It has been measured to 5%, but could it be calculated better. Dr. Dixon responded by stating that temperature and pressure corrections could be included in the calculations. A question was also asked concerning the impact of water on this reaction. Dr. Dixon responded by stating that there would be no effect from water, unless the reaction was taking place in a droplet, but because these reactions are fundamental gas-phase processes, this would not be expected.

Session V Summary of Questions and Discussions

Oxygenates: Reactivity Implications

Ian Barnes, Bergische University at Wuppertal, Germany

Eduardo Olaguer (Dow Chemical Company) commented that the ideal approach would be to learn all that could be learned about reactivity options, then decide how to design the reactivity strategy. It seems that currently, all the money goes into designing a policy index, and the science is done to make that convenient. Mr. Olaguer would prefer to do the science first.

FREE FORUM SUMMARY

Howard Feldman (Moderator) described this portion of the workshop as the opportunity for any attendee to express their 'two cents worth.' There were many experts in the audience, not all of whom made a presentation, and many others with opinions or points of view. The free forum was their opportunity to make whatever presentation they wished to make.

Kent Hokeman (Chevron Products Company) began his comments by observing that there had been talk about how desirable it was to separate policy and science issues. He expressed his opinion that, in the case of reactivity, this is impossible, and that policy is actually required to define reactivity. He continued by stating that science has been stymied by the lack of policy or, at least, a broad policy outline. In California, there is a policy definition of reactivity, but it's limited to the certification of new vehicles with respect to exhaust emissions. It was not designed to result in an ozone benefit, but only to achieve an equivalent ozone impact. Therefore, the absence of the automobile industry from this meeting is conspicuous, with the exception of Honda. This is perhaps because the California system is complex and burdensome and it does not achieve an air quality benefit. Therefore, automobile companies haven't taken advantage of the opportunity to develop their own reactivity factors, but have relied on the default values developed by CARB. Establishing the default values is a every expensive process; CARB has spent hundreds of thousands of dollars to establish and maintain their ability to determine reactivity adjustment factors.

When reactivity is applied to stationary sources and consumer products, there are some simplifications and some additional complexities. The first simplification is the absence of simultaneous emissions of VOC and NO_x from stationary sources or consumer products. This is very important when dealing with automobile exhaust. Another simplification is that, for automobiles, the VOC's are changed during the combustion processes within the car. Therefore, the fuel put into the car is not what is emitted in the exhaust. Thirdly, there is a great variability between the vehicles, between operating conditions, and between technology classes whereas this complication is not present for the stationary sources.

The first complication for stationary sources and consumer products over the mobile sources is the great diversity of chemical structures and classes of solvents. In addition, the atmospheric chemistry is not understood well. Secondly, it will be much more difficult to trade, and trade fairly, for consumer products, because the materials being traded are very dissimilar. For mobile sources, we are trading one gasoline emission mixture for another and these mixtures are very much like one another. For consumer products and stationary sources, this will require greater quantification and certainty in the reactivity of materials.

Dr. Hokeman continued by discussing two associated issues for which reactivity arguments are being used, but that he believes must remain separate: (1) to reduce the ambient ozone levels and (2) the exemption of specific VOCs. For the issue of exempting VOCs, the focus is on establishing a bright line by looking at the least reactive VOCs. For the issue of reducing the ambient ozone levels, the focus is on what materials should be controlled (VOCs, which VOCs, or NO_x) by looking at the most reactive VOCs. The attainment of the standard is a broader, more urgent issue, but a VOC reactivity policy must be developed to encompass the full spectrum of issues. It can also be asked whether or not there is any real justification for exempting anything if it contributes to ozone.

Dr. Hokeman summarized his remarks by stating that there are two main concerns for industry. The first concern deals with all of the different decisions which must be made on defining conditions, setting the scale, and measuring reactivity. There is a great deal of arbitrariness in any policy, and although this is not good, instability is worse. It is very difficult

for industry to deal with changes in the rules. The second concern of industry is that reactivity is one more appealing control measure and can be appealing to different states to a different extent. Dr. Hokeman encouraged EPA to be sure, when developing its policy, that it can be applied generally and fairly to the whole country and not as a patchwork of different requirements.

Anne Giesecke (American Bakers Association) discussed the concerns of the baking industry. Yeast fermentation releases ethanol, which is released to the air. In addition, they operate the third largest trucking fleet in the nation. Dr. Giesecke stated that this industry is encouraged by these discussions. This industry has spent about \$30,000,000 turning ethanol into CO₂ and decreasing the NO_x emissions through catalytic oxidation. The modeling discussions were interesting and this work needs to move forward. Although access to the models is important, Dr. Giesecke believes that not every state and industry needs to operate the model. The resources of many states are strained as are many industries and she suggested that modeling work could be out-sourced. Dr. Giesecke is encouraged by the work on relative or incremental reactivity or the potential for ozone formation and the shifting of the emphasis away from the 'yes or no' system currently in place for evaluating VOC emissions. She expressed the need for more sophisticated tools such as the baking industry's interest in the holistic or life cycle approach. The baking industry also recommends looking at emissions trading and how to change from the current system where all VOCs are considered equal to one where a more reactive VOC can be replaced by a less reactive VOC. This industry would like to see more effort put into the study of more reactive chemicals and those that have other complications. They would also like to see more of their money going into fleet conversion instead of ethanol control. The baking industry operates at a 2% profit margin and, therefore, they don't have a surplus of money to do both.

Leslie Ritts (Hogan & Hartson), who represents a large number of stationary source categories, commented that for 20 years billions of dollars have been spent on control strategies and on decisions that have led to moving business offshore. She expressed her concern about how the discussions held at this workshop will feed into regulations and whether or not there is a time line for such regulations.

Barbara Francis (CMA) commented that the consensus among the solvents producers is that the models are not really ready for the regulatory community to use. They believe that there is enough information available now, especially on the incremental reactivity, to implement reactivity-based regulations.

Neal Wheeler (MCNC-NC Supercomputing Center) began his comments by reminding the audience that establishing a reactivity policy wasn't going to be easy and that the issue of reactivity can't be simplified. It will take a great deal of work to apply the policy fairly and effectively.

Dr. Wheeler stressed the need for this to be a community effort and that people need to participate and to share information. He commented that there are a wide range of possibilities of how to use reactivity in the regulatory process: from setting exemptions with a bright-line (or not) to reactivity-weighted emissions. He also commented that models don't make decisions. There will be external information (scientific or policy) that will be effecting the decision making process and consideration must be given to other environmental issues as well.

He expressed the need for multiple metrics to help the policy makers and the need for the scientific community to describe the meaning of these metrics. Consideration should be given to the range of conditions from the current time out into the future. It is important to monitor an

exempt VOC both in the inventory and in the ambient environment into the future to be certain that a poor decision has not been made. He agrees that, although stability is important in a regulatory process, we can't have absolute stability, especially in light of making a bad decision. There needs to be a systematic process for dealing with necessary change based on new information.

Dr. Wheeler discussed the range of multiple metrics needed such as metrics to assess exposure, various meteorological conditions, multiple locations, multiple pollutants, and total risk. He emphasized the need to develop metrics using photochemical models with the best science available and, then, to compare the results with simpler models such as EKMA. He feels that it is very possible that such simple models could be adequate for developing a reactivity scale.

Roger Tanner (TVA) commented that the data shows clearly that ozone formation is NO_x -limited in some areas and is VOC-limited in others and that these conditions vary greatly by location and by season, depending on the sources of VOCs and NO_x . He believes that a metric is needed that scales with the actual conditions within an airshed. In order to predict ozone reduction in particular locations and at the times necessary get below the standard, a sliding airshed-specific metric is needed. Dr. Tanner believes that this type of metric can be devised with our current scientific knowledge.

Ken Schere (EPA/ORD) discussed the differences between developing assessment tools and procedures and screening tools for implementation. Between these two ends of the spectrum, there are many possibilities. The scientific tools are available to do a full scale assessment to describe reactivity as a function of various environmental variables. Dr. Schere commented that Dr. Russell showed that a sophisticated tool can be reduced down to a simple screening tool. In order to decide where on the spectrum we need to be, it is necessary to know what the policy makers need.

Randy Pasek (CARB) expressed his agreement with comments made previously about California's reactivity regulation. The regulation is limited and complex. But California has been moving ahead since the regulation was developed. From a regulatory perspective, Dr. Pasek believes that the policy must be based on good science and that the complexity should be understood. And it is very important that the policy be constant. He echoed Dr. Wheeler's suggestion to build into the policy a process for change in order to make the policy more stable. CARB has a policy based on the MIR scale, because it is a good complement to the NO_x controls. Lastly, Dr. Pasek expressed his agreement with the comment of Ms. Francis that the science is adequate to develop regulations, as has been done in California.

Dave Golden (SRI and Stanford University) believes that good models are needed to understand any complex process. He continued by commenting that although the science has advanced very far and the models are reasonable, there are a lot of things we don't know. He warned that we shouldn't think that because we can model something that the models are necessarily correct. He expressed his inability to believe in a model that predicts $\text{PM}_{2.5}$. He concluded by urging that the scientific work and the funding be continued.

George Brown (National Aerosol Association) discussed the problems caused by the huge variability in VOCs and the fact that the current regulations treat them as being equal. This situation severely inhibits the use of certain substances and outlaws the use of others. As an example, on January 1, 1999, CARB will implement a rule that allows zero VOCs in one

product. Mr. Brown believed this is ludicrous. The National Aerosol Association (NAA) has supported several reactivity studies over the last ten years and, based in these studies, they are committed to the regulatory use of relative reactivity. The NAA realizes that some substances or products will have difficulty operating under that system and they don't, as yet, have the solutions to these problems. At the present time in California, the NAA believes that relative reactivity ought to be used on an optional basis by sources having trouble meeting a mass-based standard. Lastly, Mr. Brown believes we should stop thinking in terms of cutting down the mass of precursors of ozone and begin thinking in terms of ozone limitation itself.

Phil Ostrowski (Occidental Chemical Corporation) commented about the economic benefits of reactivity regulations. Properly designed reactivity regulations should provide a tool whereby small solvent users can avoid installing costly control equipment. This will provide good environmental benefit at a low cost.

Jeff Gaffney (Argonne National Laboratory) echoed some of Dr. Golden's preceding comments. He urged the group not to forget about VOC chemistry and not limit the discussion to only the ozone-driven aspects. It should be remembered that VOCs form fine aerosols and other products such as nitro-phenols that are very toxic and water soluble. Wet deposition, cloud condensation, climate effect, and radiative properties (UV and IR absorption) of VOCs should also be considered. He made a plea for the science and the sum-level support of the science. He believes that by understanding the science better, the scientific community will be able to provide a knowledge base to allow the policy makers and the modelers to do a better job.

Tim Lawrence (Georgia Pacific and American Paper and Forestry Association) commented that, although the science has been fascinating, we must recognize the need for pragmatic regulatory tool development in parallel with the existing scientific research. At this time, EPA is moving forward with implementation plans for a national ambient air quality standard for fine particulates, ozone, and regional haze; VOC and NO_x are all listed for controls under these programs. By November 2000, 170 different industrial categories will receive MACT standards. For organic HAPs, many of the MACT floors are being set based on existing VOC controls. There is also implementation of the Kyoto Treaty that needs to be considered. Mr. Lawrence feels that there need to be two parallel tracks: (1) one track moving forward very quickly because of pending regulatory decision that have to be made and (2) the other track continuing to understand the details of the science. Regulatory tools such as those described by Donna Kenski (EPA, Region 5) are important in the near term to assess the effectiveness of proposed regulatory action.

Praveen Amar (NESCAUM) stressed the need to look at aerosol forming potential of VOCs which might be exempted, in addition to the ozone forming potential. As an example, between 33% and 40% of the fine particles in the Northeast are organics. Consideration should also be given to wet deposition, dry deposition, and toxicity.

Doug Fratz (Chemical Specialties Manufacturers Association) made comments comparing the use of regional or local reactivity scales versus the use of a linear national scale. There are a number of control types that could be controlled locally. For other sources, such as consumer products, it would not be practical to have a different product for every local region. Therefore, to use reactivity, there must be a single national scale based on a single metric. Mr. Fratz also commented on the funding of research as compared to the cost of controls. He feels

that research is still under-funded and that the ratio of money spent on controls to money spent on research is far too high.

Jeffrey Holmstead (Latham & Watkins) stated that in the regulatory arena, we operate in a legal framework that doesn't offer much flexibility. He hopes that in the long term, the framework can be changed to allow flexibility. But in the near term, there are things that can be done. Mr. Holmstead reminded that group that they already have a reactivity scale where everything is either a 0 or a 1, and he believed that it would be hard for this group to do worse than that. In the near term, he believes that the current knowledge can be used to help people move from using highly reactive compounds to using lower reactive compounds. In the long term, the scientific research needs to continue. Mr. Holmstead urged the group not to let the perfect be the enemy of the good in the short term.

William Carter (University of California) wanted to echo what Mr. Holmstead said about the near term problems. There are three approaches to using reactivity: the two currently used reactivity scales (the binary national scale and the California MIR scale) and airshed/scenario specific assessment. The scientific basis of the ethane exemption standard is not good. This is why the EPA has frozen the exemption petitions, but these can't stay frozen for long. Dr. Carter suggested that in the near term the EPA do a modeling assessment to recertify the ethane standard or identify another standard. This would then allow the present method to continue while alternative methods are being developed. In California, the regulations they are developing require a scale which, if nothing else is put forward, is going to be the MIR scale. With the demand for stability, if the MIR scale is implemented (later in the year), it will be difficult to change. Therefore, this is the time to provide an alternative. Dr. Carter strongly emphasized the urgency of this problem.

Bob Avery (Eastman Chemical Company) recommended two tracks be followed in the future. Although the modelers are improving our understanding, the necessary results will not be available for three to five years, optimistically. A more realistic time frame is between five and ten years. The current system is bad and, therefore, a better interim system is needed for the next two to five years. Mr. Avery suggested that a few dozen individuals should be able to sit down in a room and improve on the current binary policy.

Cyril Durrenburger (Texas Natural Resource Conservation Commission) discussed the Control Measure Catalog developed for the last SIP submitted by Texas. It is a metric that ranks the VOC controls based on the tons reduced, toxicity, and the reactivity using Dr. Carter's MIR scale.

Robert Wendoll (Dunn-Edwards Corporation) discussed two approaches to the policy/science issue first raised by Mr. Hokeman. The scaling approach is used to rank VOCs by some reactivity metric for regulatory purposes. There are policy decisions that have to be made and some of these will be arbitrary, by necessity. Other decisions would be arbitrary only because of the lack of scientific information. The complementary approach is the systemic approach which is the study of actual emissions into ambient air to determine their potential to contribute to high ozone levels across the full range of environmental conditions. Mr. Wendoll believes that the systemic approach is important because it is the area of research that will develop the policy-relative science or the science that links actions with outcomes. This allows the policy makers to choose action intelligently. Mr. Wendoll believes that both the scaling approach and the systemic approach should be pursued simultaneously. The policy makers must

realize that both of these approaches together are embedded in the total ecological impacts. There will be other factors that affect the regulatory decisions being made, such as the impact of the regulations, including material resource and energy consumption, waste disposal, and water quality. Mr. Wendoll echoed the comment made by Mr. Fratz about the ratio of research spending to compliance spending. He believed that the amount of money that needs to be spent on the research necessary to provide a better basis for sound regulations is minuscule compared to the cost of compliance. Lastly, Mr. Wendoll reminded the group that control costs also have indirect health impacts by reducing available income.

Dave Morgott (Eastman Kodak Company) commented that in order to assess the intrinsic impact of VOCs on the environment, the more appropriate scale is the MOIR scale and not the MIR scale. The MOIR scale provides information about the peak amount of ozone that can be formed when a quantity of VOC is introduced into the environment.

POLICY AND SCIENCE QUESTIONS SUMMARIES

Howard Feldman (Moderator) introduced this segment of the workshop by asking the group to consider what needs to be done next. A review of these policy and science questions will be a form of guidance. This is a genesis workshop and a group will be formed as a result of this workshop and will continue these discussions. Mr. Feldman reviewed the policy questions listed below and asked the group if these are the right policy questions. He also asked the group if there are other questions that should be added to this list.

POLICY QUESTIONS

1. How should reactivity policy account for interaction with other air-pollution problems?
2. How should the reactivity concept be used to both maximize environmental benefit and encourage environmentally superior product development? “Exemption” vs. “substitution”?
3. What is the maximum uncertainty level that can be tolerated for reactivity-related decision making?
4. Exemption policies:
 - _ Bright line vs. bright band?
 - _ Environmental cofactors?
 - _ Where, ethane?
 - _ Molar or mass basis?
5. Exemption protocols:
 - _ Cookbook?
 - _ Maintenance and tracking?
 - _ Automatic testing criteria?
6. Procedures for modifying exemption criteria? Grandfathering? Grace periods?
7. Substitution protocols and guidelines?
8. How should vapor pressure be incorporated into the decision process?

Bob Avery (Eastman Chemical Company) raised the issue of national standards versus regional standards, and he believes that this question needs to be added to the list.

Edward Edwards (Dunn-Edwards Corporation) was concerned about availability and whether availability will be considered when making policy decisions. Availability is the issue of the difference between what’s in the can and what’s in the air. He was also concerned about looking at the time domain used to assess the ozone impact. For example, a paint may last from between two to fifteen years, depending on how it is formulated. The question is will the ozone impact be assessed only for the one-time application or for the full life cycle of the product. These are both very critical policy decisions in analyzing how to- determine whether the VOC life cycle is important for ozone forming potential.

John Kurland (Union Carbide) made comments on question 8 that deals with vapor pressure. He stated that the issue of volatility is a subset of the general issue on how much of the content becomes emissions. There are other environmental non-evaporative fates (e.g. down the drain). Dr. Kurland believes that this question should be expanded to include consideration of

whether the policy can properly determine the actual emissions released into the atmosphere as opposed to other estimates such as gross sales.

John Durkee (Creative Enterprizes) commented that an additional policy question is needed that deals with the issue of communication of the policy to the affected community. Policy which can't be communicated may not be good policy. As the policy is developed, consideration should be given to how the policy will be communicated, because, regardless of the quality of the science, the end-user won't buy it if they don't understand it.

Howard Feldman (Moderator) reviewed the science questions listed below and asked the group if these are the right science questions. He also asked the group if there are other questions that should be added to this list or if any of these questions should be taken off the list.

SCIENCE QUESTIONS

1. Is a reactivity-based policy practical, feasible, and beneficial?
2. How do we best factor long-range transport into a reactivity-based strategy? How about co-dependencies with PM?
3. What are the uncertainties of the various possible reactivity scales?
4. What are the advantages/disadvantages of using MODELS 3 for estimating reactivity?
5. What are the merits of using speciated VOC reactivities, as opposed to lumped VOC reactivities?

William Carter (University of California) commented that several of these questions are actually policy questions. The questions on the practicality and feasibility of a reactivity-based policy are policy issues. Although the question on the benefits of a reactivity policy is a scientific issue, it would require a policy on how to measure the benefit. Also, the question on using MODELS3 (question 4) has both a policy and a science component. Whether or not photochemical grid models can be trusted is a science question, but the advantage or disadvantage to using one is a policy question.

Anne Giesecke (American Bakers Association) commented that it is difficult to divide science and policy issues. From an industry perspective, they are looking for regulatory baselines: predictability, long-term planning, and basic functionality. Baking companies currently work with a very high level of uncertainty on their emissions (+/- 30%). This is acceptable, because it provides a regulatory baseline that tells them if they are in or out of an EPA threshold for clear air requirements. For this reactivity-based policy, the same level of science and policy would be acceptable, if it establishes a regulatory baseline.

Jason Ching (EPA) wanted to clarify that MODELS3 is not a model, but it is a community modeling framework. MODELS3 is a tool, and the scientific and policy-making communities have to decide what science will be used at any given time to set policy.

Jake Hales (ENVAIR) commented that Question 4 was intended to be more generic than just MODELS3. He suggested that MODELS3 be replaced with 3-D or Eulerian models. Howard Feldman (API) suggested that a Question 4a be added: how do you use one of these models to determine a relative or incremental reactivity for substitution purposes. Other related questions are: how many simulations are needed, how good do the databases need to be for a

given urban area to do these calculations on a national level, or, if a scale is used, was the modeling used to develop the scale adequate.

Jim Vickery (EPA/ORD) would like to add a question about timing. He asked the scientists what could they produce in the next two to three years that could help guide the policy. This would allow the policy maker to decide if they should develop an interim policy or if they should wait for a permanent answer.

William Carter (University of California) wanted to add to Question 4: What is the distribution of conditions where ozone is a problem and where VOC control is relevant.

Howard Feldman (API) commented about the time period of a scale: 1-hour or 8-hour or some other time period.

Ed Edwards (Dunn-Edwards Corporation) was concerned about the sensitivity of the models and their ability to measure small changes in product formulations and how these small changes are expanded into an airshed which contain only fractional percentage of VOCs.

Jim Berry (Berry Environmental) made several comments concerning the change in 1976 from Rule 66 to the beginning of the federal program. Rule 66 was based on reactivity measurement for one solar day. Subsequent work based on multi-day exposures, recognized that many of the compounds that Rule 66 exempted actually reacted over the longer term. In earlier discussions, Dr. Jeffries stated that half of the ozone formation was the result of slower reacting materials. Mr. Berry continued by discussing the impact that Rule 66 and, subsequently the change to the federal program, had on various industries. He commented on the resources spent on reformation to comply with Rule 66 and then again to comply with the federal program. He urged that the lessons learned in 1976 not be forgotten, and that changes be made to the federal program only after there is a longer term vision.

