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National Specialty Workshop on Technical Tools for Air Toxics Assessment

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Clean Air
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National Specialty Workshop on Technical Tools for Air Toxics Assessment

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Office of Air Quality Planning and Standards
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Executive Summary

The National Specialty Workshop on Technical Tools for Air Toxics Assessment was held on June 17-20, 1997 in Research Triangle Park, North Carolina. The purpose of the workshop was to provide a forum for Regional, State and local agency personnel to learn about air toxics technical tools that are available to them, and make comments and suggestions on these tools. Over 80 participants attended the workshop, representing 33 State and local agencies, five Regional EPA Offices, and a number of other staff from various EPA groups. Workshop sessions were focused in six main areas: Elements of the Office of Air Quality Planning and Standards (OAQPS) Air Toxics Program, Ambient Air Monitoring and Data Analysis, Emission Inventories, Dispersion Modeling, Exposure Assessment, and Education and Outreach. Participants volunteered for panel discussions held for each of the subject areas. Several weekly conference calls were held prior to the workshop and panel members worked to identify issues for discussion at the workshop. The lists of issues were compiled into an issues paper for each area.

At the workshop, half-day sessions were devoted to each of the six main areas. Each session consisted of presentations, followed by a panel discussion. The presentations were intended to provide information on the current status of many activities relating to air toxics. During panel discussions, panel members presented their issue paper to the workshop attendees for discussion. Issue papers were finalized at the end of the workshop.

In general, four major themes emerged from this workshop: the strategy of the Air Toxics Program, personnel training, guidance on proper use of the tools and technical and budgetary resources. A summary of each of these main areas is as follows:

1. An overall strategy for dealing with air toxics issues needs to be developed and technical tools should be designed to fit this strategy.

   - The overall air toxics strategy would include how the various activities within Section 112 relate to each other, such as MACTs, NESHAPs, Urban Air Toxics Program, etc. If these activities could share the same data (e.g., emissions inventory and monitoring data), rather than having to recreate these data for each application, duplication of efforts could be reduced and the technical tools could be used more effectively.

   - Air toxics programs should be designed to promote closer working relationships and technical tools should promote the sharing of air toxics data (i.e., monitoring and inventory data should be provided in a format that can be used in dispersion modeling, which, in turn, should be able to be input easily in exposure models). There is a need for a coordinated working relationship between exposure modelers, the risk assessors and the decision makers at the Region and State levels in order to address the specific questions that need to be answered.

2. Training should continue to be recognized as a critical element of the Air Toxics Program.

   - State and local agency personnel need to be advised of the availability of training materials and courses. It would be hepful to have a continually updated clearinghouse of training materials, accessible to agency personnel.

   - Alternative forms of training, such as Internet courses, are useful for situations where travel time or funding is limited.

   - Training materials need to be user friendly. Training is a separate function from writing guidance documents and policy memos. The training program need to identify audiences, develop learning objectives and measurement methods, and determine suitable delivery systems.

   - Training should be built into the Air Toxics rule development process in the early stages since training is essential to rule implementation.

   - Air toxics is recognized as a priority program and additional training, i.e., MACT-specific training, is planned in FY98.

3. Guidance on the availability, purpose, and use of air toxics technical tools is needed.

   - On a new or existing website, provide an EPA-approved list of exposure models, how and when to use them, EPA expert contacts, and suggested default inputs.

   - Specific guidance on assessing HAPs is needed, such as guidance on emission inventories for point, area, and mobile sources. The role of the Emission Inventory Improvement Program (EIIP) should be expanded to specifically address HAPs and guidance and tools from State and local agencies should be obtained.

   - A guidance document is needed to instruct agencies on how to effectively collect, analyze, and present data.

4. As Federal, State, and local governments continue to downsize and are asked to do more with less, innovative air toxics monitoring tools and procedures need to be developed.

   - Opportunities, such as this workshop, could be provided for agency personnel to meet each other and develop contacts for various technical issues.

   - A contacts list for technical area experts within air toxics would be helpful as a quick reference for technical questions and would promote interaction between the various technical disciplines. An initial list of area experts based on workshop participants was developed but a more comprehensive list is needed.

In addition to the general themes that were discussed at the workshop, specific issues within the panel subject areas were identified. The major issues for the panel areas include the following:

- **Monitoring and Data Analysis:** More monitoring data are needed to define the community health concerns caused by air toxic pollutants. In many instances, monitoring has been performed, but the data from the States performing the monitoring are not centrally located or available for use by others. In those cases, the data need to be compiled for future use. For many pollutants, monitoring has not been previously or adequately performed and additional monitoring is needed.

  Update sampling and analytical methods need to be completed for monitoring pollutants where methods have not been previously available. For example, the update of EPA's Compendia of Methods for monitoring organic and inorganic pollutants in air is needed. These compendia are necessary to promote uniformity in monitoring procedures from state to state. These revised documents should be widely distributed for ease in locating information.

  As monitoring methods become available for pollutants not previously monitored, analysis methods and tools must be developed to organize and analyze the data. Projects such as the Ambient Air Quality Characterization Project help to address needs for new analysis tools.

- **Emission Inventories:** There is an overall need for more guidance on how to provide a complete emissions inventory for mobile, area, and point sources. Upgraded tools/software are needed, as well as recommended procedures for applying the tools for area, mobile, and point sources. Inventories should be consolidated where possible to reduce duplicate data collection and reporting. Overall guidance is needed on:

  - Estimating toxic emissions and uncertainty levels from highway vehicles, nonroad equipment, aircraft, commercial marine engines, and locomotives.

  - How to do a point, area, on-road and nonroad mobile sources, and biogenic toxics emissions inventory.

  - An emissions inventory suitable for modeling HAPs is needed.

- **Dispersion Modeling:** For the purposes of assessing impacts of specific sources, the existing technical tools are generally adequate, however, more guidance is needed on how to use the tools. Tools are needed to address new issues that result from modeling air toxics. For example, better algorithms are needed to characterize wet deposition, particle/gas partitioning, gas scavenging coefficient and particle size distribution, etc. More technical guidance is needed on using the models to help promote consistency in applications. For the purposes of nationwide modeling assessments, existing tools need to be assessed or new ones developed.

- **Exposure Assessment:** EPA needs to develop better tools to address exposure assessment needs. Guidance is needed for all personnel on the steps involved in performing exposure assessments. Specific areas that the tools need to consider include:

    - Assessing the exposure through the inhalation pathway versus all routes of exposure;
    - Assessing exposure to humans versus including exposure to animals and plants; and,
    - Assessing exposure in urban settings.

At the completion of the workshop, participants were asked to evaluate the workshop. The evaluation showed that the workshop succeeded in bringing together many technical disciplines to voice opinions on issues relating to areas involving air toxics assessment. Sixteen percent reported that their primary job function is monitoring and data analysis, 32 percent dispersion modeling, 20 percent emission inventory and permitting, and 32 percent classified themselves as environmental engineers. The participants gained information on how their work affects others and on the available technical tools that they may not have known about prior to the workshop. Participants provided EPA with information regarding their current and future needs. They indicated that one of the benefit of the workshop was learning who the experts are in various technical areas to help promote interaction between technical disciplines. Participants wanted to learn basic information about all of the disciplines so that they could see how their work fits into the overall air toxics approach. Those speakers presenting new information (e.g., the dispersion model AERMOD) were more helpful because they gave an idea of the current activities and what is coming, relating to air toxics, in the near future. Participants indicated that they were eager to learn more about performing exposure assessments and how EPA plans to approach exposure assessment in the future. They felt that the workshop was helpful in informing personnel of the availability of technical tools. For example, prior to the workshop, panel members developed lists of tools that would be helpful in performing their work. During the workshop, they learned that tools were already available to do many of the things they suggested.

Participants stated that they felt that the workshop was helpful in opening lines of communication between States and EPA to help get agency personnel more involved and interested. They felt that the workshop was organized and productive, and was successful in meeting its goals. The participants liked the idea of workgroup discussion prior to the workshop. They suggested that the workshop become an ongoing activity in order to promote interaction between technical personnel.

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1.0 Introduction

The National Specialty Workshop on Technical Tools for Air Toxics Assessment was held on June 17-20, 1997 at EPA's Administration Auditorium, 79 Alexander Drive, Research Triangle Park, North Carolina. Over 80 participants attended this workshop. Participants included representatives from 33 State and local agencies, five EPA Regional Offices, and a number of other EPA staff from various groups. The purpose of the workshop was to provide participants with an opportunity to learn about a variety of technical tools that are needed for air toxics assessment and provide an opportunity for Regional, State and local agency personnel to voice their opinions and define their needs as they relate to these tools. This report describes the preparation for the workshop, provides a summary of the presentations, and outlines the recommendations received from the participants.