Paul Makar (Atmospheric Environment Service) asked if it would be possible to create a hierarchy of methods for measuring reactivity that agree with one another.

Jeffrey Gaffney (Argonne National Laboratory) suggested that a question be added about the reactivity of secondary products of the primary emitted VOCs. The chemistry of these secondary products needs to be understood, because they will play a role in the long-range transport issue.

PUBLIC/PRIVATE PARTNERSHIP DISCUSSION SUMMARY

Jake Hales (Moderator) began this portion of the workshop by describing NARSTO. Dr. Hales then asked the group if it is appropriate to go into a public/private partnership to pursue the reactivity issue, either within NARSTO or separate from NARSTO. Dr. Hales described his views on the function of this committee as follows: (1) to establish the forum for communication among interested participants, including the policy community and (2) to design a plan for the future strategy for reactivity research and to provide a time table for the research. He asked the group if there were any strong feeling against forming a public/private partnership. He took the lack of response from the group as consent.

AD HOC OPERATIONS TASK FORCE DISCUSSION SUMMARY

Jake Hales (Moderator) began by describing his thoughts about generally how this ad hoc task force would operate. Anyone would be welcome to participate. At a minimum, there would be several meetings per year. There would be communications on a regular basis. Travel expenses would be the responsibility of the individuals participating.

A question was asked about whether the ad hoc task force would necessarily function under NARSTO. Dr. Hales responded by stating that the task force could be either independent or it could work as a functionary group under NARSTO. It could blend into all of the NARSTO task activities: modeling, chemistry, observations, assessment, etc. If the group was to work under NARSTO, it would have to adhere to the quality assurance and data management guidelines. It would also have to adhere to the basic NARSTO principles which are to do good research for the benefit of policy.

Dr. Hales continued by asking for volunteers to serve on the ad hoc task force. There was a show of hands. Dr. Hales suggested that a sign-up list be circulated, and that the group caucus immediately after lunch.

Dr. Hales began the discussion by asking the group if this ad hoc group should function under the NARSTO umbrella. Robert Wendoll (Dunn-Edwards Corporation) asked if NARSTO doesn't also have to agree to this association. Jake Hales described the standard procedures for NARSTO to accept a field program under its umbrella. The Science and Resource Planning group makes these decisions, but he expects no problem with this. William Carter (University of California) suggested that the group encourage European participation, who have made important contributions to this work. Dr. Hales responded by saying that NARSTO has in the past worked with the Europeans. EuroTrac is an affiliate member of NARSTO and other European efforts could be in the future.

Bob Avery (Eastman Chemical Company) asked about alternatives to NARSTO. He didn't feel that the workshop group had the information available to make the decision on whether to associate with NARSTO. Mr. Avery was particularly interested in more information about the costs associated with association with NARSTO. He asked if the EPA could provide the leadership as an alternative. Jim Vickery (EPA/ORD) responded by stating that the EPA is committed to conducting and organizing all of their ozone related research through NARSTO for two primary reasons. This has helped to coordinate all of the different aspects of the research and to effectively allocate the scarce resources of people and money. Dr. Vickery strongly recommended that the ad hoc task force operate under NARSTO.

Jeffrey Holmstead (Latham & Watkins) asked how this effort would feed into the EPA's policy decisions. He asked about the EPA's level of interest in pursuing these issues and whether the EPA is in a position to accommodate the changes in the policy that this group would recommend. Jake Hales expressed his observation that a simple liaison with a policy team is not effective. There needs to be a strong presence of EPA policy people in the partnership. Bill Johnson (EPA/OAQPS) responded to Mr. Holmstead's question by stating that this question is one that EPA's management would need to answer. Joe Paisie (EPA/OAQPS) added that as Sally Shaver (EPA/OAQPS) said in her introductory comments to this workshop, the EPA is here to listen, and has been listening, but they are not prepared to say what the results will be yet.

It was asked if this activity could enjoy equivalent status with the recent FACA process. That is, could there be direct EPA/OAQPS participation in the process.

Jeffrey Gaffney (Argonne National Laboratory) asked about extending invitations for participation in the task force to people who had left or who didn't attend the workshop, such as automobile makers. Ron Patterson (EPA/ and NARSTO) commented that several people who are no longer here did complete the commitment forms made available at the beginning of the workshop. He added that many of the automakers are members of NARSTO.

Tim Lawrence (Georgia Pacific and American Paper and Forestry Association) commented, based on his experience with several FACA processes, that the level of interest, participation, and commitment of resources, particularly by the regulating community, is directly related to their sense of just how serious EPA is about moving the process forward to a useful endpoint. He concluded that it will be very important at the beginning to see some real finite indication of EPA's level of interest.

Howard Feldman (API) commented that the next step is to develop a plan with a specified time horizon. It will be important to know what time horizon EPA would be receptive to on the policy side. On the other hand, it is important to continue to work towards the good science, because the policy makers will use it if it is there.

Jim Vickery (EPA/ORD) agrees with Mr. Feldman's comment about the importance of good science and the fact that it will feed into the policy process. He described the difference between the FACA processes and NARSTO. For the FACA process, there was a statutory driver that required an output by a certain date. There is no such a driver for the reactivity policy. Reactivity research is very much like the other ozone research organized under NARSTO. Under NARSTO, the researchers and the policy makers are brought together to organize the research in such a way as to use the resources efficiently and solve the most important questions for the policy maker as quickly as possible. The EPA policy office is committed to using good science as soon as it is produced.

Jake Hales (Moderator) summarized this discussion by stating that there is consensus to form a public/private partnership on reactivity research and there are people interested in participating in an ad hoc task force to develop the forum, the research plan and the time table. Whether this task force operates under NARSTO is a question that will be deferred to the task force itself. Everyone interested in serving on the task force was asked to meet after the conclusion of the workshop.

MINUTES FROM RRWG MEETING ON DECEMBER 2-3, 1998

Wednesday, December 2, 1998

I. Welcome and Introductions

Acting Co-Chair, Robert Wendoll, called the meeting to order and requested that the participants introduce themselves.

II. Meeting Objectives

Wendoll stated the meeting objectives: 1.) To review progress since last meeting, 2.) To make decisions on organizational structure, and 3.) To plan steps to take to develop and implement research plans

III. Organizational Issues

A. Report on Chair selection: Wendoll reported that there was a tie between two candidates for the chair position, Jake Hales and Jonathon Wiener, and that J.Hales withdrew his nomination due to worries within NARSTO about potential conflict-of-interest between the RRWG position and his position as NARSTO management coordinator. Wendoll reported also that the RRWG Chair position was reopened, and that new nominations and proposals now need to be solicited from the Group. Proposals will be posted on the NARSTO web page (<http://narsto.owt.com/Narsto/>), as will notices of phone interviews for those members of the group who are interested in participating. January 15, 1999, is the deadline for receiving nominations and proposals, and February 1, 1999, is the target date for selecting a Chairperson. There was a discussion regarding setting up a conference call to discuss selection of the Chairperson and communicate other information to the Group.

Three candidates for the Chair position, George Talbert, Don Fox, and James Berry, gave brief talks on their backgrounds and qualifications.

B. Funding Mechanisms: Barbara Francis reported that 18 organizations have contributed \$2K each towards funding the chair position and other administrative costs of the RRWG. Some other organizations (government organizations) will contract to provide their \$2K directly to the elected chairperson. There was brief discussion on how the research plan would be developed and implemented. The response was that a list of needed research projects would be developed by Group members and prioritized by the Group, and sponsors would pick those they wish to fund.

Leslie Sue Ritts reported on funding possibilities from foundations such as the Gunn, Pew, and Mellon Foundations. This would be a good source of long term funding, but takes 6-9 months for the application process. Harvey Jeffries offered to work with Ritts to write a 1-page summary of the RRWG purpose and objectives, which can be distributed to potential funding sources.

In-kind contributions (such as photocopying, mailing, conference calls, etc.) were also mentioned as a significant funding source that would reduce the total cash needed for

administrative purposes. The EPA participants suggested that if the GGWG meetings are held in the RTP area, EPA would probably be able to provide requisite meeting facilities and clerical support.

C. Voting Structure: The group discussed Basil Dimitriades' "RRWG Membership Rights and Obligations". All agreed on the first point. The group suggested changing the end of the sentence in the second point to read "free to compete for *contracts arising from RRWG activities*," and changing the 3rd point to read "...which conduct in-house *research, provide in-kind contributions*, or sponsor...". A correction was pointed out by Dimitriades, replacing the word "objective" in the 6th point with "consensus".

Much discussion ensued on what constitutes eligibility for the Executive Assembly of the RRWG. One suggestion made was that eligible would be those who provide funding above a certain level (as yet undefined), i.e. to use "those who give should get" as a way to encourage funding. On the other hand, others pointed out, for the RRWG to be a truly public-private partnership, the Group should be receptive to inputs from all, strive to reach decisions by consensus, and avoid the appearance that it is the organizations with the most money that decide what research is important. Participants noted the NARSTO "science teams" approach, by which, in practice, most of the science team decisions are made by consensus with little need for voting. Wendoll suggested an interim solution: those organizations which have contributed the initial \$2K to the administrative fund, will be the ones eligible to vote on how this fund is to be used (for the chair position). He suggested, further, that the Organizing Committee will make the final selection of the Chairperson with the input of these funding organizations. Decisions on eligibility to vote on future issues, such as, e.g., for development of research and assessment plans, were put off for later.

D. Standing Committees: The RRWG examined the NARSTO model of science-based teams, and compared it with its own current structure of three committees/teams - - Organizing Committee, Science Assessment Team, Policy Assessment Team. The Group agreed that it might be premature to start development of a Research Plan and new committees before the Assessment effort is finished. In the meantime, it was proposed that the Organizing Committee continue to exist until a full-time Chair is appointed.

During discussion on finalizing the assessment reports, Wendoll suggested appointing a Synthesis Team to integrate the work of the Science and Policy Teams. The Synthesis Team will create one integrated document that addresses all of the issues raised in the charge to the Initial Assessment task force, and will contain a Synopsis and an Executive Summary. Due to the fact that the assessment reports are not finished yet, assignments for the Synthesis Team were not made.

Dimitriades suggested that the Group should have all assessment reports (once they are finished) reviewed, and formally endorse them. Then they can be published if desired by the authors, but can be used by the RRWG in the meantime.

IV. NARSTO Update

Ron Patterson presented the revised NARSTO Charter including the reactivity work, and asked the RRWG for comments prior to its final presentation at the NARSTO meeting in January. He discussed the process of becoming a sponsoring or participating or associate partner in NARSTO, and reported that the first NARSTO product, the State-of-Science Ozone Assessment reports are available on the web. They are scheduled to be reviewed by the NRC in December, 1998.

Thursday, December 3, 1998

V. Initial Assessment Reports

A. Progress Review and B. Discussion - - Science Assessment

1. Atmospheric Chemistry: Dave Golden highlighted important parts of the report, emphasizing the dependence of the ozone reactivity of a VOC on the ability of the VOC to initiate radical formation and on the VOC/NO_x ratio. The inorganic chemistry is pretty well known, with the exception of uncertainties in the formation of HONO and in the primarily heterogeneous hydrolysis of N₂O₅ to HNO₃. Uncertainties in the organic chemistry follow those outlined by Atkinson in the NARSTO assessment; major ones include the lack of data on the reactions of intermediate radicals, questions about pressure dependence and the special role of H₂O as a third body, reactions of aromatics, and reactions of O₃ with alkenes. He suggested that ab initio theoretical calculations of potential energy surfaces can be very useful, but are currently underused in the tropospheric chemistry community.

Bill Carter discussed chemical mechanisms. Important considerations in using a mechanism include how up-to-date the mechanism is, what estimation methods it uses to treat uncertain chemistry, the degree of condensation (especially for reactive products that can become important when concentrations of integrated radicals are high), the extent of evaluation of the mechanism (this is especially a problem at low VOC/NO_x ratios where the mechanisms have not been evaluated), and whether the mechanism is suitable for reactivity assessments.

Aerosol Forming Potential: Prasad Pai discussed the two paradigms for secondary organic aerosol (SOA) formation presented in the assessment. The saturation method is used in most models (such as RADM2 and SAQM) and assumes that aerosol formation does not occur until a saturation vapor pressure is reached. The absorptive partitioning method, which describes SOA formation in terms of the initial aerosol concentration, a partitioning coefficient, and a stoichiometric coefficient, better explains the wide variation in experimental measurements, and is used in a few models such as the CIT and revised UAM-AERO models.

It is currently not clear to what extent ozone formation and SOA formation are correlated. It is also unclear what fraction of PM_{2.5} is "typically" composed of SOA.

Emissions: Paul Makar discussed emissions as they relate to airshed model input as well as volatility and availability issues in emissions determination. Sensitivity analyses need to be done to determine the effect of uncertainties in emissions source and temporal approximations, and they need to be done in different environments. There are still many uncertainties in biogenics emissions, such as the role of genetic variability, wounding, and chemical losses at the source. The volatilization rates of chemicals are not well handled in the models.

Jeffries commented that the models must be able to differentiate between weekday and weekend emissions and correctly model concentrations on both types of days.

Air Quality Models: Gail Tonnesen highlighted topics that are covered in the models assessment document. Box and trajectory models have been used in the past for reactivity calculations, but researchers are starting to use Eulerian grid models more. The differences between the two types of models are important because box models can't correctly represent transport and dispersion, which can significantly affect the reactivity calculations. This assessment document identified different types of sensitivity tests that can be performed, and discussed errors in model evaluations.

Environmental Conditions: Jay Olaguer discussed the role of long-range transport in reactivity assessments, and how penetrating convection can bring ozone and PAN to the surface from above the boundary layer. Transport across the domain boundaries must also be considered. These additional sources of radicals will change the calculated VOC reactivities. Carter stated that we must also study the role of differences in environmental conditions (VOC and NOx levels) used in the MIR calculations, since most of them were done using EPA's "39 cities" study which is not well documented.

Persistent Organic Pollutants: Phil Ostrowski discussed the need to consider the environmental fate of "persistent, bioaccumulative, toxic" (PBT) pollutants. Jeffries stated that the toxicity of a replacement compound should be considered in reactivity substitutions, not just its ozone formation potential, i.e. we must consider reactivity in a "one atmosphere" sense.

Reactivity Assessments: Carter presented things that must be considered when performing a reactivity assessment. These include how you quantify the VOC impacts on ozone air quality (impacts on peak ozone, integrated ozone, other), what type of model to use (box/trajectory or grid), how to assess the variability of the measure (how to account for time/space/scenario differences), and how the uncertainty in the chemical mechanism affects the reactivity scale. The chemical mechanisms probably have at best +/-30% uncertainties.

Jeffries stated that we don't currently know how to do a reactivity assessment related to exemption policies, using an Eulerian model, i.e. how to match techniques with policy needs. He discussed how the treatment of radical source strength and loss processes determine the reactivity, and how, therefore, differences in calculated reactivities (i.e. Derwent vs. Carter) can be explained by differences in the radicals. He mentioned that most ozone formed in a multi-day episode is due to the previous days' organic reaction products. He also cautioned that the group be cognizant of the distinction between how much a VOC contributes to ozone formation versus how much the O₃ changes with decreases in VOC emissions. The latter sensitivity measure is the information needed for use in control strategies. The former, however, is also important in that it helps explain the sensitivity of ozone formation to VOC changes (i.e. know not just "what happened" but also "why it happened"). The RRWG must also figure out how to communicate

its conclusions to policymakers. We must be sure that reactivities that we calculate using current conditions are applicable to future conditions, where many other variables will change in ways that are difficult to quantify at the current time.

Jeffries suggested that the assessment documents be considered “living documents” to be updated from time to time.

A. Progress review and B. Discussion - - Policy Assessment

Tom Helms discussed the work of the Policy Team. He presented and briefly discussed the 12 draft documents compiled thus far:

1. Outline of Draft White Paper (Dimitriades)
2. Overview of an Ongoing Investigation on Approaches to Controlling VOC Emissions in Industrial Nations (P. Lambert)
3. “Policy Statements and Other Publicly Available Documents Related to Reactivity”(W. Johnson)
4. “A VOC Reactivity Plan Using Community Multi-Scale Air Quality Models with Advanced Chemical Mechanisms” (Jeffries)
5. “The Role of Low Vapor Pressure Organic Compounds in Atmospheric Ozone Formation (R. Avery et al.)
6. “Definition of VOC: Rationale” with attachments including “experiments on the Distribution of organic Pollutants between Airborne Particular Matter and the Corresponding Gas Phase”
7. “Scientific Basis of an Improved EPA Policy on Control of Organic Emissions for Ambient Ozone reduction” (journal article to appear in the May-1999 issue of JAWMA)
8. “White Paper on VOC Reactivity Exemption Options” (R.Wayland)
9. Enhance EKMA Diagram (J. Dege)
10. “Volatility” (J.Berry)
11. “California’s Low Emission Vehicles and Clean Fuels regulation” (R.Pacek)
“Developing a Hydrocarbon Reactivity Based VOC Control program for Consumer Products (R.Pasek)
12. “Consumer Products Industry Policy Proposals on Reactivity” (D.Fratz)

VI. Research and Assessment Plans (Discussion put off to next Group meeting)

VII. Tasks/Assignments/Deadlines

The following timetable was agreed upon:

- | | |
|--------------------------------------|-------------------|
| - Comments on White papers: | 12/31/98 |
| - White Papers Internal review: | 1/15/99 |
| - Final Drafts: | 2/1/99 |
| - Complete draft “Executive Summary” | 3/1/99 |
| - review by NARSTO: | Within two months |

VIII. Other Business (None)

IX. Next meeting and Adjournment

- Next meeting of RRWG: 3/24-25/99 (at EPA/RTP)
- Following RRWG Meeting: 6/9-10/99 or 6/16-17/99

Minutes from RRWG Meeting on March 24-25, 1999

Wednesday, March 24, 1999

I. Welcome and Introduction

Acting co-chair, Robert Wendoll, called the meeting to order and requested that the participants introduce themselves.

II. Organizational Issues

The first order of business was the installation of Dr. Don Fox as chairman of the RRWG. Robert Wendoll symbolically handed a gavel to Dr. Fox thereby signifying the assumption of the chairmanship by Dr. Fox. Basil Dimitriadis then expressed appreciation to Mr. Wendoll for his efforts in helping organize the RRWG, in serving as acting co-chair, for presiding over early meetings and conference calls, and for providing valuable services in producing and distributing agendas and other written materials necessary for the operation of the RRWG. The attendees applauded Mr. Wendoll for his contribution. Don Fox thanked Basil Dimitriadis for also serving as acting co-chair of the RRWG during the organizational phase. From this point in the meeting, Don Fox chaired the proceedings.

The next order of business was consideration of the proposed steering committee. The size of and the need for a steering committee were discussed. Some members felt that a smaller steering committee consisting of the chairman and co-chairs of the science and policy teams would be sufficient. Others expressed a concern that no one who wished to participate be left out of participation in decision making. Harvey Jeffries pointed out that the proposed steering committee is very similar in size and composition to the informal organizing committee, which had served in the early stages of the RRWG formation. A motion to postpone the steering committee decision until the next day was made and the motion passed by vote.

The next organizational item was a report by Barbara Francis of the Chemical Manufacturers Association, concerning funding of the RRWG, which is used to compensate the chairman. Ms. Frances said the CMA had contracted with the University of North Carolina, where Dr. Fox is on the faculty, for \$30,000 for one year of Dr. Fox's service. This represents several \$2,000 contributions from individual companies. A first payment of \$6,000 has already been made. EPA and State governments will transfer their contributions by contracting directly with UNC.

Leslie Ritts gave a report on her efforts to ask charitable foundations for support for the RRWG. She said that the following foundations have been

contacted:

Pew
Gunn
John S. Mott
Andrew Mellon
Rockefeller
Ford

Funding in the level of \$40,000 to \$60,000 has been discussed. One problem has been that neither the RRWG nor NARSTO is registered as a tax-exempt organization. There is a possibility that money could be given to the University of North Carolina and be used to support RRWG through Dr. Fox's participation.

III. NARSTO Update

Dr. Jake Hales of NARSTO gave an update of NARSTO activities that are relevant to the RRWG. Fine particulate matter research is being undertaken by NARSTO. Dr. Hales noted several recent NARSTO related conferences and documents concerning ozone. The current assessment document for ozone is under review by the National Academy of Sciences. Information about much of this is available on the NARSTO website. Dr. Hales said that all RRWG members would soon receive an invitation to join NARSTO.

IV. Integration of Science Assessment and Policy Assessment Draft Documents

Don Fox gave a PowerPoint slide presentation concerning integration of Science Assessment and Policy Assessment. Copies of this slide presentation were made available to attendees. This presentation summarized and synthesized the draft VOC reactivity science assessment and VOC reactivity policy white paper. Copies of drafts of both of these documents were also available at the meeting. Dr. Fox discussed how these draft assessment reports fitted into the framework of the RRWG as expressed by the RRWG mission statement. Dr. Fox reviewed various possible control strategies and also discussed various science uncertainties.

A discussion followed Dr. Fox's presentation. A comment was made that the last bullet in Dr. Fox's presentation is of key importance. That bullet asks, "Will changing the VOC reactivity of anthropogenic emissions to the atmosphere limit the formation of ozone and/or PM?" Another person asked whether we are talking about peak ozone or average ozone. Some one else asked whether utilization of reactivity would allow us to attain the NAAQS in a more cost-effective manner.