Plans for the workshop had been discussed for many months. On March 25, 1997 a letter of invitation was sent to Regional, State and local agency personnel defining the purpose of the workshop. This letter is included in the report as Appendix A. The workshop mission statement was defined as:

Regional and State contacts have expressed an interest in learning about the technical tools required to support many sections of the Clean Air Act regarding the air toxics program so that:

1. They can better support requirements under Title III such as the newly published Risk Management Plans under Section 112(r), residual risk and de-listing requests under MACT rules, the Urban Area Source Study, the Great Waters Studies, etc.

2. They know who the air toxics topic area experts (office level identification) are across EPA and the State and local agencies in order to obtain rapid assistance.

3. They can better communicate the magnitude of air toxics issues facing the technical analyst and the success in solving air toxic problems.

Based on this invitation, very positive response was received from over 75 persons. Based on this response, the workshop date was set to begin on June 17, 1997. The workshop was divided into seven sessions. The first day devoted half-day sessions to Elements of the OAQPS Air Toxics Program and Ambient Air Toxics Monitoring and Data Analysis. Half-day sessions on June 18, 1997 were devoted to Air Toxics Emission Inventories and Dispersion Modeling. On June 19, 1997 sessions were devoted to Exposure Assessment, Case Histories of Multi-Pathway Modeling, and Education and Outreach. On the final day of the workshop, June 20, 1997 two hands-on computer training sessions were provided on the use of dispersion models and emission estimation tools. The final workshop agenda is included in this document as Appendix B. A list of all workshop attendees is included as Appendix C.

The first part of each session included speakers who provided information regarding the current status of many activities relating to air toxics. Many speakers provided handouts of their presentation slides either prior to or during the workshop. Copies of these presentations are included in this report as Appendix D. The second part of each session was used for panel member discussions. Panel members had been in contact prior to and during the workshop to define issues in each subject area as they relate to air toxics assessment. The panel discussions were framed around three basic questions:

1. When are the present technical tools adequate in helping you do your job?
2. When are they deficient?
3. List possible solutions that may alleviate some of the items on the deficiency list.

A series of conference calls were held for each panel where panel members answered the questions and developed issue papers. The final issue papers were presented at the workshop during panel discussion. Workshop participants commented on the issues and added suggestions. Panels met at the end of the day following the workshop discussion and revised the issue papers according to the discussion. The final versions of the papers are included in Section 3.0 of this report.

Over the course of the workshop, each participant was asked to indicate his or her area of expertise in air toxics issues. The list was designed to meet the second workshop mission of helping provide a quick reference so that personnel working in air toxics can stay in contact with each other after the workshop. This list is included in this report as Appendix E. At the end of the workshop, participants completed a Workshop Evaluation Form that gave them an opportunity to voice their opinions on the workshop and make suggestions for improvement for future workshops. A brief summary of the responses can be found in Section 4.0 of this report. The evaluation form and a more complete listing of the responses is included in this report as Appendix F.

Overall, this workshop will provide an opportunity for Regional, State and local agency personnel to inform EPA of their needs over the next few years. Major issues will be summarized into a workshop report, and major recommendations will be presented to senior management. A copy of all presentations will also be included in this workshop summary. Mr. Touma closed by discussing workshop logistics with participants and introduced the first speaker, William F. Hunt.

William F. Hunt, Jr.,Director, Emissions, Monitoring and Analysis Division (EMAD)

Mr. Hunt, welcomed participants to the workshop and reiterated the importance of the role of technical tools in the air toxics program. The purpose of Mr. Hunt's presentation was to provide an overview of the air toxics infrastructure, discuss challenges ahead for the air toxics program, and give a few examples of how these tools have been used in the past. Mr. Hunt began by describing the current sense of direction of the Air Toxics Program and the current activities involving infrastructure development. A significant amount of technical tools are available to the Regional, State and local agency personnel for monitoring and data analysis, dispersion modeling, and emission inventories. Although these tools were designed for criteria pollutants, they may be applicable to air toxic pollutants also. Although there is no explicit mandate in the Clean Air Act (CAA) for infrastructure development, technical tools are needed to carry on several mandated programs including air toxics, which pose unique challenges. Since funding is limited, efforts to develop or improve existing tools must be prioritized and efforts must build upon the programs already in use.