Dr. Gary Whitten gave a short talk describing UAM modeling of ozone caused by the addition of a compound to the air shed over the Los Angeles area. The modeling was done to represent a two-day period. Dr. Whitten said this work showed that xylene produced 5 times the ozone as ethane over this period (although the MIR of xylene is much higher than 5 times that of ethane.)

Ed Edwards showed a slide of VOC reactivity and NO_x reactivity at high VOC/NO_x ratios. He said that this graph demonstrates that some VOCs have a negative reactivity at high VOC/NO_x ratios.

Harvey Jeffries referred to a passage in the 3/24/99 draft version of the policy white paper which said: "The discussion of the benefits of substitution above presupposes that higher reactive compounds have less ozone generation potential over the atmospheric lifetime of the compound than a low reactive compound over its lifetime. This hypothesis would need to be clearly demonstrated before restrictions on total mass of VOC emissions were relaxed. Any existing supporting data needs to be published so that all policy makers involved are able to take it into consideration." Dr. Jeffries said this is a key issue with policy makers, which needs to be answered to their satisfaction.

The discussion turned to NO_x limited areas. Ed Edwards said that it might be reasonable to market separate product lines for VOC limited areas and for NO_x limited areas. It was suggested that an important research goal might be to determine which geographic areas are VOC limited and which are NO_x limited. Gary Whitten said that big grid squares in a model may make most areas seem NO_x limited. If you go to smaller grid sizes, some of the areas would begin to appear as VOC limited. Someone asked whether sections of the country may be sometimes VOC limited and at other times NO_x limited.

Dr. William Carter summarized the discussion by seeking a response to the question "Is reactivity a good idea?" Harvey Jeffries said that if we find reactivity is worthwhile, as we well might, that there is still much work left to be done.

Thursday, March 25, 1999

Dr. Fox called the meeting to order. He then discussed the possibility of changing the location (and possibly even the date) of the June 9-10 RRWG meeting. There has been an annual meeting of ozone scientists from Germany and the USA in alternative years in either the USA or Germany. This year the USA/Germany meeting may be in southern California where they will discuss European involvement with smog chambers with Dr. William Carter. By moving the RRWG to the Los Angeles area, we can hold the meetings jointly and gain the advantages of additional expertise. It was thought that it would be appropriate to hold a RRWG meeting on the West Coast in any case. Since the USA/Germany meeting will be all week, it was suggested that the RRWG

meeting be shortened to one full day, perhaps on June 10. A definite decision was not made on this. Basil Dimitriadis said that the date for the European visit should be firmed up in 2 or 3 weeks. A final decision to move the RRWG meeting cannot be made until then.

V. Reactivity science Assessment

Dr. William Carter gave a talk on Reactivity Science Assessment. This was a thorough discussion that lasted much of the morning. During this talk various research areas for RRWG were identified and listed on flip charts for later prioritization. A summary of these research areas is listed as an attachment.

There were periods of discussion from the audience during Dr. Carter's talk. At one point Dr. Jeffries said that there is a lot of smog chamber data from Australia and from TVA on low NO_x conditions. He said this data has not yet been analyzed due to lack of funds.

Dr. Fox led a discussion of how the VOC Reactivity Science Assessment document should be treated. He asked whether the group had concerns on whether the science document is ready to be released to the public. After discussion, a vote was taken to put the science document on the NARSTO web site with "DRAFT -version 1" written on it. Dr. Carter said the thought the science document is close to being final except for some minor editing that needs to be done.

VI. Reactivity Policy White Paper Discussion

After lunch, Dr. Fox introduced Tom Helms who gave a talk on the VOC Reactivity Policy white paper (March 24, 1999 draft version). Mr. Helms said that we have omitted controversial items on which people had voiced disagreement. He mentioned that EPA lawyers had asked us to put a disclaimer in front of the white paper saying that document does not represent EPA official policy, nor does it necessarily represent the views of any particular company that participated in the preparation.

Mr. Helms asked if the white paper had missed any important issues. Dr. Gary Whitten said there needs to be a discussion to distinguish between impacts on overall air sheds versus things that affect individual sources, i.e. overall gross impacts vs. individual sources. Mr. Helms asked Dr. Whitten to write a short summary of that issue for the policy white paper.

VII. Session Summary

Dr. Fox summarized the discussion in this way:

1. The policy team will redraft the policy white paper and post it on

the NARSTO password protected site before the next meeting

2. The science team leader (Dr. Carter) will work with Mr. Helms to get a draft of the research plan for the next meeting.

3. Dr. Carter wants any final edits on the science document by the end of the next week (i.e. by April 2, 1999). Dr. Carter will then send this edited version to Don Fox to post on the NARSTO public web site.

The current version is not necessarily the final version, but it is close.
4. We will send a typed version of the research tasks identified during Dr. Carter's presentation to RRWG members by e-mail.

Don Fox will prepare an executive summary to be used as a preamble to the science and policy assessment papers that will be around 5 pages. A shorter one-page version of this will also be prepared for briefing outside persons such as possible funding organizations.

Bob Avery suggested a computer bulletin board where researchers could say that they would be interested in performing certain types of research. Potential sponsors could express interest in sponsoring certain types of research on this bulletin board as well. The group expressed interest in this idea.

Barbara Francis said that the budget process for the year 2000 would end by the end of June 1999 for many companies. We should earmark research money now to have it available to use during 2000. Even the June 9-10 meeting will be late to identify research needs for year 2000 funding cycle.

Harvey Jeffries recommended that documents to be distributed to the RRWG be sent to David Sanders of EPA as a central point and have Mr. Sanders distribute the documents. Mr. Sanders said he would be willing to do this. Having a central distribution point should result in less confusion than if many people are trying to distribute things.

The group discussed a tentative date for the Fall RRWG meeting. October 6-7 was chosen.

The question of the steering committee was raised again. Don Fox said he would like to postpone a decision on this until a later date. Dr. Fox thanked the organizing committee for getting the RRWG to the current point. The meeting was then adjourned.

Outline of Reactivity Science Research Issues

Basic Laboratory Studies

For:

- General effects

- gas/surface phase
- heterogeneity
- Multi-day chemistry
- Individual VOCs
- Improving analytical methods
- Synthesis of reactive intermediates

Evaluate/Improve Estimation Methods

For:

- Structuring reactivity methods
- *ab initio* methods
- Neural net techniques

Evaluate/Improve Chemical Mechanisms for Models

For:

- Appropriate level of condensation

Evaluate/Improve Smog Chambers

For:

- Better characterizing of chamber effects
- Analytical instrumentation improvements
- Distinguishing Simple vs. Complex surrogates
- Identifying gaps in current chamber studies, tests, databases

Develop Lower Cost/ More Applicable Screening Methods

For:

- Brute force/mass analysis (empirical analysis) of reactivity
- Method 24 improvements

Evaluate Aerosol Forming Potential

For:

- Chamber studies of aerosol yields
 - black light vs. sunlight yields
- Improving representation of aerosol formation in models
- Obtaining more data on composition of ambient aerosols
- Analytical development of aerosol studies
- Aerosol fate

Characterize Distribution of Conditions with Respect to Total VOC, NO_x, Reactivity Composition

For:

- Sensitivity composition changes
 - incremental analysis for NO₂

Atmospheric Analysis/Indicator Species for Model Evaluation and Compositional Changes

For:

- Atmospheric radical sources
- Improving atmospheric monitoring (e.g., NO₂)
- Atmospheric analysis for evaluating emissions inventory

Investigate Role of Long-range Transport

For:

- Improving representation of long-range transport
- Improving model representation of regional/multi-day transport
- Characterizing NO_x transport and fate (NO_x/NO_y in rural areas)

Identify Important Sources of VOC in VOC Impacted Areas

Develop Model Evaluation Criteria for Assessment

Improve Sensitivity Analysis Methods

Conduct Uncertainty Analyses

Make Models More User Friendly - More Generally Available

Improve Emissions Processing Modules

For:

- Resolving simplicity vs. complexity problem

Evaluate/ Improve Emissions Data

For:

- Speciation profiles
- Biogenic inventories
- Effects of emissions uncertainties
- Determining emissions variations resulting from changing policies

Availability and Fate

For:

- Improving availability information for various source types
- Improving representation of alternate fates and depositions in models
- Improving analytical methods
- Evaluating fugacity models
 - implement/incorporate fugacity model into atmospheric model

Persistent Organic Pollutants

Reactivity Assessments

For:

- Relative reactivity on all spatial and temporal scales

Evaluate Alternative Reactivity Metrics

Evaluate Effect of Small vs. Large Changes

Evaluate Reactivity for Present-day Base Case Scenarios and Attainment Scenarios

Improve Enforcement and Compliance

Using:

- Appropriate instrumentation

Summary of RRWG June 9-10, 1999 Meeting

I. Welcome and Introductions

Don Fox (UNC-Chapel Hill) called the meeting to order at 12:10 pm and welcomed everyone to North Carolina. After introductions by participants in the meeting, the agenda was presented.

The action items for this meeting are:

1. Select Near Term Research Projects (probably limited to 8-10)
2. Identify a variety of funding approaches.

Other items:

- (3) Discussion of Policy White Paper
- (4) Initial Assessment Executive Summary
- (5) Future Meeting Scheduling

II. Review and Discussion of Draft VOC Policy White Paper

Presentation by Tom Helms

The draft VOC Policy White Paper was distributed at the meeting. The Policy Team met on May 17-18 and generated a list of Policy-relevant research plan questions, which were distributed before and during the meeting. This information and the discussion at the June meeting are to be incorporated into Chapter 6 of the draft Policy White Paper.

Reactivity Policy-Relevant Questions Needing Scientific Investigation

1. In those areas where VOC reductions may be required, does “reactivity” make a difference (relative to mass-based reductions) in O₃, PM, and Regional Haze (RH)?
 1. How big a compositional change is needed?
 2. How widespread is the effect?
 3. How consistent spatially and temporally are the responses in O₃, PM, and RH?
2. What are the alternative ways of expressing the “differences” in question one above, and what are their advantages and disadvantages?
3. What are the ways of comparing the differences in VOCs found in question one above?
 1. What are the scientific data needed to do the comparisons?
 2. What are acceptable ways of adding new compounds to the system?

3. How consistent are the different approaches?
 4. Which ones are applicable for multiple pollutants (O₃, PM, RH)?
 5. Which are most appropriate for multi-day and multi-episode scenarios?
 6. Do any methods have “gaps” in the response by different VOCs?
4. What are the sources of total VOCs that can be influenced (locally, regionally, nationally) by regulatory reactivity policy?
 1. Which are the VOCs that can be influenced?
 2. What are the forecasts for emissions under a changed policy?
 2. If more compounds are exempted, what may be the impact on O₃, PM, and RH?
 3. What is the impact on total mass of VOC emissions?
 4. What are the likely forecasts of emissions under a changed policy?
 5. Can we quantify “uncertainty”?
 1. What are ways to accommodate incremental improvements in science?

Future Policy Committee Questions

6. What are the issues related to implementing, verifying, and enforcing regulatory reactivity rules?
 1. What test methods are needed?
 2. What record keeping is needed?
7. What are the likely costs of doing any of the activities identified in question one above?
8. What do we do with “uncertainty”?
 1. Is the uncertainty small enough to determine if the regulation is directionally okay?

Some Specific Questions That Need Good Answers

9. What are the roles of transport and multi-day stagnation?
10. What are the global implications on Global Warming Potential (GWP), Stratospheric Ozone Depletion Potential (ODP), persistent organic pollutants (POP), and formation of toxic secondary products?
11. What role does “atmosphere” availability play?
 1. Vapor pressure or evaporation rate?
 2. Fugacity?
 3. Water-gas phase partitioning?
 4. Particle-gas phase partitioning?
 5. Life cycle?

12. From the perspective of a reactivity policy, what does “integration” mean?
1. How can we do this?

Discussion

Tom Helms responded to a question about the legality of this process by stating clearly that EPA and the RRWG were not doing this activity under FACA. This was a free exchange of information for the express purpose of prioritizing research. The decisions that could ultimately be made after getting this technical information were not a subject for discussion.

The policy team framed these questions where the answers would make policy-relevant contributions by providing information to assist policy makers their deliberations to maintain or change the existing policy or generate a new policy.

Role of Biogenics

Distribution of biogenic emissions and their contribution to the reactivity of ambient mixtures in a particular region should be considered. Others commented that improvements in the chemical representation of biogenic compounds are occurring, but there are still uncertainties in the ability of models used to generate biogenic inventories to produce reliable predictive outcomes.

Spatial Scale

Applicable spatial scale was referenced. How big should a non-attainment area be? This issue becomes a testable condition once appropriate assessment tools are developed.

Role of NO_x

In response to a question asking for the RRWG develop a comparable NO_x document, several participants responded that the role of NO_x is explicitly described and considered in the VOC science assessment document and the draft policy white paper.

III. Presentation of Draft Research Plan

by Bill Carter

Science Assessment Document Categories

1. Reactivity Assessment
2. Atmospheric Chemistry
3. Emissions
4. Availability and Fate
5. Environmental Conditions
6. Air Quality Models
7. Analytical Methods
8. Persistent Organic Pollutants

Bill Carter posed a series of topics and options that follow:

Concerning Reactivity Regulations

- Are reactivity regulations a good idea?
- vs. How best to do reactivity regulations.

Types of Assessments

- Evaluate alternative exemption standards.
- vs. Develop better reactivity scales.
- vs. Improve methods to evaluate specific substitution scenarios.

Ozone vs. PM

- Develop ability to assess PM Impacts.
- vs. Reduce and quantify uncertainties in ozone impact assessments.

Type of VOCs

- Research on low reactivity VOCs for substitutions.
- vs. Research on VOCs that contribute most to the current problem.

Comment from Audience.

This framework is helpful but the research needed is generally not an “either – or” scenario.

Dr. Carter presented three major categories of questions and then presented a plan that described where the results of the different tasks identified in the science assessment document would contribute to answering the questions below.
(See Appendix - Matrix of Research Tasks and Relevant Questions)

3 Major Categories for RRWG Policy Questions
RRWG Research Plan

What will be the effects of reactivity-based controls?

- How will reactivity based controls affect emissions?
- How will reactivity-based controls affect air quality in different areas?
- What are the effects of changing the exemption policy?

How do we develop optimum reactivity based controls?

- How do we quantify impacts on O3, PM, RH and other pollutants?
- If the impacts depend on conditions, what conditions, or weighting for multiple conditions should be used.
- How will the policy deal with differing relative reactivities for different impacts?
- How does policy deal with uncertainties in reactivity assessments?
- How does policy deal with changes in knowledge?

How do we enforce reactivity based controls?

IV. Selection of Priority Near Term Research Projects (Fox)

An initial list of 11 research projects based on the draft research plan was placed before the group. Considerable discussion ensued from the floor with issues of available data or information, chamber and observational measurements, uncertainty and degree of importance, level of effort and cost. One research project was dropped from the list and the remaining ten were prioritized by the group by a voting on each project. (See Table Below) The notation refers to the corresponding section of the science assessment.

Table 1. Priority Near Term Projects

- Assess effects of large-scale reactivity-based substitutions on regional air quality using existing models [1.2.A] (25 votes)
 - Evaluate alternative reactivity metrics [1.5.1]
 - Uncertainty analysis [1.6]
- Analyze available information relevant to how much of the environmental would be sensitive to VOC controls, and the distribution of conditions appropriate for reactivity assessments [5.1.1A & B] (20 votes)
- Improve information on atmospheric availability of VOC with low volatility, [4.1], and evaluate existing fugacity models [4.3](13 votes)
- Survey amounts of emissions that are suitable for reactivity-based controls [3.1.1] (10 votes)
- Develop appropriate scenarios for general reactivity assessment [5.1,3]. (7 votes)
- Survey existing modeling assessments [1.1] (4 votes)
- Develop model criteria for reactivity assessments [6.1] (3 votes)

- Improve emissions processing modules in models [6.3.2] (2 votes)
- Use existing models to evaluate exemption standard [1.3.A] (3 votes)
- Evaluate existing chamber data base [2.4.1] (1 vote)

V. Possible Funding Sources

The discussion started in a very general manner with several topics raised by the group including generation of RFPs, scope and level of effort, individual or collective funding, research investigator involvement, and communication. Several process suggestions were made ranging from requesting proposals from investigators, development of research project white papers, forming ad hoc working groups for specific projects, to forming a funding group or committee. To proceed, relevant projects must be identified and the scope the work must be appropriate for an initial funding scenario. [At this meeting, the RRWG prioritized the near term research projects.]

RFP writing teams comprised of knowledgeable sponsors were proposed. It was suggested that the RFP development process be iterative – identify minimum need and proceed from there. The full level of detail might not have to be defined in the early iteration before making material available to the research community. At some point, pre-proposals or brief white papers by investigators to refine a research project or to identify research interests and capabilities could be solicited. Elements suggested include:

Elements of a Pre-Proposal/Scoping Paper

- Relevant Policy Topic
- Research Task
- Approach/Methodology to Solving the Problem
- Capabilities they possess
- Deliverables
- Some Indication of Level of Effort (e.g., time, money, etc.)
- Estimated Time Frame/Cost

Any of these approaches do not preclude a group of funders interested in a particular from coming together and contracting with researchers on a given project.

Process Question from Floor. Do all of our projects have to be reviewed by NARSTO?

The consensus was a combination of proposals and research projects will develop with some within the RRWG and others outside. The NARSTO review process is available for RRWG work. The quality assurance aspects of any research project are extremely important for credibility and any future value in the policy arena.

Summary of Research Priorities Discussion

Fox proposed the group work with priority projects listed in Table 1.

Fox requested the RRWG members do the following: (1) over the course of a short period of time (2-3 weeks), potential funders (at \$25,000 or above) are requested to identify themselves to Chair. In addition, specify the topic(s) of funding interest. Anyone interested in a specific topic would then become a sub-group working on this topic, and they could begin to identify potential researchers. The subgroup would then define the scope of the project with a funding level in mind. The chair agreed to distribute the list of self-identified sponsors to the membership.

VI. Draft RRWG Executive Summary

Presentation by Don Fox

Purpose of Initial Assessment Report - Executive Summary

- Introduction and General Overview
- Convenient Summary for Potential Sponsoring Organizations
- Marketing Tool for New Members

Contents

- Conceptual Framework
 - Policy-relevant science on reactivity issues
- Genesis of the RRWG
- Summary of key issues
- Major research recommendations

Discussion Points

The document needs explicit disclaimer that all this research may or may not be performed and perhaps a blanket disclaimer up front like EPA uses in its documents.

Some participants were concerned about potential liability with their names associated with this executive summary.

It was agreed that a disclaimer would be added to the draft executive summary. It was also agreed that if a company or organization had objections based on potential liability they would provide such comments to the Chair by July 15 th.

VII. Ongoing Reactivity and Related Research

• **NARSTO by Ron Patterson**

NARSTO Program Planning included a Modeling Intercomparison Study (U.S., Canada, Mexico - using the same data sets and best models available). These investigations are using the NARSTO-NE studies, along with some of the SOS data. The study is a two phase model intercomparison- (1) everybody models the same real estate for the same time periods using their own inputs (i.e., meteorology and inventories); (2) is much more constrained with common inputs for all modelers. Different versions of CB-IV as well as the Canadian models may be used. SOS - Nashville and Atlanta Intensive Field Studies for summer 1999, starts 6/15 in Nashville, July in Atlanta through August. For PM Research, meetings had occurred to begin planning on a Tropospheric Aerosol Program. NARSTO has established a PM Measurements Research Subcommittee and the QSSC Data Management research process is operational. Planning for the Texas 2000 Study on O3, PM2.5, and Regional Haze a field study, primarily run by NOAA; is underway currently. It comes under the Air Collection program of Texas - numerous aircraft involved and will cover the Gulf Coast to Oklahoma.

NARSTO has a total of 57 sponsoring members and 21 participating partners. NARSTO continues to publish a newsletter, it along with the draft ozone assessment report, critical review papers, QSSC Methods Compendium documentation, information from PM research planning workshops are all available on the NARSTO Website www.cgenv.com/Narsto/
The NARSTO data center is set-up to specifically handle requests from NARSTO participants for QA/QC.

• **Ongoing Research Activities at CARB**

Presentation by Eileen McCauley - California Air Resources Board (CARB)

- (1) Atmospheric Chemistry of Mineral Spirits
 - Product studies on three C10 alkanes
- (2) Development of Improved Reactivity Measurement Methods
 - Next generation reactivity techniques
- (3) Uncertainty Analysis of Chamber Data
 - Determine chamber parameters which contribute the most to uncertainty
- (4) Review of August 1998 MIR Values
 - Peer review of Carter's most recent mechanism
- (5) Reactivity of Stationary Source VOCs
 - determine reactivities and uncertainties of several compounds associated with consumer products

New Projects for This Year

- Improved Aerosol Speciation Profiles
 - Speciated profiles of up to 40 compounds
- Investigation of Low Reactivity Solvents for use in Consumer Products
 - Produce a public database of solvent properties
- Reactivity Values Using Airshed Models
 - Calculation of reactivity values using a 3-D airshed model (Ted Russell, PI) - using MAQSIP for San Joaquin Valley region and the CIT model for LA Basin

1999-2000 Research Plan

- MIRs for VOCs in Architectural Coatings
 - Based on the 1998 Architectural Coatings Survey
 - Estimate MIRs and degree of uncertainty
 - Support possible voluntary reactivity-based standards for SCM

CARB has reactivity research activities in several divisions with ~ 10 staff members involved daily and another 10 having reactivity as part of their tasks.

- **Activities in Canada (Environment Canada and Atmospheric Environment Service, AES)**
Presented by Paul Makar

AURAMS - Atmospheric Environment Service Unified Regional Air Quality Modeling System

Using a variety of different atmospheric models to determine their performance characteristics. This system will eventually replace the current ozone modeling. It will encompass particles, and look at the total atmospheric chemistry picture.

VIII. RRWG October 1999 Meeting

Plans for the Fall Meeting of the RRWG were discussed to coincide with two other workshops where reactivity and chamber studies are to be presented and discussed. According to Basil Dimitriadis, the next annual meeting of the joint U.S. -German workshop on reactivity and ozone science is tentatively scheduled for the first week in October and the opportunity is available to hold this workshop at UC-Riverside. In addition Bill Carter intended to schedule a workshop on environmental chamber design the same week at Riverside.

The RRWG agreed to schedule the Fall Meeting in October 7, 1999 as a one day meeting following the two workshops on October 4-6, 1999.

Future Tentative Meeting Schedule

February 2000 at Research Triangle Park NC

IX. New Business

What about the operational funding for this work group?

The chair will continue to work with interested parties to seek sustainable funding for the operational aspects of this group. Completion of our documents and the executive summary will be helpful for this activity.

Are the policy questions going to be matched with the Research Plan?

One suggestion would be to have Bill Carter and Tom Helms work together to mesh that activity and delineate and identify those tasks. They could obviously rely on their respective team members to assist them in this process.

EXPRESSION OF APPRECIATION -- Bill Carter

Fox asked the group to recognize Bill Carter for his untiring support of this process. These plans didn't simply jump out that word processor; he has contributed great deal of time and effort to this process.

Adjourn

APPENDIX

Matrix of Research Tasks and Relevant Questions

What will be the Effects of Reactivity-Based Controls?

How will reactivity-based controls affect emissions?

- 3.1.1 Survey amounts of emissions that are suitable for reactivity-based controls
- 3.1.2 Survey potentials for substitutions
- 3.1.3 Evaluate compositional implications of current control strategies

How will reactivity-based controls affect air quality in different areas?

- 1.1 Survey existing model assessments
- 1.2 Assess effects of reactivity-based substitutions on regional air quality
 - 1.2.a Assess effects of large-scale reactivity based substitutions on regional air quality using existing models.
 - 1.2.a1 Assess ozone and PM reactivities over the Eastern United States.
 - 1.2b Assess effects of large-scale reactivity-based substitutions on all applicable scales using advanced, state-of-the-science models.

How will reactivity-based controls affect air quality in different areas (continued)?

- 1.4 Assess impacts on PM
 - 1.4a Determine contribution of VOCs to PM_{2.5} exceedances and role of VOCs in meeting PM standards
 - 1.4c Determine effect of O₃ reactivity-based substitutions on aerosol levels.
- 1.5.4 Evaluate the relative benefits of VOC reductions for local and regional-scale ozone and pm_{2.5}
- 6.3.2 Improve emissions processing modules in models

What are the effects of changing the exemption policy?

- 1.3a Use existing models to evaluate whether ethane and other low reactivity VOCs meet a given policy-defined criterion of “negligible” ozone reactivity. (Highest research priority need to support exemption policy)
- 1.3b Evaluate air quality impacts of changing the exemption standard.

How do we develop optimum reactivity-based controls?

How do we quantify impacts on O₃, PM, other pollutants?

- 1.4B Develop scales for secondary organic aerosol formation potential from VOCs
- 1.5.1 Evaluate alternative reactivity metrics
- 1.5.2 Evaluate effects of large vs. Small changes in VOC emissions
- 2.1 Improve our understanding of atmospheric reactions of VOCs
 - 2.1.1 Compile, review, and evaluate kinetic and mechanistic data.
 - 2.1.2 Improve estimation methods
 - 2.1.x Laboratory and chamber studies of individual reactions and VOCs (gas and aerosol)
- 2.2 Improve our understanding of general atmospheric chemistry
 - 2.2.1 Improve understanding and ability to model surface reactions
 - 2.2.2 Improve understanding and ability to model nighttime and multi-day chemistry
 - 2.2.3 Study fates of ambient aerosols

How do we quantify impacts on O₃, PM, other pollutants (continued)?

- 2.3 Develop improved mechanisms for reactivity assessment
 - 2.3.1 Develop improved methods to represent chemical detail in models (various near and long term projects)
 - 2.3.2 Evaluate appropriate level of condensation for mechanisms in models.
 - 2.3.3 Develop mechanisms that can predict secondary aerosol formation
- 2.4 Environmental Chamber Studies
 - 2.4.1 Evaluate existing chamber data base
 - 2.4.x Conduct more comprehensive chamber studies using improved facilities
 - 2.4.5 Conduct chamber studies of aerosol formation potentials of VOCs.
- 2.5 Develop improved and lower cost reactivity assessment methods

How do we quantify impacts on O₃, PM, other pollutants (continued)?

- 4.1 Improve availability of information
- 4.2 Improve representation of alternate fates and deposition in models
- 4.3 Evaluate and apply fugacity models
 - 4.3.1 Evaluate existing fugacity models
 - 4.3.2 Incorporate existing fugacity models into the atmospheric modeling system
 - 4.3.3 Provide a consistent basis for estimating and applying “down-the-drain” factors
 - 4.3.4 Establish correction factors for VOC in consumer products discarded in landfills
- 5.1.2 Improve data and models for specific regions
- 5.3 Improve information on long range transport

- 5.3.1 Evaluate the importance of long-range transport in 3-D Eulerian models
- 5.3.2 Understand the regional budget of reactive nitrogen

5.4 Obtain data on atmospheric composition of aerosols

How do we quantify impacts on O3, PM, other pollutants (continued)?

6.1 *Develop Model criteria for reactivity assessments*

- 6.3 Improve model components
 - 3.2 Improve emissions inventories
 - 6.3.1 Make models more generally available
 - 6.3.2 *Improve emissions processing modules in models*
 - 6.3.3 Improve representation of long-range transport
 - 6.3.4 Develop methods for incorporating measurement data into models
 - 6.3.5 Improve representation of aerosol processes in models
 - 6.3.6 Improve methods for evaluating reactivity effects on varying scales

7 Analytical Methods

- 7.2 Improve analysis methods for volatility and fate assessment
- 7.3 Improve method 24 or equivalent methods
- 7.4 *Develop low cost reactivity screening methods*
- 7.5 Improve methods for aerosol monitoring

If VOC impacts depend on conditions, what conditions, or weighting for multiple conditions should be used?

1.5.3 Evaluate reactivities in attainment scenarios

3.2 Improve emissions inventories used for modeling ambient conditions (various projects)

5.1 Characterize distribution of conditions

- 5.1.1 *Survey of available information*
- 5.1.2 Improve data and models for specific regions
- 5.1.3 *Develop appropriate scenarios for general reactivity assessment (highest priority for policies using a general reactivity scale, e.g., CA's reactivity-weighting regulations)*

5.2 Improve atmospheric monitoring and assessment methods

- 5.2.1 Use indicator species to assess sensitivities to VOC and NOx controls
- 5.2.2 Develop improved atmospheric monitoring methods (particularly for NOx species)

5.3 Improve information on long-range transport

5.4 Obtain data on atmospheric composition of aerosols

How will the policy deal with differing relative reactivities for different impacts?

1.4 *Assess reactivities for aerosol formation potential*

1.5 Conduct more comprehensive reactivity assessments

1.5.1 Evaluate alternative reactivity metrics

1.5.4 Evaluate reactive benefits of VOC reductions for ozone and

PM2.5

2.1 Improve mechanisms for reactions of VOCs

2.3.1 Improve methods to represent chemical detail in models

2.3.3 Develop mechanisms that can predict secondary aerosol formation

2.4.5 Conduct chamber studies of aerosol formation potentials of VOCs

4.2 Improve representation of alternate fates and depositions in models

5.3 Improve information on long-range transport

6.1 Develop model criteria for reactivity assessments

7.2 Improve analysis methods for volatility and fate assessments

8.0 *Assess state of science for persistent organic pollutant issues related to reactivity.*

How does policy deal with uncertainties in reactivity assessments?

1.6 *Conduct model uncertainty analyses for reactivity predictions.*

3.2.2 Quantify emissions uncertainties for model uncertainty studies.

6.2 Improve model sensitivity analysis methods

How does policy deal with changes in knowledge?

2.1.2 Develop improved estimation methods for atmospheric reactions of VOCs

6.3.1 Make models more generally available

How do we enforce reactivity-based controls?

7.1 *Improve analysis methods for enforcement*

7.4 *Develop low-cost reactivity screening methods*

Summary of October 7, 1999 RRWG Meeting at Riverside, CA

I. Welcome and Introductions

Chairman Don Fox called the meeting to order at approximately 8:15 am. He asked everyone to introduce himself or herself. Approximately 50 people were in attendance. The meeting included several guests from Europe who had earlier in the week been in attendance at the U.S./German photochemistry workshop held in Riverside. Dr. Fox presented the meeting objectives:

1. To accept the remaining working papers generated by the RRWG to date
2. To review initial research activities
3. To establish working subgroups to facilitate research program

Other Items

Future Meeting Scheduling

- Next Meeting February 2,3 or February 9-10 at USEPA RTP, NC.
- Subsequent Meeting will be in May/June 2000

II. Update on Studies Underway

John Dege Review of Existing Low NO_x Studies. John Dege said all of Dr. Carter's work was done at above 50 ppb of NO_x and said that at 20 ppb or lower VOCs supposedly have little impact. He mentioned that Harvey Jeffries had said at a previous meeting that the Sydney, Australia and TVA chamber runs were done at low NO_x conditions, but much of the data has never been analyzed. John Dege said Harvey Jeffries had proposed a work plan to model existing data from low NO_x chamber experiments. This effort would look at:

- a. Outdoor chamber data of the Commonwealth Scientific and Industrial Research Organization (CSIRO), Sydney, Australia
- b. Indoor chamber of Tennessee Valley Authority.

These two smog chambers have data sets at lower concentrations of nitrogen oxides (as low as 12 ppb) and VOC than work done in the University of California at Riverside and University of North Carolina chambers. Don Fox recapped this discussion by saying that this effort would fall within the RRWG priorities of evaluating existing chamber databases.

Dave Morgott CMA research initiatives. The CMA atmospheric chemistry technical implementation panel (AC TIP) has a number of projects in core areas, which it wants to investigate. Among these are:

- AC-1 Atmospheric degradation pathways
- AC-2 Aerosol microphysics and chemistry
- AC-3 Organic compounds in global atmospheres
- AC-4 Urban to global modeling and reactivity
- AC-5 Atmospheric formation and transport of persistent organic pollutants

Dr. Karl Becker, Jay Olaguer and Harvey Jeffries commented on the role of vertical transport and the need to consider it in modeling.

Dan Baker Atmospheric reactivity task group Solvent Council of CMA. Among activities he mentioned are:

1. Assess strengths / weaknesses and similarities / differences in approaches to develop chemical mechanisms (they are working with Dr. David Golden on this).
2. Initial scouting of concept of incorporating "atmospheric availability" into a model like EKMA.
3. Jump-start laboratory setup to study HONO photolysis for radical generation.
4. Mapping where/when VOC controls make sense.

Objectives of the above studies are to use existing data, identify areas where more data is needed, and link results to policy.

Ed Edwards made a formal presentation with overhead slides on the role of low NO_x and reducing ozone in the Los Angeles basin. He said current approaches would not allow achievement of ozone attainment by the year 2010. Mr. Edwards focused on methods to achieve very low atmospheric NO_x concentrations for most all atmospheric conditions. Mr. Edwards proposed consideration of OH radical generators as a way to alleviate ozone exceedences in the LA basin. He used EKMA type diagrams to explain his rationale for recommending this approach.

Level of initial research funding

Don Fox said he would like to have some idea of the level of funding for each project. Dave Morgott said all the projects he had talked about are funded at \$50,000 or less. Fox announced that Dunn-Edwards has committed \$25,000 for each of the RRWG top priority research areas for a total of \$125,000.

Possible Research Workshop

Karl Becker said that we should have a workshop on HONO chemistry

sometime. He said some industrial sponsorship of such a meeting would be beneficial. Bob Hamilton said it will be difficult to get money for pure research if it is not more related to policy. Dr. Becker replied that the US/German workshop could not recommend policy for all Europe since representatives of all affected parties are not present.

III RRWG Working Papers

A. Final Draft of VOC Policy White Paper Don Fox

Don Fox indicated that Tom Helms was unable to attend the meeting and asked Don to lead a discussion on the policy white paper. He said the changes in the white paper since June include removing references to the 8-hour ozone NAAQS and NOx SIP call since implementation of these have been held up indefinitely by Court decisions this May. Also Chapter 6 has been added to the white paper which summarizes research priorities which were discussed at the June RRWG meeting.

A discussion on the white paper ensued. Bob Avery said that since we have visitors, we should recognize that this is a document that had input from many people, but that everyone would not necessarily agree with everything in the report. Gary Whitten asked if there could be an additional review period for the white paper. He said the current version was only distributed for review a few days before this meeting and that some of his previous comments (concerning Rule 66 and multi day problems) had not been included. Doug Fratz also asked for an additional review period. Fox proposed that any additional comments be considered by the Policy Team for this version or a future version of the VOC Policy White Paper. In the mean time, any comments on the policy white paper should be given to Tom Helms by November 15.

B. RRWG Initial Assessment Executive Summary Don Fox

Don Fox presented the final draft of the Executive Summary that included the following modifications: 1.) Addition of a disclaimer 2) Modification of the Research Table 1 to be consistent with initial RRWG priorities. Question asked who is the target audience for the executive summary. Don Fox said the audience was managers of companies that may participate in the RRWG programs who want short summary of the program. It also might be used to request funding from outside foundations. Comments on the Executive Summary should be given to Don Fox by November 15.

Updating of Assessments

Bill Carter discussed the possibility that the science white paper and the policy white paper may need periodic updating to emphasize subjects that may have received small attention before, but seem to be important later. Fox indicated that Tom

Helms has already discussed with policy team members the need to continue to interact and discuss the research agenda and its utility to inform potential policy options. Brian Keen proposed that the working papers be considered as living documents with updates when the RRWG considers it appropriate. The membership endorsed this approach.

Web based Communication Tools

Carter asked how about a web site discussion group. Joyce Graf asked if a web site would be open to the public or just to the work group. There was further group discussion of options for a web site to share information. Terry Keating said the NARSTO web site has a discussion site. Some one questioned whether this site is up to date on web technology enough to allow an on-going discussion. The group agreed to consider further a web site.

III. Research Task Groups

Don Fox then introduced a major topic for discussion for the day. He proposed to establish a set of research task groups whose goal is to bring research plans to funded programs. In order to do that, this approach will bring together interested stakeholders on particular topics. This will allow the task group to establish a realistic scope, identify potential researchers and sponsors.

The goal is:- to bring research projects to funded programs

Tasks would include:

- to identify specific research tasks
- to identify level of effort and funding
- to identify possible researchers
- to identify /obtain the funding for contracts

Don Fox said the approach of getting a pool of money, then directing it to tasks has not worked. Rather we should identify tasks, then seek funding.

There was a discussion of researchers role in these task groups. Should they be involved? The consensus answer was yes they should be involved. They may want to excuse themselves if it is obvious that they may bid on a particular contract.

Don Fox listed the ten research areas that were ranked with highest priority at the June meeting and which were listed in the minutes for that meeting. He proposed forming a task force for each research area with the purpose of achieving the goals listed above. He asked interested persons who want to participate on a particular task-force to sign a sign-up sheet for that area. After a break to give people a chance to sign

up for the various project areas, Don asked for volunteers who would chair each of the various groups. Below is a summary of the ten project areas with the number of people who signed up to participate on the task group and the group leader who volunteered to lead the group:

Task Subgroups

1. Assess effects of large-scale reactivity-based substitutions on regional air quality using existing models (21 sign-ups) (task leader, Jay Olaguer epolaguer@dow.com)
2. Analyze available information relevant to how much of the environment would be sensitive to VOC controls and the distribution of conditions appropriate for reactivity assessments. (21 sign-ups) (Dan Baker dcbaker@equilon.com)
3. Improve information on atmospheric availability of VOC with low volatility, and evaluate existing fugacity models (18 sign-ups) (Jonathan Kurland KURLANJJ@UCARB.COM)
4. Survey amounts of emissions that are suitable for reactivity-based controls (14 sign-ups)(Dave Morgott dmorgott@kodak.com)
5. Develop appropriate scenarios for general reactivity assessment (7 sign-ups)(combined with task 1)
6. Survey existing modeling assessments (1 sign-up) (combined with task 1)
7. Development model criteria for reactivity assessments (6 sign-ups)(combined with task 1)
8. Improve emissions processing modules in models (5 sign-ups)(Basil Dimitriades dimitriades.basil@epamail.epa.gov)
9. Use existing models to evaluate exemption standard (7 sign-ups)(combined with task 1)
10. Evaluate existing chamber data base (6 sign-ups) (Paul Makar paul.makar@ec.gc.ca)

As noted, some of the tasks which received a smaller number of volunteer participants were combined into task 1, since the tasks were thought to be somewhat similar to task 1 anyway.

Don referred to an earlier statement by Paul Makar that there needs to be a central archive of data for chamber results to which researchers from around the world could have access.

The object of the task groups will be to write a scope of work that can be given to a contract researcher to perform specific research projects. This document will also be used to inform the rest of RRWG and to attract sponsors. There should be a draft by December 15, 1999 that the team is willing to share with the rest of RRWG. The December 15th draft will be considered a 1st draft, even though there may have been earlier working drafts within the subgroup.

IV. New Business

NARSTO Membership

Don Fox emphasized the desirability of individual companies participating in the RRWG signing up as members of NARSTO. Don encouraged every one to do this. Company representatives desiring to sign-up their company for NARSTO membership should contact Ron Patterson who can assist them with the process.

Journal of Environmental Science and Pollution Research

Jay Olaguer mentioned an article he had prepared for the journal Environmental Science and Pollution Research on the RRWG. This short article gave a one page overview of the background and purpose of the RRWG. The editor of this journal that is published in Germany has asked if we want a permanent monthly column to discuss RRWG activities. Don Fox said it is too early to start a regular column, but that we may want to consider it later.

UC-Riverside New Chamber Program

Bill Carter discussed a possible role for RRWG in planning experiments for his new smog chamber. Collaborations are anticipated between interested persons in the U.S., Europe, and Mexico. The RRWG may want to have a role also, but it was not obvious now what such a role would be. Don Fox asked Dr. Carter to think about what role the RRWG might play and to perhaps discuss this at the next meeting.

RRWG Organization Funding

Don Fox discussed finances for the group. He said he had \$30,000 for a 12 month commitment. He said EPA had indicated a grant of an additional \$10,000 would be forthcoming. (This grant has not yet been awarded.) This grant along with the other funds already received would provide resources into the May/June time frame. Don said he will approach foundations and other groups to see what other funding may be available. Barbara Francis of CMA said she had collected \$24,000 of the funds Don has received.

RRWG Steering Committee

Don Fox proposed establishing an RRWG steering committee. The committee would assist the RRWG in achieving the RRWG goals by:

- Interacting with the Chair between meetings to promote the activities of the RRWG.
- Focusing activities on critical issues.
- Identifying interested stakeholders

The make-up of such a committee should be composed of about 3 members from government agencies and about 5 members from industry. Don proposed that the

industry representation should be from trade associations rather than individual companies. He felt this would give broader representation. Don said he will continue to work on putting the steering committee together.

Brief Summary of the two preceding workshops on Oct 4-6, 1999

Don Fox gave a concise summary of the Combined US/German Ozone/Fine particle Science and Environmental Chamber Workshop that was held during the 3 days which preceded the RRWG meeting. Some of the RRWG participants had not had an opportunity to attend the 3 day workshop although the topics that were discussed there are relevant to the interests of the RRWG.

VI. Adjournment

The meeting ended around 4:30 PM on October 7.

Prepared by Don Fox October 26, 1999



**REACTIVITY
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Summary of February 9-10, 2000 Reactivity Research Working Group (RRWG) Meeting at Research Triangle Park, NC

I Welcome and Introductions

Don Fox called the meeting to order at 12:15 pm on February 9. He asked attendees to introduce themselves. Approximately 45 people attended the meeting. A speakerphone hook-up was used to tie in persons from the California Air Resources Board and EPA Region IX (in San Francisco). Don Fox gave an overview of the accomplishments to date of the RRWG, which included production of the policy and science white papers. The rest of the afternoon was taken up by reports by team leaders of the various Task Groups that had been formed in Riverside during the October 1999 meeting.

II Task Group Updates

Task Group (1,5,7,9) Reactivity Assessment

Jay Olaguer the team leader for subgroups 1, 5, 7, and 9 talked about the work of these combined groups. This effort involved assessing effects of large-scale reactivity based substitutions on regional air quality using existing models. In opening his presentation, he discussed basic philosophy and said we should ask, "Will it work?" before "how will it work?" He went through each of the projects that were itemized in his outline that was presented to members by e-mail before the meeting. These research priorities were broken into (I) short, (II) medium, and (III) long term research priorities for regional reactivity assessment.

Jay described one significant item among short-term goals as a proposed project to substitute ethane for all VOC emissions in one or more model runs. A discussion ensued on this subject. Would we substitute ethane for all natural emissions (i.e. from trees)? Jay said only manmade

emissions would be substituted. It was suggested using only a 50% change in VOCs during runs rather than a 100% change because a 100% change would be a radical change in chemistry. Other questions asked included: What would we expect to see from this experiment? Who will decide what is an acceptable model for the runs? Jay said the contractor selected to do the project would work out details of the modeling. Tom Helms suggested we should rely on techniques and modeling decisions generated by the Ozone Transport Assessment Group (OTAG) that spent a lot of time investigating aspects of modeling.

Another item suggested for short-term priorities is to determine the zone of influence of VOCs in the model run described above. What areas of the country would be covered? Jay said that California and the OTAG region would be looked at. What would account for the results obtained with models? Jay said changes in NO_y and radical budgets. He said that he is not trying to get into the fine details of models, but wants to look at big impacts.

After looking at big impacts in the short term, goals for the medium term include adopting plausible VOC substitution scenarios and use existing models to evaluate these changes. An RRWG participant questioned whether changing one aspect of a model gives any meaningful information about reactivity. Another mentioned the Coordinating Research Council is pursuing this issue.

For long-term goals of the task group, advanced assessment scenarios were discussed including rigorously characterizing meteorological conditions of exceedence sites and other modeling details

Task Group (2) Where to consider Reactivity-based Controls

Dan Baker described the work of subgroup 2, which he chairs. The purpose of this group is to analyze information relevant to how much of the environment would be sensitive to VOC controls and the distribution of conditions appropriate for reactivity assessments. The focus of this discussion was on analyzing existing monitoring data. Someone said asked where reactivity would apply, and said that in NO_x limited situations VOC control probably wouldn't matter. One possible project mentioned was to collect ambient samples and irradiate these samples in a smog chamber.

Question: Will it be important to improve instrumentation for NO_x or VOC? Harvey Jeffries said a new instrument had recently been

announced in the scientific literature that can accurately measure NO₂ at very low concentrations.

Task Group (3) Atmospheric Availability

Jonathan Kurland made a presentation on subgroup 3, which is concerned with atmospheric availability and environmental fate. He proposed having a workshop on this subject sometime in June, perhaps on two days just prior to the next RRWG meeting. He proposed inviting distinguished scientists in several fields related to this topic, including atmospheric photochemical modelers and indoor air pollution experts. It was recommended that people other than just the invited speakers should be allowed to listen, since others could learn from the gathered experts. Don Fox said the RRWG is an open group, and he would encourage this environmental fate team not to place restrictions on who could participate.

Task Group (4) Emissions Suitable for Reactivity-based Controls

Dave Morgott, team leader for subgroup 4, made a presentation on the efforts of this team that is concerned with surveying the amounts of emissions that are suitable for reactivity based controls. He recommended postponing several (if not all) of the projects suggested for this team until the work of Task Group (1,5,7,9) is further along. He questioned whether some of the projects would actually fall under the heading of "science" research. Among the projects his team is considering is:

1. Survey emissions by mass and reactivity
2. Survey sources of emissions
3. Look at compositional information and the amenability of sources to substitution to determine the practicality of reactivity-based VOC policy

Discussion

Discussion on relationship of reactivity and composition ensued. If we don't know the current composition, how can we have a plan to change composition? Bill Carter said that we do have a way of defining reactivity by using his MIR scale. He said the biggest criticism of his scale is that it may exaggerate the reactivity differences between compounds.

Doug Fratz said his association (the Chemical Specialty Manufacturers Association) has already done some work on the profile of

emissions from consumer products in California. Much of this work is published in a Sierra Research report.

Someone pointed out that the carbon bond IV (CB-IV) mechanism for handling reactivity in some photochemical models only has 12 reactivity categories into which all organic compounds are lumped (according to which category the compound's structure most resembles). The question was raised of what good is detailed speciation of composition if every chemical is assigned one of 12 reactivities in the model and most of the detail is lost anyway.

Harvey Jeffries said that for modeling work done by the State of North Carolina, the ratio of xylene to toluene that was used in modeling did not match that which was measured by ambient air modeling. The State realized there was some discrepancy and made an effort to get better inventory data which was more specific to North Carolina. (The previous inventory data had come from California.)

Task Group (6) Existing Model Assessments

John Dege, team leader of subgroup 6, presented the efforts of that group whose purpose is to survey existing modeling assessments. Dupont has contracted with Environ to conduct a comprehensive survey of recent North American modeling runs and also to see what information exists for Europe. The cost of this contract is \$15,000. Dupont is paying for this now, but is looking for someone to share the cost.

Task Group (8) Improving Emission Processing Modules

Bill Benjey of EPA, who spoke for Task Group 8, described the Sparse Matrix Operator Kernel Emission Processor (SMOKE) for use in modeling the effects of chemical compound reactivity. SMOKE is an emission processor that can be used as a module of EPA's third generation air quality modeling framework (Models-3) and will allow this airshed model to take into account the actual reactivities of individual compounds. The reactivities will be species specific and not "wired" to any set of pollutants, as is CB-IV with its 12 categories of lumped organic species reactivity. A SMOKE tool will create files to be fed into SMOKE. However, considerable contractor work remains to be done before SMOKE is ready for use. The summary of subgroup 8 activities that was sent out by e-mail before the meeting summarized the activities concerning SMOKE that still need to be

completed. More information about Models -3 can be found on the world wide web at: <http://www.epa.gov/asmdnerl/> under Models 3. A description of SMOKE is available at: http://envpro.ncsc.org/EDSS/edss_register/.

Discussion

It was brought up that one issue not being considered by any task group is the validation of emission inventory records.

Task Group (10) Existing Chamber Studies

Paul Makar, leader of subgroup 10, presented a summary about the task of surveying and compiling existing chamber databases. He addressed the question of "what's out there" and described known chambers. He plans to put data from the various chambers into a standardized format and make this available to researchers throughout the world. He said that more than one iteration at compiling data may be needed due to problems that may arise. Paul estimated that it would take \$30,000 and 4 months to complete this task

As the last presentation of the day, Harvey Jeffries gave a talk on the TVA chamber. He has been involved in an activity to summarize and place data from this chamber into a standard format and to place this information on the world wide web to be available to all. More information on the TVA chamber and data on chamber runs may be found on the web at: <http://airchem.sph.unc.edu/research/tvadata/>. Harvey said a repository of data may not meet all needs, although it may meet one need. There is a need for a unified format.

Second Day (February 10)

The morning started with coffee, which was graciously provided by Brian Keen of Union Carbide. At 9:15 am, Don Fox began the meeting with an overview which summarized issues that had been discussed so far.

III. Discussion of Drafting RFPs

The time between Don's introductory talk and the next break was taken up by a long group discussion about the subgroup summaries which

had been presented the previous day. Here is a sampling of these discussions.

Tom Helms said that OTAG has already done a lot of work on modeling. We don't need to reinvent the wheel. Jay Olaguer said that RRWG is not trying to develop a new model, but is trying to use existing models. Tom expressed concern that if models lump all organic chemicals into 12 reactivity bins, will there be enough sensitivity to distinguish between reactivities of numerous compounds. Ted Russell said that we would not have to use CB-IV (which uses the 12 bin approach) in the future.

Doug Fratz asked what would a model show if VOC is reduced instead of substituted. He said his Association had investigated this question with airshed modeling work (carbon bond IV in UAM) in California.

Robert Wendoll said the question before the RRWG is what intentional changes in emissions will be optimally effective in reducing air pollution.

Tom Helms said he had been asked why EPA does not talk more and tell what EPA wants. Tom said that this is not an EPA group. Why is EPA participating? In order to get more research done which may bear on ozone control. We should concentrate on research that can be done which will help convince EPA that it should revise and update its reactivity policy. Lets determine what is the most effective information that will help EPA decide to revise its policy. Tom also said that people should keep in mind that a policy must be fairly simple to be workable and that anything too complex would be difficult to administer. Implementation and enforceability should be of concern to all parties.

After the break, Don Fox said that we are ready to spend some money on actual research. He said that the policy team is ready to look at the process to see if what we are spending money on would be useful.

Bob Avery said that the policy team should think about what are the possible outcomes of research and what are the policy implications. Bob said we don't have to and cannot do everything at once. We need to decide what can be usefully done in the short term.

Ted Russell said he would put Tom [Helms] on the spot. If the group could show that substitutions in reactivity make a big impact on

ozone would EPA care? Tom replied yes, but if research showed that a reactivity scale is good for Los Angeles but not for Atlanta, EPA would not recommend it for national use (although it might be useful on a local basis in California.) If research shows that a common reactivity scale holds up in different areas of the country, and a simple way can be found to implement/enforce it, EPA would consider that approach.

IV. Discussion of Funding Stage

Barbara Francis asked what company representatives can do to assure their management that research, which they are being asked to fund, has been approved by the policy group.

The group outlined the following points:

- Group consensus on a list of projects
- RFPs for each specific project
- Short (1-page) summary of project
- Near term outcomes

V. Additional Discussion of Parallel Activities

California is going ahead with an ozone control rule based on reactivity. As part of the California rule, industry and the State of California will address issues related to record keeping, compliance testing and other implementation issues. It was also pointed out that MACT standards already required consideration of individual chemical species.

Paul Makar give a short summary of a Canadian project, called Pacific 2001, which intends to study the sources of PM and ozone in the lower Fraser Valley (near Vancouver) to provide credible guidance on appropriate strategies to reduce human health risks. This project is being done in cooperation with NARSTO. There is great deal of Canadian interest.

Paul wants to encourage U.S. interest in this also. The project will look at how much of VOC is going to form particulate rather than reacting to form ozone. The budget is 1 to 2 million dollars (in U.S. currency). Pilot projects will begin this summer with more detailed studies later.

VI. Next Meeting Date

The group discussed dates for the next meeting. The group settled on the dates of June 27 and 28 for the environmental fate workshop and June 29 and 30 for the RRWG meeting.

VII. Chair's Status Report

Don Fox discussed his status as chairman of the group. He recounted the accomplishments of the group since his assuming the position in March 1999. These accomplishments included completion of the science and policy white papers. Don offered his services for the next year. He discussed the finances for the RRWG. He has received \$30,000/year (which includes \$2,500 for travel and expenses). \$24,000 has come through CMA. CARB has committed to providing \$2,000 per year over 5 years. EPA has budgeted \$14,000 for a grant (or cooperative agreement) with the University of North Carolina to be applied toward RRWG activities and Don Fox's chairmanship. Don said he is still negotiating with the University to make sure that most of that money goes to directly to RRWG and not to University overhead. This grant has not yet been submitted to EPA. Don is also interested in pursuing foundational funding for RRWG. This was discussed at earlier meetings, but needs follow-up.

Don said the RRWG steering committee consists of the following individuals:

Tom Helms, EPA
Barbara Francis, CMA
Doug Fratz, CSMA
Bob Nelson, NPCA
Eileen McCauley, CARB

Don said any comments / dissatisfactions with his chairmanship should be taken up with this steering committee.

The meeting was adjourned at 12:53 pm.



**REACTIVITY
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Summary of RRWG Meeting for June 29-30, 2000

(A meeting document folder of PowerPoint presentations is included in this distribution as a ZIP file)

I. Welcome and Introductions

At 1:15 pm on June 29, 2000, Don Fox gave introductory remarks and welcomed attendees.

II. Task Group 3 Environmental Fate and Air Pollution Modeling - Workshop Summary – Jon Kurland

Jon Kurland who gave a summary of the environmental fate workshop that had been held during the two and a half days that preceded the RRWG meeting (See Meeting Zip File – Fate Workshop Preliminary Summary.pdf). Dr. Kurland acknowledged sponsors of the workshop that include the American Chemistry Council, Dunn Edwards Corporation, the National Paint and Coatings Association, and the Soap and Detergents Association. He also acknowledged the persons who led the workshop, especially the leaders of the three breakout sessions. He then summarized the major conclusions of the workshop by showing a series of summary slides whose content is summarized below:

1. It is feasible to link level IV fugacity models with photochemical models
2. Various sectors are involved such as air, water, soil, vegetation and films on buildings.
3. Combining environmental fate and air quality modeling is feasible
4. Research priorities are development of screening box model, investigation of chemistry and mass transfer rates, and development of grid model.

Discussion

Comment that workshop highlighted the problem that people can assign different meaning to technical terms such as for wet and dry deposition. It is important that terms are defined to make sure we understand each other. This task group will prepare a summary of the workshop, a brief article for publication and possible additional research tasks.

III. Focus of RRWG Don Fox

Don Fox made a presentation in which he summarized the mission and accomplishments of the RRWG (See Meeting Zip File – Primary Mission.pdf). Some of the things he highlighted are:

- RFP to develop model comparison criteria, review existing models, identify test scenarios
- Review existing model assessments
- Clarification of NO_x and HC limited regions
- Workshop on environmental fate modeling
- RFP for improved emission processor for Models 3 CMAQ modeling system (SMOKE)
- Need to develop RFP on chemical classes based on reactivity properties
- RFP for inventory of photochemical chamber data bases for chemical mechanism testing (e. g. TVA data)

In summary Fox encourage us to focus our main efforts on near term research that would use selected 3D models with the most current chemistry and test a limited number of variables.

Discussion

The question was asked if we would do any thing for task 4 (emission inventories and classification of reactivity) and task 10 (data bases). Fox replied that work will be necessary in most of the priority areas identified by RRWG.

There was a discussion about criteria for exempting compounds as

VOC. It was asked what is the evidence for deciding a VOC is not a pollutant and how credible is this evidence. What measurements would be good enough for EPA. Two approaches would be to make Models 3 better or to use existing models.

Past discussions were referred to about whether ethane is the proper cut point and whether a bright line cut point is correct. The comment was made that EPA needs better tools to make more refined decisions. The RRWG was reminded that this is not a FACA group since it is not balanced with environmental groups, so policy development is not the purpose of the group. If the RRWG can provide improved scientific information, EPA can consider whether this information can be used to improve EPA's reactivity policy. If RRWG doesn't provide any new information, EPA has an existing reactivity policy that EPA can continue to use.

The comment was made that EPA's reactivity policy is a 0 or 1 system (either reactive or exempt). The commenter said the only worse system would be if everything were considered reactive. Another response indicated that there are people who don't believe VOC composition makes much difference in ozone outcome. The California reactivity based aerosol coating rule has viewed by many people as a pilot program. These people were surprised to hear that EPA did not fully support this rule. The comment was made that the California experience will show what people will actually use as substitutes. These experiences will be real results, not just hypothetical speculation.

The issue of enforcement testing under a program such as the California aerosol rule was discussed. The question was asked what labor burden would be involved in testing for compliance under such a program.

IV. Policy Team Reactions to RFPs Tom Helms

Tom Helms gave a formal talk about Policy Team activities (See Meeting ZIP File). He discussed policy relevant questions needing scientific investigation. Questions include 1.) In those areas where VOC reductions may be required, does "reactivity" make a difference (relative to mass reductions) in O₃, PM, and regional haze? 2.) What are the roles of transport and multiday stagnations? 3.) What are the issues related to implementation, verifying and enforcing regulatory reactivity rules?

V. Task Group 6 Existing Model Assessments (See Meeting ZIP File Existing 3D Modeling Studies.pdf) Don Fox

Discussion.

Initial survey identified a number of studies in various regions of the country with a using a variety of grid scales and modeling approaches. RRWG members were aware of additional studies that should be included in the report.

VI. Task Group (1 5,7,9) Reactivity Assessment Draft RFP Discussion John Dege

Task Group chair Jay Olaguer has recently changed professional affiliations and requested a new chair be appointed. John Dege and Dan Baker have assumed leadership of this task group. John Dege talked about regional reactivity assessment. He identified the following three tasks that should be done:

1. Identify scenarios in California and other regions that serve as the basis for a preliminary regional reactivity assessment.
2. Model scenarios in which ethane is substituted for other compounds.
3. Repeat modeling with other compounds (methane, acetone, etc.)

Discussion

There was a discussion of problems with using all ethane in a modeling run. Some people suggested this might not be realistic and that a more realistic scenario should be used.

It suggested that we should consider putting out a request for proposal (RFP) asking people who are already have work going to piggyback the RRWG studies onto existing studies. This would be a more cost effective way to proceed.

There was general agreement that the draft RFP should be revised to request pre-proposals for this piggyback concept. This alternative approach is expected to provide innovative tests of incorporating reactivity in 3D air quality models that will encourage more detailed modeling in the near future.

VII. Status of Models 3 (Task Group 8) Ken Schere

Ken Schere of EPA's Office of Research and Development gave a presentation of the SMOKE emissions preprocessor which is being developed for use with Models3 (See meeting ZIP file – Schere June 2000 Models 3.pdf). He emphasized that the development of SMOKE is crucial to the successful use of Models 3. EPA has already provided \$70,000 through RRWG for development of SMOKE. It was asked if additional industry money could be channeled through RRWG and piggybacked onto existing SMOKE development work.

VIII. OBM Classification of Regions Task Group (2)-- Charles Blanchard

Charles Blanchard of Envair gave a presentation on spatial mapping (Draft Report on NARSTO Site). This work involves an analysis of ambient air monitoring data to:

- identify where and when VOC or NOx controls would help reduce ozone concentration
- identify regions where further study of reactivity based controls is warranted.

One result discussed is lowered concentrations of NOx on weekends. There were strong NOx reductions and modest VOC reductions on weekends in the study area. A question raised about the study is whether emissions inventories are adequate to support modeling results. A report on the Envair study will go through the NARSTO review process and may be published.

IX. Summary of Draft RFPs

Paul Makar reported on the work of subgroup 10 which is reviewing smog chamber results and compiling and standardizing formats. Similar work is underway at UNC-CH on TVA data.

X. Possible Funding Sources

Don Fox said that the RRWG is at the point where we need to commit funds to specific projects. If a company or trade association wants to support SMOKE development they should contact Deborah Luecken of EPA's Office of Research and Development since Basil Dimitriadis is out of the country for several months. Debra can coordinate with the proper EPA officials.

The comment was made that the American Chemistry Council is doing projects through its various task groups that are relevant to the RRWG, but not everyone understood what these projects involve. The option of posting information on the NARSTO website about ACC projects was discussed and will be pursued.

Question was asked if the development of SMOKE would hold up the other projects RRWG is planning. The answer is no - work can go ahead independently of improvements in SMOKE, although it will be more difficult and expensive to do all the projects without SMOKE.

Question asked if OTAG could do something to help RRWG research. OTAG no longer exists. Some other organizations such as LADCO and OTC have picked up some of the OTAG work and may be of help.

Question asked if we are still pursuing foundations as a source of funding. No contacts have been made to date.

XI. Scheduling Next Meeting

The last item of business was selecting dates for the next RRWG meeting. After a short discussion, October 4 and 5, 2000 were selected.

Adjourn at 12:30 pm

Attachment

June 2000 Meeting ZIP.zip Contains PowerPoint .pdf files:

- Fate Workshop Preliminary Summary
- Primary Mission Fox
- Policy Team Comments
- Existing 2D Modeling Studies DRAFT
- Schere June 2000 Models 3



**REACTIVITY
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Summary of RRWG Meeting for October 4-5, 2000

Attending: Bob Avery, Jim Berry, Bill Carter, Ed Casserly, Janet Catanach, John Dege, Basil Dimitriadis, Barbara Francis, Joyce Graf, Jake Hales, Madelyn Harding, Tom Helms, Jeff Holmstead, Bill Johnson, Brian Keen, Jonathan Kurland, Jan Meyer, Bob Nelson, Bruce Moore, David Morgott, David Sanders, Bob Stallings, Stanley Tong, Jeffrey West, Robert Wendoll, Fred Whiting, Bernie Zysman, Don Fox

I. Welcome and Introductions

After introductions, Don Fox reviewed the agenda for the meeting

II. Task Group 1, 5, 7, 9 John Dege, Dan Baker

Dan Baker and John Dege have drafted a revised RFP (request for pre-proposal) which was sent out a few days ago for the task being done by combined task groups 1,5,7,and 9. This combined group was often referred to during the discussions as group or task "1579". Don Fox summarized the approach in a series of slides. (See Attachment A). This is a preliminary investigation that will take a relatively inexpensive, but not comprehensive, look at reactivity. The study will examine how various variables could be adjusted to see how the end result in ozone formation would change. The purpose of the request for preproposal is to clarify issues relating to VOC reactivity and the use of air quality models. There will be an open solicitation advertised over the NARSTO website. Anyone who is interested could respond. The submission preproposal response should have a 6 page limit, and responders should plan to give final results in nine months. The proposal is to be submitted to Fox, Dege, or Baker.

A discussion on this topic followed. It was suggested that it may be easier to get 5 different groups to model the areas they are already

working on rather than getting one group to model five different areas. Dave Morgott said that this request for preproposal is a scoping study that doesn't cover everything. Barbara Francis said we must make sure we have the money to cover all the work we are requesting. There would be no use in putting out an RFP unless we have funds committed to pay for the work. About a dozen organizations would be expected to respond to this solicitation. However anyone can submit a pre-proposal. Brian Keen summarized the project as trying to determine when and where reactivity makes a difference (relative to mass reductions). Don Fox added the need to determine if our tools are good enough to determine this effect.

Bob Avery suggested a meeting of the review team (and perhaps some policy team members along with Helms' staff members) near the end of the year to review what has been submitted and then funders could decide on funds around the first of the new year.

III. Task Group 6 Existing Model Assessments John Dege

Don Fox introduced the second item on the agenda, which is a review of efforts by task group 6. John Dege discussed the summary of modeling assessments. He is already having work done by a contractor done on this task. He asked if anyone knew of any modeling that is not already included in the study. He asked the participants for funding to pay for evaluating different models

IV. Task Group 3 Environmental Fate and Air Pollution Modeling Summary Document and Draft RFPs – Jon Kurland

Jon Kurland gave a summary of the preparation of the final report of the environmental fate workshop which was held in June. He had a handout of a draft final report. He said there is a possibility of a journal article being published which summarizes these workshop results. These results explore the technical feasibility of integrating environmental fate studies and air quality models.

Paul Makar said there is work going on in Canada which is related to the results of the environmental fate workshop which is being funded over a 3 year time frame at \$100,000 (US) per year. Several RRWG members

expressed interest in inquiring more into this work.

Group 3 lead by Jon Kurland will review RFPs for development of box models for multimedia studies. Dave Morgott said he will take up multimedia box model development with the environmental TIP (of ACC). They will likely consider funding a project to develop a multimedia box model. This work is expected to start in early 2001 and be completed by mid 2001.

The three action items for Group 3 are:

1. RFP on screening study for multimedia fate modeling
2. Development of a multimedia box model by the ACC TIP
3. Short article for publication

There was a discussion of confidentiality agreements for reviewers of proposals. Dave Morgott said the ACC TIP used these. Jake Hales of NARSTO recommended that all RRWG reviewers sign such an agreement.

V. Discussion of Task Group 4 and 10

Don Fox discussed the work of group 4 which is to look at chemical compounds which would be available to classify by reactivity. Such a "binning" approach may be useful in certain regulatory schemes. Don Fox said he had discussed with Tom Helms the possibility of using EPA staff to do some of this work.

Paul Makar discussed the task he is involved in to examine existing chamber data. He said he needs one person year of labor to get the smog chamber data base in shape. He has asked the Canadian Foundation for Climate and Atmospheric Science for a grant to help fund this. In a similar project, John Dege is working with Harvey Jeffries of the University of North Carolina to review TVA and Australian smog chamber data.

Barbara Francis suggested the distribution of draft meeting minutes prior to finalization. This will allow RRWG members to correct any mistakes which may be present.

VI. Task Group 8 SMOKE Emissions Processor RFP Status

Deborah Luecken of EPA gave a status report of the development of the SMOKE emissions preprocessor for Models3. She said Bill Benjay of EPA had written an RFP for SMOKE development. EPA has decided to make SMOKE JAVA based which will delay the development time and also delay integration into Models3 until November 2001. However, the development costs will be a bit lower, even though taking longer. EPA is still looking for outside funding. Dave Morgott said industry money for FY 2000 will be committed before the SMOKE modifications will begin and at this time funding is not identified in FY 2001. He added he thought the changes that would delay SMOKE development until 2001 were valuable changes.

Dave Morgott said he thought it would cost around \$60,000 to do what Bill Benjay had described previously. Barbara Francis said that it is unlikely that the ACC can pay for all of SMOKE if it slides into 2001, although it is a worthwhile project. She asked if other members of RRWG might want to contribute (in the 40 to 60 thousand dollar range).

Tom Helms said that SMOKE development should be a high priority. If we don't have the SMOKE tool, it will be difficult to develop a new policy. Barbara Francis said ACC supports its development and will fund part of it, but can't fund the whole thing. Again she said other companies or associations need to contribute.

Bob Avery asked if SMOKE development will be done in parallel with other projects. Several people said this could be done. The group asked Deborah Luecken to organize efforts to track this and see that this happened. She said she would do this or get another EPA person to do this.

VII. Task Group 2 – OBM Classification of Regions

Barbara Francis gave an update on the Charles Blanchard (Envair) project to study VOC/NOx ratios in certain areas. She said a report on this is now on the NARSTO website. This study will be published in a peer reviewed scientific journal. Charles Blanchard will report results at a professional meeting (perhaps AWMA) sometime in the future.

Bill Carter asked about the possibility of a critical review of task 2 (the Envair study on VOC/NOx ratios). He said we should get independent scientific review to see if everyone agrees the study is completely credible. Tom Helms said he agreed with Dr. Carter. Barbara Francis said since this is on the NARSTO web site, would NARSTO be responsible for having a peer review? Tom Helms said the science and policy groups should at least review the paper. Dr. Carter said that we may have to pay someone to critically review the report. Such a review could be a good deal of work. While several people had contributed much labor to write the science assessment white paper, it is unfair to expect that such labor go uncompensated all the time. Brian Keen suggested that RRWG set aside funds for this. Bob Avery said it was his understanding that NARSTO is supposed to do this type of review. He thought that is one of the reasons RRWG agreed to affiliate with NARSTO. The group asked Bill Carter and Robert Wendoll to follow up with NARSTO on this issue.

VIII. Milestones for RRWG

Don Fox gave a talk on a chart titled "Milestones for Current Priorities of RRWG" which is a 3 year time line chart of what RRWG is doing. (See Attachment B) Although several tasks are being done, the work of group 1579 seemed to form the main thrust of RRWG efforts. Jake Hales suggested he would like to put this chart on into the NARSTO newsletter along with a short article explaining it. Bob Avery said we need to determine who would post Task Group 1579 results on the (NARSTO) website. Brian Keen said we should consider updating the policy and science assessment white papers as new information comes available.

Referring to Don's chart, Robert Wendoll said that rather than saying RRWG alone will not be able to do all that may be necessary to answer all ozone related questions we should say that RRWG will work with others to synthesize available material. Don said this is a good suggestion. (Change included in Attachment B)

Discussion turned to a possible workshop to summarize results coming out of the group 1579 study at some time during the fall 2001. It was

suggested we might do this in connection with some larger scientific body . RRWG members participate in AWMA committees and would be willing to coordinate with AWMA if that would be helpful. Others mentioned the long lead time to get on programs of organizations such as AGU or AWMA. It may already be too late for next fall. Someone suggested that trying to pull in large organization such as AWMA may overly complicate things. Others suggested it might be better to keep this a relative small RRWG meeting at this stage.

Don Fox led a discussion on follow-up on air quality modeling. Dan Baker is the leader of this effort which is to plan for using an air quality approach. Bill Carter will also be involved. Plans are to:

- Organize a group by Nov 1
- Develop a preliminary presentation for next RRWG meeting
- Refine the issues over the summer
- Draft an RFP for Fall 2001

Someone asked how this is different from the present work of group 1579. The reply was that this is essentially a reorganization of group 1579.

IX. EPA and RRWG Research Tom Helms

Tom Helms gave a presentation beginning with a discussion of the status of the ozone program in EPA. He said EPA is placing a lot of emphasis on NOx reductions to control ozone. He discussed various court decisions which affect the NOx SIP call. He talked about 1-hour ozone standard attainment problems, and mentioned how the Ozone Transport Commission is looking for new VOC reductions. He discussed the 8-hour ozone standard which EPA is not now implementing due to a Court decision (which is currently being appealed), but said that the designation process is on going.

Tom then showed a series of slides with the title "Thinking about a New Ozone Policy." The elements of a new reactivity policy would have to include:

- Be scientifically sound, easily understood, and directionally correct

across the country.

- Be compatible with ongoing air management efforts such as trading offsets, and rate of progress determinations.
- Consider the overall effects of VOCs on the environment
- Require reasonable record keeping for compliance and be simple to enforce.

Basil Dimitriadis asked how an 8-hour standard would affect a reactivity definition. Tom said that it is important to consider since he believes that eventually some sort of 8-hour standard will be adopted, even if it may be somewhat different than the 8-hour standard which is now before the courts.

Tom showed a slide of policy possibilities. Included were:

- no consideration of reactivity, i.e. everything reacts
- keep the existing policy
- keep the existing policy but adjust it for new science
- have a new policy based on reactivity bins, scales, etc.
- a new comprehensive policy, which may be different from any of the above.

In another slide, Tom discussed aspects of implementing a revised policy:

- scientific impediments to revising policy, i.e., will RRWG work answer all questions
- National and regional air quality differences
- enforcement difficulties
- record keeping requirements
- integrating new policy into current air quality management scheme
- public understanding about policy changes

Don Fox discussed new business before the RRWG. He asked what we might discuss at the next RRWG meeting. He suggested a follow up of the modeling exercise being done by group 1579.

Jeff Holmstead asked about the timing for the RFP for the 1579 task. This schedule was given:

- comments to Dan Baker by October 11
- finalize request for preproposal
- make recommendations about who should receive request for preproposal. Send recommendations to Don Fox. Some suggestions include NARSTO website, NARSTO e-mail list, RRWG mailing list, other parties.

Bill Carter said that since we need to contact NARSTO about peer review we can ask them about e-mail distribution of the request for pre-proposal. We need to do this by October 18, 2000 and ask for preproposal submittals by December 1.

The date for the next RRWG meeting was discussed. January 17 and 18, 2001 was tentatively selected. Brian Keen suggested that we preschedule all meetings for 2001, so people can plan ahead. He suggested 3 meetings. The steering group will look at this recommendation.

Bob Avery asked that we get a list of action items summarized on one page within a week.

X. *Adjournment.*

The meeting adjourned at 11:30.

Attachments

Attachment A. Air Quality Modeling 1579.pdf

Attachment B. RRWG Milestones.pdf



REACTIVITY
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**Summary of RSWG Meeting for January 17 and 18, 2001
Research Triangle Park, NC.**

Attending: Sarav Arunachalam, Bob Avery, Dan Baker, Jim Berry, Bill Carter, Janet Catanach, John Dege, Basil Dimitriades, Don Fox, Barbara Francis, Doug Fratz, Bruce Gay, Bob Hamilton, Madelyn Harding, Tom Helms, Jeff Holmstead, Bill Johnson, Jon Kurland, Deborah Luechen, Dave Morgott, Eileen McCauley, Ted Russell, David Sanders, Bob Stallings, Stan Tong, Jeff West, Robert Wendoll, Fred Whiting

I. Welcome and Introductions

After introductions, Don Fox reviewed the agenda for the meeting.

II. Policy Team Meeting

Tom Helms made a presentation on the Policy Team concerns. He said, in answer to those who have asked when we are going to do something, that we are now ready to do something that could have a big impact on what future policy will be. Tom then gave a quick summary of policy options and problems with options that he had presented in more detail at the October 2000 meeting. Then he asked Bill Johnson to go over a list of policy concerns that we would use to judge the pre-proposals that we had gotten for Task 1579.1. Bill presented the following "Policy Interests for Evaluating RFPs":

1. What is the hypothesis that we want to test?
2. What would be the affect on ambient air levels of substituting low reactive compounds for highly reactive ones?
3. Would controlling only the most reactive compounds (while exempting lower reactive compounds) have any significant impact on ambient ozone levels?

4. How would low reactivity compounds emitted in large volume affect ambient ozone levels? Could widespread exemption of lower reactive compounds cause the ambient air quality standard to be violated in certain locations?
5. What is the geographical validity of reactivity scales? Are scales valid over the whole country or only in certain locations? If not, how large are variations? What would be the cause of the variations?
6. How do initial conditions affect reactivity scales (i.e., VOC/NO_x ratios)?
7. How does meteorology affect scales?
8. Do reactivity scales shift if reactivity is evaluated over different lengths of time? (i.e., would a scale evaluated over 8 hours differ from a scale evaluated over 5 days?)
9. What is sensitivity of scales to different conditions? For example, do compounds' position on the scale flip-flop with different conditions?
10. Should we be looking at other kinds of scales than MIR scales? What other scales should we look at? Would we want to evaluate how other types of scales vary with varying conditions?
11. What atmospheric model is used to evaluate validity of reactivity scales? Is this model one that is widely used and available to various independent researchers so that work can be verified and peer reviewed? Is a proprietary model of value if it is not widely accessible to everyone? (*Questions 12 and 13 below are technical questions, but they have policy implications.*)
12. What is the sensitivity of reactivity in the model? Are all compounds lumped into a few bins? Is carbon bond IV, which lumps compounds into 11 reactivity bins, sensitive enough to evaluate reactivity scales? Is there a better way of handling reactivity in models? If so, what?
13. Are effects of grams versus moles being considered? If a certain percentage of VOC is being reduced in a model, is this by weight or by number of moles? If one compound is being substituted for another in a computer run, is this substitution being made by weight or by number of moles? How will this affect the outcome of the experiment?

Basil Dimitriades and Doug Fratz commented that the "policy issues" presented by Bill Johnson are really mostly technical issues. Tom agreed that Basil and Doug had a point; but that these are technical issues that must be addressed to EPA's satisfaction before there can be any realistic hope for a revision to EPA's present reactivity policy.

There was a discussion of various reactivity scales. Bob Avery

commented on the use of MIR scales. He said a lot of work had already gone into this and it is widely accepted. There is no use of reinventing the wheel, so to speak, by trying to develop some other scale. Deborah Luecken said a key question before us is how robust are scales over various geographic areas. Some one suggested that all the scales developed to date, including Carter's MIR, MOIR, EBIR and Derwent's POCP, are similar and correlate well with each other, although there may be small differences.

Madeline Harding asked if the information you would get by using CB-IV would have enough specificity to aid in making policy revisions. Doug Fratz said the CB-IV data would be directionally correct. The initial studies are designed to get an overview, not to answer all questions that might arise. Bob Avery expressed the opinion that if bins were used to group compounds then CB-IV would be good enough. Doug Fratz asked whether people would have disputes about compounds that are near the border of the bins concerning which bin they should be in.

John Kurland asked how important it is to look at other endpoints than ozone, such as particulate matter. Tom Helms said that ozone is of primary concern; however, EPA management has responsibility for multi-pollutants so they may be interested in other components than ozone.

III. TASK 1579.1 PreProposal Technical Evaluation Panel Meeting

The group reconvened after a break. Don Fox said that this part of the day's discussion would be used to evaluate the pre-proposals, which had been received in response to the Task 1579.1 RFP. Don said that this session would be restricted to persons who agreed to sign a confidentiality agreement, which stated that participants would not divulge the contents of proposals to outside parties. This was done to protect the privacy and work of the submitters of proposals. The submitters of the pre-proposals, some of whom were regular participants in the RRWG, did not attend this session to avoid any appearance of conflict of interest.

There were 11 pre-proposals submitted. Five of the pre-proposals were judged too narrowly focused on certain topics to answer the questions, which the RFP had posed. The group discussed at length the six remaining pre-proposals. Of these, three were selected as being the most responsive to answering the questions that RRWG wished to address. The RRWG members present agreed that RRWG should attempt to fund all three of

these studies. It was thought that if the three independent approaches gave results that showed good correlation, that would be a significant finding which would lend confidence to the results. All the pre-proposals that were not selected were judged to have merit. There was a general agreement that perhaps some of these other projects might be worth funding at some later time. The three pre-proposals were not going to be identified publicly (or even to the submitters of the pre-proposals) at this time, since firm funding commitments to proceed with the work had yet to be obtained. RRWG members did not think that it is appropriate to tell submitters that they have been selected to submit a proposal unless money was in place to pay for the work.

After lunch the group discussed possible funding of the three pre-proposals that were selected for immediate funding. The total combined cost of the three was in the range of \$180,000. The American Chemistry Council said they would provide \$60,000 toward these studies. Robert Wendoll said the Dunn Edwards company was prepared to fund \$25,000 of this research. Doug Fratz said the Consumer Speciality Products Association would probably fund several thousand dollars toward this project. Bob Nelson of the National Paint and Coatings Association was not present. EPA, both OAQPS and ORD, were expected to contribute but no exact amount was given at this time. Doug Fratz said he had been working with the Ozone Transport Commission and he would contact the OTC to see if they would be interested in funding part ~~of~~ of this project.

(Thursday, January 18th)

IV. Task Group Reports

Don Fox called the meeting to order. Don said that today's meeting would be devoted largely to a discussion of other tasks being done by RRWG in addition to the Task 1579.1.

Task Group 10 Survey and Compile Existing Chamber Databases

There was a short discussion of Paul Makar's work in evaluating existing chamber databases. Since Paul was not in attendance at this meeting, Don Fox led the discussion. Don mentioned several sources of Canadian funding that Paul had contacted.

Task Group 8 Emissions Processors

Dave Morgott reported on work of Task Group 8 and indicated that an ACC TIP has agreed to sponsor an RFP for developing the SMOKE emissions pre-processor. The RFP will ask for a 9 to 12 month development period for SMOKE development work. The ACC TIP will provide funding for doing this SMOKE development work. Dave will distribute the RFP to RRWG members for a brief review, then post it on the NARSTO website to request proposals.

Task Group 4 Suitability for Reactivity Based Controls

Task Group 4 was to identify specific chemical groups that would be useful in consideration of reactivity. Don Fox said that this project is still alive, but currently moving slowly. Don Fox asked Tom Helms if perhaps some EPA staff might be available to help with this. Tom said yes, although no specific work was assigned.

Task Group 2 VOC or Nox Limited Regions

Dan Baker reported on the work of Task Group 2 whose purpose is to analyze available information relevant to how much of the environment would be sensitive to VOC controls and the distribution of conditions appropriate for reactivity assessments. He said the Blanchard report, which had been done under contract, concerning VOC/NOx ratios has been posted on the NARSTO website. In addition, data have been collected for the Lake Michigan area for the 1990s. Data have also been collected for the Northeast and Southeast. Charles Blanchard is the contractor for this work on these three regions. Another small task has also been done in rendering data from UNC and an Australian smog chamber into a useable format.

There was a discussion of presenting some of this information at an Air and Waste Management Association meeting. Also a paper may be prepared for publication in the Journal of the Air and Waste Management Association (JAWMA). Deborah Luecken asked about whether NARSTO has reviewed this work. Don Fox and Robert Wendoll said they had talked to Jake Hales of NARSTO and Jake Hales had said that NARSTO would provide peer-reviewing services. RRWG needs to identify what needs to be reviewed and what time frame we are interested in. Someone asked if there is

a cost for this NARSTO review. Several people thought NARSTO had funds set aside to cover peer reviews.

Task Group 3 Environmental Fate and Availability

Jon Kurland discussed the work on environmental fate. He was proposing to publish some of the results of the Environmental Fate Workshop held on June 27-29 in Research Triangle Park so that this information might reach a wider audience. He suggested several publications which might publish some sort of notice about this work and at least refer readers to the NARSTO website where a summary of the workshop could be posted. The publications he mentioned are Environmental Science and Technology, Atmospheric Environment, and Journal of the Air and Waste Management Association. Environmental Health Prospective, an NIEHS publication, was mentioned, but the group decided this publication was not a good fit for the particular information.

Jon Kurland said Task Group 3 had drafted two RFPs and he passed out draft copies. The first would identify compounds predicted by environmental fate modeling to have significant destruction pathways other than oxidation in air. This task would determine the potential importance of environmental fate corrections to emissions and provide the data set for investigating the ozone forming potentials of VOC in a box model.

The second RFP would be for creation of a simple screening air quality model (e.g., a box model) including compartments and transport properties of common environmental fate models. The model would be publicly available as a tool with which one could test representative compounds of various chemical classes to see whether the same oxidation is predicted with complex meteorology as with the environmental fate model. After some discussion, Jon said we might not limit ourselves to a box model, but might be open to other approaches.

Jon said he had funding almost lined up for these tasks through Sue Lewis of the American Chemistry Council who has some money left over from the previous environmental fate workshop.

Tom Helms asked how task 3 results would be expected to play in policy modification. Jon said that it would be important to learn how large the universe of compounds is that might be removed from the atmosphere

by various processes. If this is small, we might want to forget about it. If it is large, we might have to consider this in ozone control policy. Bob Hamilton said some compounds are not very volatile and don't get into the air. Bob Avery said some compounds might get into the air, but not stay very long. Robert Wendoll said this work might help solve apparent discrepancies between emission inventories and ambient air measurements.

V. *Proposal Review Procedures Discussion*

Barbara Francis asked if we would handle this RFP in a similar fashion to the way task 15791 had been handled, with review by the whole RRWG of various proposals that were received. This led to a discussion of exactly what the procedure is for reviewing proposals or pre-proposals. Don Fox said he would write up a summary of the review process and distribute this to the RRWG membership

Discussion continued on the approval process. Robert Wendoll said proposals don't have to get approval from RRWG. Bob Avery said RRWG doesn't approve anything; we just review and comment.

Tom Helms said people should not just go out and do something and then represent it as an RRWG product. To be represented as an RRWG product, it should undergo wide review so that the product doesn't represent only the view of a particular person or group.

Robert Wendoll said that as to the question of how a work product becomes a NARSTO (or RRWG) product, there is a procedure spelled out by NARSTO, and we should follow this. Robert asked Jeff West, who represented NARSTO at the meeting, to explain the procedure.

Eileen McCauley expressed concern that the public could see approval of something by the RRWG Policy Team as essentially the same thing as EPA approval.

Dave Morgott said in response to this discussion that he will submit the SMOKE RFP to the whole group for review.

VI. *Funding Process for Task 1579.1*

For those who were not present on the previous day, Dan Baker

gave a review of the task 1579 activities that took place the day before concerning the review of the pre-proposals. He said the purpose of task 1579 is to use existing tools (models, data, etc.) to see what questions we can begin to answer in regard to how reactivity affects air quality.

Don Fox said we are close to having sufficient funds to support the 3 projects identified as most useful. The RRWG will respond to all investigators who submitted pre-proposals by the end of January. Don Fox said that the 3 projects should be completed in a 9-month period. It will take up to 2 months to get the money together. This should give us results in the November - December 2001 time frame.

Barbara Francis said she had agreed to be the contract manager for part of the 1579 projects, but that her compensation from CAA might not cover her work for that. She said part of the money the CAA had collected for salary compensation for Don Fox had not been used. She asked if she could be compensated for her time out of that money. No one objected to this. Don Fox said his compensation was being covered mostly by his University as a public service. The only money he needs from RRWG is for expenses such as photocopying, telephone calls and soft drinks/coffee served at meetings. Money that EPA had set aside for Don Fox compensation could go toward funding one of the research projects.

Don Fox discussed the timing of the next meeting and its purpose. An earlier meeting could give input to the preparation of the proposals. A later meeting could look at how work was proceeding and discuss needed corrections. It was decided that two tentative dates would be considered: April 4 and 5 or April 11 and 12. A decision on meeting date will be made later. Either of these times is a rather late date for early input to the proposal development process. It was decided that early input into this process could be made through conference calls among interested parties.

VII. *Adjournment*

The meeting adjourned around noon. Twenty-eight people had attended all or part of the meeting.



**REACTIVITY
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Summary of the Reactivity Research Working Group Meeting for April 11 and 12, 2001 in Research Triangle Park, N. C.

Attending: Zac Adelman, Sarav Arunachalam, Bob Avery, Dan Baker, Jim Berry, Bill Carter, Janet Catanach, John Dege, Basil Dimitriadis, Susan Eastridge, Don Fox, Barbara Francis, Doug Fratz, Bob Gross, Amir Hakami, Adel Hanna, Madelyn Harding, Tom Helms, Bill Johnson, Terry Keating, Jon Kurland, Deborah Luecken, Rohit Mathur, Bruce Moore, Dave Morgott, Eileen McCauley, Monica Nichols, Bob Nelson, Bill Rawson, Paul Reed, Ted Russell, David Sanders, Bob Stallings, Stan Tong, Jeff West, Robert Wendoll, Fred Whiting

I. Welcome and Introductions, Review of Agenda

At 1:00 pm on April 11, Don Fox called the meeting to order and gave a preview of the meeting. He presented three primary goals for the meeting:

- Preliminary AQ Modeling Initiative
Improve overall results from interaction of three research groups with RRWG membership
- Review and Consensus on three RFPs
HC Availability – Partitioning
Integration of AQ & Fate Models
SMOKE – Emissions Processor
- Develop roadmap and scope for Extensive Air Quality Modeling Project

He reviewed issues from the last meeting that still had to be dealt with, and discussed what constituted an RRWG effort. He discussed current research efforts, and how results could be disseminated. One possibility is having results published in scientific journals to reach a wider audience.

However, some journals consider posting on a web site, such as the NARSTO site, to be a publication and won't publish articles that have already been published. This raises a concern about how best to distribute the results of RRWG research products.

Would we disadvantage an investigator, who has written a paper on an RRWG research project by posting a manuscript or report on the NARSTO website? Would this keep them from publishing their paper in a journal?

Eileen McCauley said that it was her understanding that the format of a journal article is copyrighted by the journal, but the information in an article is not copyrighted if it is paid for by a government grant.

Barbara Francis advised that we change our report dissemination criteria from "report will be posted on NARSTO website" to say report will be "published." Others indicated that the objective is to get the information out and many considered a journal article to have more impact and taken more seriously than a web site posting. Dave Morgott said that the SMOKE project has a requirement that work will be published in a journal within 6 months of finishing or else will be posted on the NARSTO website.

II. RRWG Research Development Process

Don Fox introduced a discussion of the milestone summary chart (See Attachment) and various projects being carried out by the different task groups. He reordered the Tasks to focus on the priority issues of the RRWG. Don went over the chart and discussed each task.

There was a short discussion of Task 4 which involves identifying chemicals and conditions for their emissions. The question was asked if an RFP exists for this task. The expectation may be that this question will be answered, as the tools are developed to conduct the assessments. There is not an active effort on this task at this time.

III. Updates on Task Group Activities

(Task Group 3) Jon Kurland provided an update on the environmental fate effort. The two proposed RFPs related to this effort have been rewritten to make them clearer. Don suggested that the RRWG approve the changes which had been made in the Task 3.1 and 3.2 RFPs. No one objected. Don will check with the NARSTO coordinator to see what we have to do to get the workshop results on the NARSTO website

Jon requested that the Task Group 3 members be permitted to review pre-proposals and make recommendations to funders between

meetings. The RRWG approved this request for review of the Task 3.1 and 3.2 submissions by e-mail or conference call with the signing of confidentiality agreements. There was a question from Jon about whether signed confidentiality forms were universal or do we have to sign a new form for each project. Don Fox indicated the forms were universal. Bill Carter suggested that there may be some value in having separate confidentiality forms or “non-conflict of interest” forms. Don said we would request a “conflict of interest” form with use for each new task.

(Task Group 8) Dave Morgott discussed the project for SMOKE development. Some potential bidders on the project were in the room and Dave indicated they could listen to the discussion, but he would not take any comments on this subject from them. Dave said three research organizations were being targeted to receive the RFP. These are MCNC, SAIC and W. P. L. Carter. In addition, proposals will be accepted from the public. After the RFP is approved by the RRWG, the ACC TIP which will be paying for the work will do the evaluation of proposals. Bill Carter asked if it would be possible to submit a proposal which addressed only part of the RFP. Dave Morgott indicated that would be acceptable. Also, collaboration between different groups in submitting a proposal will be permitted.

Bill Benjey described the RFP for the SMOKE project which will cover SMOKE tool development. The SMOKE tool will aggregate compounds into groups which SAPRC uses. SMOKE can now be used for CB-IV and RADM2. It is desired to modify the emissions processor so that SAPRC can be used.

Dave Morgott said that he interpreted the discussion on the SMOKE RFP to constitute concurrence to post the RFP. He said he was looking for 4 or 5 peer reviewers.

(Task Group 2) Dan Baker gave an update on Task 2 involving the use of ambient data in assessing where reactivity may make sense as part of a control program. This included a discussion of Charlie Blanchard work which pulled together efforts of other groups. Robert Wendoll said that Charlie Blanchard’s work which is posted on the NARSTO website is being peer reviewed by the NARSTO science team.

Robert Wendoll asked the group to consider seasonal as well as geographical validity. Some organic chemicals may have a seasonal pattern associated with use and release. Robert suggested we add “environmental availability” as something to consider.

Bill Carter asked how far can we go with a discussion on next steps until we see the results of some of these assessments. We need to see some results before we can develop other RFPs and find the monies to support the work. Bob Avery said that we can think qualitatively about these issues in the mean time until we get results from the assessments.

(Thursday, April 12, 2002)

IV. Task 1579.1 Preliminary Modeling Goals and Objectives
Dan Baker

The next morning, Don Fox reopened the session at 8:40 am. Dan Baker was moderator for the morning session. The morning session was focused on discussing the three contract studies that were being supported by the combined Task Group 1579.1. Dan summarized the purpose of group as follows:

- Task 1 - Assess effects of large-scale reactivity-based substitutions on regional air quality using existing models.
- Task 5 - Develop appropriate scenarios for general reactivity assessment.
- Task 7 - Develop model criteria for reactivity assessments.
- Task 9 - Use existing models to evaluate exemption standard.

Research Group Presentations. Representatives for the three groups of scientists selected (from the larger group who had submitted pre-proposals) by RRWG to submit proposals gave presentations about their proposals.

Bill Carter presented “Investigation of VOC Reactivity Effects Using Existing Regional air Quality Models” which described work he proposed to do under RRWG funding. The reactivity screening project will focus on the East coast scenarios. In this project there is insufficient funding for use of SAPRC97 mechanism. Incorporation of SAPRC97 would require an additional \$6,000. The project will use the CAMx model. There was a discussion of CB-IV versus SAPRC. It was pointed out that CB-IV does have standing with regulatory agencies. Dr. Carter presented various scenarios which he proposed to test how a reactivity scale will predict ozone caused by substitution in various scenarios.

Amir Hakami who described the work proposed by Ted Russell’s

team at Georgia Tech under RRWG funding gave the next presentation. He indicated organic reactivity assessment is difficult to do in a smog chamber since it is difficult to simulate the atmosphere in a smog chamber. Air quality modeling will be the Georgia Tech approach. The models solve atmospheric diffusion equations. Different assessment techniques include brute force sensitivity analysis and DDM sensitivity analysis. The relative importance of VOCs depends on the way the results are processed and interpreted.

Ted Russell gave a further summary of Georgia Tech's proposed project. He plans to apply SAPRC 99 to the eastern U.S. Bill Carter said that what the Carter team is planning to do is complementary with Ted Russell's work. Bill said it would be preferable for all three projects to present results on a similar basis so that comparisons would be more obvious.

Dr. Sarav Arunachalam of MCNC presented an "Investigation of VOC Reactivity with Comprehensive Air Quality Models" which described the modeling effort which MCNC plans under RRWG funding. Dr. Arunachalam said the "reactivity" of a compound depends on the compound's unique properties, and the conditions of the ambient environment in which it is reacting. This talk presented various modeling scenarios and VOC substitution scenarios. Scenarios include modeling for the eastern U. S. with emphasis on North Carolina, and modeling for the Southeastern U. S. with focus on the Houston-Galveston area. Model options include MAQSIP/MM5/SMOKE with CB4 chemical mechanism and CAMx/SAIMM/SMOKE with CB4 chemical mechanism. RADM was discussed as a possible mechanism for certain VOC substitution scenarios. Numerous metrics can be used to assess impacts from VOC substitution.

Don Fox requested an accounting of funding resources from RRWG members. The following organizations reported:

National Paint and Coatings Association - money is available
Dunn Edwards Company - money is available
Consumer Specialty Products Association - money is available
American Chemistry Council - money set aside
EPA - Money committed,

Sufficient monies are available to execute these three projects.

Don and the funding sources will work out the funding details with these three organizations.

Barbara Francis said the we need to make a decision of exactly what MCNC is going to do before a contract can be written. Someone said that it would be desirable to use CB-IV mechanism for both the Carter and MCNC work so that the overlap between the two efforts can be looked at on the same basis.

Bill Carter asked why a mole substitution is going to be investigated by MCNC as one of their scenarios because an evaluation could be estimated by a linear calculation. The ensuing discussion indicated that RRWG wanted to see the actual modeling results.

Bill Carter asked if we will have a meeting which can serve as a mid-course correction. Don Fox said these projects should be finished by the end of January 2002. Barbara Francis asked what pieces of work would have to be complete before mid-course reviews. The answer given was the Carter project on DDM with Environ. Bill Carter thought he can get this done by the date of the next meeting in the late August or early September time frame.

V. Schedule of Next Meeting

Don Fox led a discussion about when the next meeting should take place. August 28-29, 2001 was selected as the preferred date. October 3-4 was the back-up date selected.

VI. Adjournment

The meeting was adjourned around noon on April 12.

Attachments

RRWG Milestone Chart



**REACTIVITY
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**Summary of the Reactivity Research Working Group Meeting for
January 16 and 17, 2002 Research Triangle Park, NC.**

I. Welcome and Introductions. Review of Agenda

At 1:00 PM on January 16, Don Fox called the meeting to order and introduced the agenda and goals for this meeting. He indicated there were three action items for the meeting:

- To review the results so far of the three photochemical modeling contracts
- To consider an advisory committee for the University of California at Riverside chamber
- To outline the next policy questions to be considered.

II. Milestone Review of Tasks 3.1, 3.2, and 8

Don Fox gave a summary of the environmental fate modeling effort (Tasks 3.1 and 3.2). (Dr. Jonathan Kurland, Task 3 group leader, was not present at this meeting.) Two companies had bid on the effort. SENES Consulting LTD., a Canadian company, has been awarded the contract. They will develop an environmental fate box model and then use the model to assess the environmental fate for several common compounds. The Glycol Ether Panel of American Chemistry council (ACC) had received a petition for funds to pay for this work.

Dave Morgott gave an update on Task 8, which is SMOKE emissions processor development. One proposal from MCNC was received in response to the proposal.

*III. UCR – New Chamber Update – Bill Carter
(See Attachment A Website address.)*

Bill Carter gave a presentation on the new smog chamber being

developed at the University of California at Riverside (UCR) that is initially funded largely by EPA. A summary of the slides presented during the talk entitled “Development of a Next-Generation Environmental Chamber Facility for Chemical Mechanism and VOC Reactivity Research” was made available to the attendees. Dr. Carter showed pictures of the facility that has already been constructed and described the analytical instrumentation in the facility. He described his current funding and a summary of experiments in his draft research plan. He concluded by recommending that RRWG be a main vehicle for providing oversight and input into the overall project.

Robert Wendoll concurred with Bill Carter’s recommendation that RRWG serve as an advisory group to provide oversight to the UCR chamber work. Mr. Wendoll would like to see a subgroup established for this purpose.

Don Fox asked the group if we have agreement that we develop such a workgroup and work with CARB Reactivity Science Advisory Committee (RSAC) on UCR chamber work. No dissenting opinions were heard.

IV. Task 1579.1 Preliminary Modeling – Dan Baker

This session was devoted to hearing progress reports from the three contractors who are doing modeling studies to address the Task 1579 issues. These studies are funded by the RRWG and include the following organizations:

- Georgia Institute of Technology – Ted Russell PI
- Microelectronics Center of North Carolina – Sarav Arunachalam PI
- University of California at Riverside / Environ – Bill Carter PI

IV A. Georgia Institute of Technology Presentation

Dan Baker introduced Dr. Ted Russell for a presentation entitled “Three Dimensional Regional Reactivity Assessment for California and Eastern United States.” (See Attachment B) He is finishing up a 3-D reactivity assessment in California. He is using MAQSIP, SAPRC-99 and DDM-3D applied to central California. CIT, SAPRC-99 and DDM-3D is used in the Los Angeles area. He is beginning an eastern US reactivity assessment using URM, SAPRC-99 and DDM-3D. Dr. Russell’s work gives population weighted MIR values which emphasizes ozone impact in

populated areas. In his summary, Dr. Russell concluded that DDM is a reliable tool for sensitivity and that 3D reactivity modeling captures temporal and spatial variability in meteorological and chemical regimes. He concluded that the California and very preliminary eastern U.S. 3D results show a consistency with prior modeling studies that he has conducted.

IV B. UCR – Environ Presentation

Dan Baker introduced Bill Carter for a presentation entitled “*Investigation of VOC Reactivity Effects Using Regional Air Quality Models*” (See Attachment C.) Dr. Carter made copies of his slides to the audience. The objectives of his research project are:

Assess VOC reactivity effects using existing Regional Modeling database representing the eastern U.S. Assess relative incremental ozone impacts of VOC model species with respect to:

- Variation within the modeling domain
- Derivation of various reactivity metrics
- Comparison with reactivities calculated using EKMA models
- Predictions of effects of selected large scale substitution

Assess approach for deriving a general reactivity scale representing regional O₃ impacts.

Some of Dr. Carter’s preliminary conclusions are:

- NO_x control is more effective than VOC control in most of this modeling domain
- VOC control is effective in some large urban areas where O₃ is high
- Relative reactivities are highly variable, but variability is less in more VOC-sensitive cells
- EKMA scales underestimate reactivities of slowly reacting species (e.g. ethane)

Tom Helms asked what people thought about bins versus scales. Are there obvious breaks in reactivity to draw lines between bins? The initial response was that reactivities are fairly continuous among all organic compounds with no obvious breaks.

IV C. MCNC Presentation

The next presentation was by Sarav Arunachalam of MCNC titled “*Investigation of VOC Reactivity with Comprehensive Air Quality Models.*” (See Attachment D.) He explained various tasks in his modeling scenarios. Some runs involved substitution of compounds for others. One run involves reducing VOC across the board by 15%. He said MCNC has just recently received funding and has just started work.

Bill Carter asked if the ethylene glycol substitution planned for one scenario is a good representative compound. Dr. Carter agreed to talk to Harvey Jeffries, who is helping MCNC, outside the meeting about this.

The first day adjourned at 5:50 PM.

Thursday, January 17, 2002

Don Fox began by summarizing the time line for projects underway. He presented these dates:

- preliminary modeling results, April - May
- additional project RFPs outline, April - May
- RFP given to contractors, August - September
- contract performance period 6 to 9 months, ending April 2003

IV. Associated Federal Air Quality Research Groups

- a. *National Institute of Standards and Technology – Robert Huie*
- b. *National Oceanic and Atmospheric Administration – Pai-Yei Whung*

The meeting proceeded with additional speakers. The next two speakers were invited guests from Federal Agencies other than EPA who have an interest in the activities of the RRWG.

The next speaker was Bob Huie with the National Institute of Standards and Technology (NIST). He talked about “Environmental Measurement Activities in the Experimental Kinetics and Thermodynamics Group.” He described, among other things, a flash photolysis fluorescence method to measure k_{OH} values easily within 2% accuracy. He also

described studies comparing ^{14}C and ^{13}C ratios and asked do carbon isotopes have a role in chemical mechanism and VOC reactivity research. (See NIST Presentation.)

The next talk was by Pai-Yei Whung with NOAA in Maryland. She gave an overview of NOAA research related to international transport of pollutants from the Gobi desert including oxidants, aerosols and their precursors. She said the NOAA desired to work with RRWG through NARSTO.

V. Models III Update – Bill Benjey

The next speaker was Bill Benjey of EPA who gave an update on Models3/CMAQ and SMOKE development status. (See Models III Update)

VI. Future Directions Science to Inform Policy Issues - Don Fox

Draft Timeline

Don Fox then discussed the time line for finishing up current projects and the need for funding for future projects. He would like preliminary modeling results from the current contracts in the April - May, 2002 time frame. He suggested the following time frame if follow-up work is needed. RFPs to conduct such additional analysis might be developed in the August - September 2002 time period. The contract work could be conducted in the 6 to 9 month period ending in April 2003.

The discussion turned to more general issues. Bob Hamilton said you could research something forever. He said he would like to encourage this group to make specific recommendations based on the research. He said California has two rules based on reactivity concepts: an auto exhaust rule and an aerosol spray paint rule. He suggested that this should give others an impetus to adopt something with reactivity; either adopting what California has adopted or takes some alternative approach. Dave Morgott replied that we are making progress with the current research approach we are pursuing, and we should keep following our current line of research. Tom Helms said he thought that the discussion of scientific issues the previous day was one of the best sessions we have had. Tom said that he wants to do more evaluations of these preliminary studies. He said that EPA needs to look toward moving to a new policy. He said his dream is to be able to wrap this up in 18 months or so. He expects that EPA may be

able to put more money toward this work in the future than it has over the past two or three years.

Harvey Jeffries said that we need a funded workshop to analyze results of the modeling. Bob Avery said such a workshop could take place meeting after next since the next meeting would be to report on results.

Policy Scenarios

Bob Avery said he would like to ask Tom Helms what sort of policy direction Tom envisioned us going in. Tom said we currently have a +/- scale reactivity scale (i.e., controlled or exempted) that we have been using for a long time. Tom said it is apparent to him that we need to do something different. The options he sees are:

1. Keep current policy
2. Let areas do what they want regarding reactivity as long as they can demonstrate attainment
3. Adopt some form of reactivity scales
4. Use reactivity bins. With bins you are only concerned with the margins between bins. Individual reactivity numbers are of not so great a concern.

Tom said a more sophisticated consideration of issues uncovers a new layer of complication. For example, any adoption of a policy based on scales or bins raises the question of how you do trading or how you do NSR offsets using them.

Bob Avery said he doesn't like bins because whether you have 3 bins or 6 bins you have bright lines to argue over. Scales get you away from this. He cited the example of California that will fix scales for a certain period of time, and then revise them at stated intervals if additional research shows that this is necessary.

Eileen McCauley said that California has adopted reactivity scales on a source-by-source basis for carefully studied sources, not as a blanket approach to all sources. She said it seemed like she was hearing that EPA may consider adopting a reactivity approach that would apply to everything across the board. Tom Helms replied that we are just brain storming now.

Summary and Near Term Ideas

Don Fox summarized the discussion so far by saying that we have a series of projects (i.e., the three modeling studies related to combined tasks 1579) underway looking at the late May time frame for initial results. There are hints that these studies may be more fruitful than initially expected, but more analysis of results may be needed. This analysis must be funded and would be used in preparation for a workshop. In addition, we have work on SMOKE underway, which will improve our ability to ask certain types of questions. Also atmospheric availability and fate modeling are being pursued with a 6 to 9 month time period for response. Also, we talked about the need to outline any future research in order to get a parallel funding stream started.

Dave Morgott said that he would volunteer to be part of a group to prioritize future work if Don wants to constitute such a group. As an example of possible future work, he envisioned a statistical analysis to see if binning is a good idea.

Don Fox said he would send an e-mail to the group members asking for a response on two issues:

1. Advisory committee for steering Bill Carter's chamber work.
2. Group to advise on future directions for RRWG projects.

Don Fox discussed the next meeting. He recommended that the next two meetings be held in Research Triangle Park, NC. May 15 and 16 was selected as first choice for the next meeting date. The next meeting beyond that would be a technical review workshop to be held in late July or August.

Bill Rawson asked if the workshop would just be a more vigorous exchange among current RRWG participants or do we want to attract some wider external audience. We need to agree among ourselves on the nature of the workshop to see how long it will take to plan it. Don replied that he envisioned perhaps some outside review, but that the main focus would be current participants.

Bill Carter said that in planning for the workshop there will probably need to be some follow-up by the contractors based on comments received at the May meeting. Don Fox replied that we will not be able to

know what the follow-up work will be until we see the results in April, but we could consider adding money in the interim in anticipation of such additional work.

Someone asked about what additional outside people might participate in the workshop. Tom Helms said he saw a need for getting some representatives of environmental groups involved at this stage.

Don Fox asked the MCNC representative at the meeting if MCNC could have a draft report by May 1. MCNC said that this would be difficult since they are just now starting work due to the delay in receiving funding. MCNC said they would put their interim report on the web so that it would be available to RRWG members sooner than otherwise.

VII New Business - UCR Chamber Advisory Committee

Don Fox asked if there is any new business. Bill Carter asked what is the process for forming the new chamber group. Don said that RRWG traditionally operates in an open manner so that anyone who wishes to participate can. Bill asked if we had a volunteer to head the chamber group. Don said that Deborah Luecken of EPA would lead the chamber group.

Barbara Francis asked if we could get some idea of how much the follow up assessments for the three modeling studies might cost. We need to follow up with telephone conversations to reach agreement on the cost.

The meeting adjourned at 12:30 PM.

Attachments

- A. UCR – New Chamber Presentation
<http://pah.cert.ucr.edu/~carter/epacham/rrwgch1.pdf>
Progress Report <http://pah.cert.ucr.edu/~carter/epacham/>
- B. Russell GIT Presentation RRWG Jan 02 PDF
- C. RRWG UCR-ENVIRON Progress Rept Jan 02
- D. RRWG MCNC Presentation Jan 02
- E. NIST RRWG Presentation
- F. Benjey RRWG Models 3 - Smoke Update Jan 02



**REACTIVITY
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DRAFT

Summary of the Reactivity Research Working Group Meeting for January 8-9, 2003 Research Triangle Park, NC.

Wednesday January 8, 2003

Attendees: Bob Avery, Dan Baker, Rick Brown, Ed Casserly, Andy Collantes, John Dege, Basil Dimitriadis, Susan Eastridge, Don Fox, Barbara Francis, Doug Fratz, Bob Hamilton, Tom Helms, Bob Hinrichs, Andrew Jaques, Bill Johnson, Jon Kurland, Deborah Luecken, Dongmin Luo, Paul Makar, Bruce Moore, Dave Morgott, Bob Nelson, Bill Rawson, Doug Raymond, Ted Russell, Bob Stallings, David Sanders, Stan Tong, Robert Wendoll, Jeff West,

I. Welcome and Introductions. Review of Agenda

At 1:00 PM, Don Fox, RRWG Chair called the meeting to order and introduced the agenda. Attendees introduced themselves. The primary focus of this meeting was a review of the Task 1579.1 objectives and modeling results and discussion of subsequent research questions.

II. Task 1579.1 Objectives and Research Results - Don Fox

A review of Task 1579.1 objectives and research results was presented by Don Fox. (Appendix A. Task 1579.1 Summary of Modeling Results). Task 1579.1 is comprised of the three modeling studies which were carried out under contract by three different research organizations: Georgia Institute of Technology (GIT), University of California at Riverside (UCR), and MCNC from Research Triangle Park, NC (now part of the UNC Carolina Environmental Program). Don Fox summarized the overall objectives of the modeling studies which were to develop reactivity metrics,

to investigate large geographical domains with multiday episodes, to compare different chemical mechanisms and to test the impact of substitutions. Don said that GIT and UCR evaluated relative reactivity metrics while MCNC evaluated performance metrics. Don Fox gave a summary of each of the research projects.

The GIT study used URM-SAPRC99 for two multiday episodes. A multiscale model with grids of 24 km² to 192 km² was used. Among findings of the study is that the relative reactivities are consistent with each other, independent of which metric is chosen; MIR-3D, MOIR-3D, or LS-RR, and for different averaging periods. The metrics compare reasonably well (for most species) among different episodes, different emissions scenarios and different domains. The results suggest that relative reactivity scales present a fairly robust method for ranking organic species based on their potential effect on ambient ozone concentration for the test conditions in each study.

The UCR approach used a CAMx version 3.01 with DDM. Several different approaches were considered for deriving regional reactivity scales including regional maximum ozone, regional maximum incremental reactivity, regional MIR-MOIR, and regional average ozone. These metrics varied in how representative they were of the modeling domain. The first two reflected impacts only at one location, the Regional MIR-MOIR scales represents 4-7% of area in the full domain. The regional average ozone gives urban impacts the least weight of all the metrics considered. The study compared nine different metrics in regard to how wide the spread was between lowest reactive compound and highest reactive compounds. The results varied by a factor of three depending on which scale was used. This is a significant finding in that the scale chosen for regulatory purposes would influence how much credit was given for solvent substitutions. This study showed that scales derived from urban air shed models did not differ greatly from scales derived from more simple EKMA modeling, indicating that easier to use EKMA modeling might be valid to use in the future. This study also indicated that the position of individual chemicals in the various scales did not change a great deal from scale to scale. There was occasionally some shifting of a chemical by a few positions, but highly reactive chemicals remained highly reactive in all scales and low reactive chemical remained of low reactivity. Another significant finding was the averaging time for daily O₃ (i.e. 1-hour or 8-hour) does not significantly

affect relative reactivities.

The MCNC project used state-of-the-art modeling systems like SMOKE-MAQSIP over diverse chemical regimes and geographical regions to design and perform various VOC substitution scenarios and their subsequent analysis. MCNC studied several substitution scenarios using high versus low reactivity substitutions. They did substitutions by gram, mole and mol C. Among the MCNC conclusions was that, overall, more sensitivity was seen in the Eastern US domain than in the South central US domain, but both are dominated by biogenics. Gram-based substitutions yield relatively more sensitivity than mole-based or mol C-based substitution. Substituting highly reactive compounds with low reactive compounds does have an effect on ambient O₃. VOC substitution strategy gives the same directional sense as a VOC reduction based strategy in improving air quality.

Tom Helms summarized what he had heard by saying he saw several things which we should take from this meeting. These include:

1. averaging time (1-hour or 8-hour) doesn't seem to matter in devising scales.
2. the spread between the lowest and highest reactive compounds can vary considerably depending on the scale used.
3. both removal and substitution of VOC are good ways of controlling ozone.
4. the ranking order of compounds on scales seems to hold up using different scales.

In response to item 4, Ted Russell said that there are exceptions in that a compound may switch three or four places on scale, compared to a different scale. Bill Rawson said we should not let the perfect be the enemy of the good in devising scales. Bill Carter said that the reactivity scale values have a $\pm 30\%$ variability, so if policy can't stand that there is a problem. Tom Helms summarized by saying that relative position may change a little, but not much. If substitution is used, it should be among compounds that are far apart of the scale, not right next to each other.

One interesting discussion occurred after someone said that lowering mass of VOC could sometimes lead to more ozone formation

because the solvents in the reformulated low VOC product may be chemicals of much higher reactivity than the original solvents. This could lead to more ozone being formed. They said that lowering reactivity would never lead to more ozone. Deborah Luecken replied that there are circumstances where switching to a lower reactive solvent can lead to more ozone, if more of the lower reactive solvent is used after the substitution. This could occur when the solvent is transported over several days in an air mass. There is experimental evidence that the MIR values of two compounds which are wide apart in reactivity can become closer in reactivity over a several day reaction period. If there is more of the low reactive solvent than the originally high reactive one, the reactivity of the low reactive one may approach that of the high reactive solvent and make more ozone. Bill Carter concurred that this could happen in some situations.

Thursday January 9, 2003

Don Fox called the meeting to order at 8:00 AM.

II RRWG Milestone Review – Don Fox (See Appendix B Milestone Review)

Don Fox initiated a review of the status of projects being sponsored by the RRWG other than task 1579.1. Jon Kurland gave an update of the SENES, Ltd. effort to develop a model to predict environmental fate of chemicals and then to test the model on several chemicals. Dave Morgott said that Task 8 which is development of the SMOKE emissions pre-processor is on track. There was a discussion of Task 4 and whether the name of that task, i.e. "suitable source categories" or "suitable chemicals for reactivity," may be misleading. [Post meeting review of Task 4 history reveals the effort to focus on evaluating emissions suitable for reactivity-based controls]

Paul Makar described a Canadian project (funded at ~\$200,000 US) in which a graduate student was looking at partitioning of organic chemical between water and air. This work is being done in connection with Marion Diamond who is doing ambient air modeling and Paul Makar who is doing regional modeling.

Dan Baker said that another outcome of Task 2 is to determine if the

episodes we are using to model are typical of all episodes. He said we would determine this by looking at a larger number of episodes.

*Session IV. List of Additional Research Tasks
Discussion by Group
(See Appendix C.)*

Don Fox discussed follow up work. He proposed that RRWG have a team to review the three modeling reports and give comments. We need to have a date to finalize the reports for placing them on the internet. Bill Carter had a question about whether posting the larger reports on the NARSTO website would interfere with the authors publishing a summary article in scientific journal. Jeff West said that was not the past experience.

Don Fox said that comments on the three reports should be received within 5 weeks. Bill Carter said that after incorporating these comments the reports should be considered final reports. Don Fox suggested a team of four individuals to review the reports and to coordinate collecting comments from others. These individuals are:

Dan Baker
Deborah Luecken
Jon Kurland
Bob Stallings

After discussion, Dongmin Luo's name was added to the list of reviewers to represent CARB which had funded the GIT study. We should not post the GIT report on the NARSTO web page until CARB has reviewed this.

There was a discussion of what further work we might get contractors to do. These are project that were listed.

1. Re-analyze the GIT output file to derive new metrics similar to those developed by the Carter report.
2. Evaluate the metrics and pick possibly two metrics to focus future efforts on. Dr. Carter said some of the metrics could possibly

be eliminated for scientific reasons, but that for most of them the decision on which to keep would be a policy decision. He recommended a one or two day workshop to focus on this issue and make decisions.

3. Robert Wendell said that he is interested in identifying uncertainties related to low NO_x conditions. He said at 20 to 25 ppb low NO_x conditions many compounds have low or even negative incremental reactivities. Dr. Carter said that low NO_x conditions are one of the things that the new UCR smog chamber is slated to be used for.

4. Deborah Luecken wanted to fund a project on transport down wind to see what impact changes in reactivity in one location have on down wind areas. There was widespread agreement that this question should be put to rest by doing this type of modeling study. Deborah suggested Dr. Carter do this. Dave Morgott suggested that Dr. Russell also do this type of study using SAPRC.

At one point in the meeting, it was requested that the scientists in the room who expected that they might try to get contracts for future RRWG studies leave the room as the group was going to discuss funding and other specific aspects of projects. Some people did leave, notably Bill Carter and Ted Russell.

The question was asked, how is RRWG going to fund this new work? EPA representatives said that EPA currently has adequate budget to fund this work. The question is how to get the money contractually to the people whom RRWG thinks are most competent to do the work. EPA seemed to think that this might be worked out through existing contracts.

It was emphasized that we need to fund this new research as it would be an imposition to ask the current researchers to do more without further funding. The feeling was that RRWG had already gotten quite a bit from the current contractors for the amount of money already spent.

There was a discussion of the timing of future funding. If EPA takes 6 weeks to get the money out, it will be March 1 to start new work. If

the contractors do the work in 60 days, it will be late May or early June before results of the new work are available.

David Sanders suggested that we stay in frequent telephone contact with each other so as not to let momentum slide.

A tentative date of May 21 and 22 was suggested for the next RRWG meeting. There was some mention of possibly having the next meeting in Riverside, California so that everyone could tour the new UCR smog chamber. Initially at the formation of RRWG, there had been discussion that some RRWG meetings would be held on the West coast to accommodate members from the West. However, it appeared that the next meeting will be scheduled for Research Triangle Park, NC.

The meeting adjourned at 11:55 AM. There had been 37 people in attendance during all or part of the meeting.

Adjournment

The meeting adjourned at 11:10 AM.

Appendices

- A. Task 1579.1 Summary of Modeling Results –Fox
- B. January 9 03 RRWG Milestone Review
- C. List of Additional Research Projects Jan 09 03



**REACTIVITY
RESEARCH
WORKING
GROUP**

**Summary of the Reactivity Research Working Group Meeting for
November 3-4, 2004 Research Triangle Park, NC.**

Attendees: Praveen Amar, Sarav Arunachalam, Bob Avery, Dan Baker, Jim Berry, Bill Carter, James Carver, Edward Casserly, John Dege, Ron Eritano, Don Fontaine, Don Fox, Barbara Francis, Doug Fratz, Bruce Gustafson, Bob Hamilton, Madelyn Harding, Harvey Jeffries, Bill Johnson, Laura Haynes, Bob Hinrichs, Jonathan Kurland, Sylvie Lemoine, Dongmin Luo, Paul Makar, Michelle Mebust, Arlean M. Medeiros, Mehran Monabatti, Bruce Moore, David Morgott, H. Everett Myer, Bob Nelson, Vladimir Orkin, Bill Rawson, Doug Raymond, David Sanders, Rob Sliwinski, Stan Tong, John Weeks, R. Wendoll, Jeffrey West, Xinqiu Zhang,

Wednesday AM November 3rd

8:30 AM – 12:00 Noon

**Pre RRWG Meeting
Conversation on Fate and Availability Modeling**

Prior to the formal opening of the Reactivity Research Working Group meeting at 1:00 PM, there was a workshop on Environmental Fate from 8:30 AM until around noon. This workshop reported on research findings of interest to RRWG committee 3 which was investigating environmental fate. This workshop was attended by most of the same people who would attend the RRWG meeting proper later that day. Speakers included Dave Morgott, Dongmin Lou, Bill Carter, Diedra Murphy who discussed EPA's TRIM model, Paul Makar from Canada and Mehran Monabatti of Senes Consultants, who is doing contract modeling work for the RRWG committee 3.

Wednesday PM November 3rd

I. Welcome and Introductions, Review of Agenda

At 1:00 PM Chairman Don Fox called the RRWG meeting to order. As usual, people in attendance announced their name and affiliation. About 50 to 60 people attended all or part of the meeting.

II Review of Status of RRWG – Don Fox

Don gave a summary of the projects that RRWG currently has under way. This was useful since the RRWG had not met for over a year (since July 9 and 10, 2003). (See Attached Presentation)

III.. Reactivity-related Chamber Projects at UCR – Bill Carter

Bill Carter gave a summary of reactivity-related chamber projects at UC--Riverside. He described a series of studies conducted to test mechanisms using the UCR EPA chamber. Preliminary results of two coatings reactivity studies with selected water-based solvent VOCs and petroleum distillates were presented. Future directions for the use of this facility include continued O3 reactivity and mechanism evaluations studies, investigations of secondary organic aerosol formation for model development and evaluation. This facility has special features to control temperature, humidity and irradiation conditions and the ability to investigate photochemistry under low NOx conditions. (Presentation attached and also available at: <http://pah.cert.ucr.edu/~carter/RRWG/>)

IV. Reactivity Research at EPA – Deborah Luecken

Deborah Luecken of EPA described preliminary results of an EPA in-house modeling study using CMAQ with DDM.

V. Comments by Jeff Holmstead – EPA Assistant Administrator

Air and Radiation

Jeff Holmstead said that he does not think that it is likely that the ozone national ambient air quality standard will be changed any time soon. He said he does not see VOC control being a major effort within EPA in the future. He does not see national reactivity based controls, except perhaps application of the reactivity concept to architectural and industrial maintenance (AIM) rules. He does see local efforts using reactivity scales. He would like to see an advance notice of proposed rulemaking (ANPR) on VOC control policy come out by the end of the year which will take an advocacy position for reactivity based concepts.

Several attendees asked questions after Jeff's talk. Rob Sliwinski from New York State Department of Environmental Conservation asked how a reactivity based AIM rule would fit in with local measures. Praveen Amar asked how VOC policy will affect PM₁₀ control efforts.

In reply to questions about applying the reactivity concept to regulations, Jeff said that he doesn't think we will go back and revisit rules which are already in place. The reactivity concept might find some use in new regulations. He observed that the MIR scale is the only scale in regulatory use currently.

Ellis Cowling asked if we would ever have a secondary ozone standard. Jeff said he doesn't expect that there will be a more stringent standard for non health effects (i.e., ecosystem and property) than for the health standard.

VI. Additional Analysis of Reactivity Matrices - Georgia Institute of Technology Ted Russell

As the last talk of the day, Ted Russell of Georgia Institute of Technology described additional analysis of reactivity matrices including three additional reactivity metrics AVG, AVS and M2M (common with the UCR Bill Carter project), assessment of the sub-domains variability of the reactivity scales, and Russell's assessment of the attributes of the various reactivity metrics and the resulting scales.

The last element of his talk of high interest to the RRWG attendees was Dr. Russell's evaluation of metrics for expressing reactivity.

Below are the metrics which in his opinion are the best, along with some of the metric's properties:

1. Least Squares - relative reactivity (LS-RR) [i.e., relative reactivity of the species which gives a least square fit to the line.]
 - Based on multiple cells
 - Robust (consistent)
 - Inherently designed to minimize "risk" of being wrong
 - Nothing in its formulation suggesting bias toward any "group"
2. Regional MIR to MOIR (M2M)
 - Based on multiple cells
 - Robust (consistent)
 - Conditions where VOC controls are beneficial
3. MIR-3D
 - Robust
 - Designed to work well in a VOC-limited area
 - Most readily comparable to a box model calculation
 - Based on single location
 - Likely most protective of highly populated areas
4. MIR-Box
 - Reasonably consistent with robust 3D scales
 - Ease of calculation
 - Too much spread - increased likelihood of biased substitutions

The metrics which he thought were less desirable were:

1. MOIR-3D
 - One cell, extreme conditions, often more NOX-limited, driven by a few species
2. Regional Average Ozone over Standard (AVS)
 - Less consistent across sub-domain
 - More sensitive to base calculation (how much of domain above standard)

- Designed more for heavily populated areas that have high ozone
3. Regional Average Ozone (AVG) Less consistent across sub-domain
- Not designed to protect people

In addition to the global evaluation of these metrics, Ted Russell et al., presented their analysis of the performance of several of the metrics on sub-domains including rural vs. urban comparisons. They concluded that M2M, MIR-3D, and LS-RR were consistent and show relatively little variability.
(See Attached Presentation.)

Thursday November 4, 2004

Some of the talks which had been rescheduled from yesterday due to the unexpected Holmstead presentation were given on this day. A couple of talks were deleted. For example, Mehran Monabatti had been scheduled to speak on the environmental fate modeling report. He said that he had covered most of what he had to say at the Wednesday morning workshop and that most attendees had already heard that. Tom Helms said that he did not need to speak since Jeff Holmstead had already covered the issues he had planned to talk about.

VIIa. Task 1579 Photochemical Modeling Review – Praveen Amar

Praveen Amar, who is a scientific advisor for NESCAUM, discussed a review of task 1579 on photochemical modeling. He had done this work under contract to EPA, which had felt it is useful to have a review by someone who had not been involved in developing the 1579 task. Dr. Amar preferred the global metrics with high consistency (for example LS-RR or M2M). He suggested if possible, a combined scale(s) could be used; for example a combination of LS-RR with MIR-3D. He said in the future, EKMA based scales should only be used in the context of using it as a "screening model." (See Attached Presentation)

VIIb. Task 1579 Photochemical Modeling Review – (Luecken for) Richard Derwent

Deborah Luecken described a similar review of task 1579 by Richard Derwent under EPA contract. Dr. Derwent had been in the EPA Research Triangle Park facility a few weeks before the RRWG meeting and had gone over his report with EPA. Due to the distance from England, he was not able to come back to the RRWG meeting. Deborah attempted to present Dr. Derwent's views. Dr. Derwent seemed to prefer the EKMA-MIR metric since it incorporates the best chemical kinetic information that we know, and gives the largest effective range. A large effective range would be desirable for regulatory purposes he indicated. He thought some sort of merging of the EKMA-MIR scale and his own POCP scale would be effective.

VIII. SMOKE Progress Report Jeff Vukovich

Jeff Vukovich gave an update on SMOKE development. He is employed with the contractor who is working on SMOKE. Contract will be completed in next few months. (See Attached Update)

IX. Fate and Availability Pre-Conf Summary – Jon Kurland

Jon Kurland gave a report on Fate and Availability. The issue of a 0.1 mm Hg vapor pressure cutoff was discussed. Some thought a precedent for this had been set by historical use and that any change would be counter-productive. Bill Carter said he is uncomfortable with a vapor pressure cutoff as high as 0.1 mm Hg, e.g., ethylene glycol can get into the gas phase in his smog chamber.

Someone asked how important is to have a low vapor pressure cutoff. If it is important, how do we do it?

Jon Kurland announced that he was retiring from his company, Dow Chemical. He said he would not be able to come regularly to future RRWG meetings. The attendees at the meeting applauded him for the contributions he has already made since the RRWG's formation. Jon asked Dave Morgott to take over the lead of RRWG committee 3 which works on environmental fate.

X. ARB MIR Update -- Dongmin Luo

Dongmin Luo gave an update on ARB MIR work. He said California ARB planned to continue using the MIR scale until they are convinced some better

scale is available. They are currently looking at the use of reactivity for consumer products and architectural coatings. (See Attached Summary)

XI. EPA Reactivity Update – Tom Helms

Tom Helms summarized the meeting by saying that he was impressed by the amount of scientific information the RRWG had generated and that he believes the RRWG has made real progress.

XII. Possible Dates for Future Meeting

Don Fox set March 9 and 10, 2005 as the tentative date for the next RRWG meeting. It was felt that interest will be generated in a meeting at this time due to several anticipated EPA actions such as the ANPR and expected VOC exemptions.

Adjournment

The meeting adjourned at 12:15 PM.

Appendices

Fox RRWG UPDATE Nov 2004
Carter Chamber Update RCT1104
Russell RRWG 11-04-2
Praveen Amar Reactivity Metrics Final Nov 2
RRWG Smoke Update 4 Nov 04
Luo MIR Summary