Mr. Hunt provided information on some of the current activities within the EMAD in support of technical tool development. These are:

- Emission Inventories and Factors Programs - National, State and local air toxics inventories and emission factors are being developed to meet various Section 112 requirements. There are gaps in available air toxics data. Data from State and local agencies are needed to fill these gaps. Nationwide, approximately 39 percent of emissions are from mobile sources, 26 percent are from point sources, and 35 percent are from area sources.

- Dispersion Modeling - Some of the tools available for dispersion modeling are still applicable. There are, however, some new issues that need to addressed within this area. These issues include dense gases, particle and gas deposition, and atmospheric chemical transformations of toxic pollutants.

- Air Monitoring - There is a lack of technology related to monitoring all toxic pollutants. Current efforts have been unable to develop quality assurance (QA) procedures. There would be great expense in monitoring all pollutants in all parts of the country. A project is underway that is considering requiring States to submit air toxics data.

Mr. Hunt reviewed an example of how interpretation of monitoring data can make a difference in the results. The example is from the Urban Air Toxics Program (UATP) and shows how determining trends using monitoring data is difficult due to changes in monitoring site location. In 1995, sampling for 1,3-butadiene was performed at 16 sites across the nation. The Port Neches, Texas, site results conflicted with emission inventory results. The emission inventory reported a decrease in emission from 1990 to 1995, while the monitoring data showed an increase. A team of specialists is needed to understand the complex issues involved. These complex issues included the fact that different sampling sites were used for monitoring in 1990 and 1995 and the emissions inventory had undergone changes.

Mr. Hunt continued with a discussion of air toxics indicators and trends. The goals of air toxics indicators include synthesizing data collected from different programs and showing national trends and patterns. Two challenges in meeting these goals include limited data availability on air toxics and a lack of consensus on calculating relative risk. Some ongoing work in this area includes the Government Performance and Results Act, developing a strategy to measure progress towards reduced health risks resulting from programs (e.g., MACTs), and exploration of indicators. One example of how indicator information is used includes analysis of some sampling data from PAMS. In this example, between 1994 and 1995, 19 sites were sampled for various air toxics pollutants. Between these times, the Reformulated Gasoline regulation came into effect. For these sampling sites, all pollutants tested decreased except for ozone and formaldehyde. In a comparison of the PAMS data and monitoring data from a California location, the data showed similar trends. A comparison was performed in 1993 of chemicals in the New England states and the Midwest states. This comparison also showed that during episodes of increased ozone, the formaldehyde concentrations also increased. These examples show how the data can be used as indicators and for trending.

Within the area of education and outreach, EMAD is currently working to do the following:

- Expand opportunities for education and outreach;
- Develop additional training on technical tools for monitoring, emission inventories, modeling, and exposure assessment,
- Prepare training materials;
- Utilize multi-media training vehicles such as the Air Pollution Distance Learning Network telecourses, internet, CD-ROM, and classroom lectures;
- Provide workshops that bring together multi-disciplines to foster communication and information exchange; and,
- Establish a list of area experts to allow for quicker communications and solutions.

Dialogue is needed with the State and local agencies as to what type of Education and Outreach needs exist. Some training materials are available (through the internet as well as written materials), but guidance is needed on which other types of training are needed.

Mr. Hunt listed current activities within ORD relating to exposure assessment as:

- Continuing to develop guidance and tools to evaluate multi-pathway human exposures for multi-pollutants. Scientific capabilities must be expanded to measure multi-media environmental and human exposures and biological markers of exposures; and,

- Characterizing residential multi-media exposures. Quantifying contributions from indoor and outdoor sources including source-receptor relationships are needed, as well as understanding relationships between exposure, dose and effect.

Some of the accomplishments include:

- Expanding the National Air Toxics Emission Inventory database;
- User friendly air dispersion models capable of addressing new concerns;
- Several years of PAMS monitoring data and easier ways to collect data;
- Developing useful air quality indicators;
- Developing a strategy to measure effectiveness of Air Toxics Program;
- Continuing research on exposure assessment methodologies; and,
- Expanding education and outreach opportunities.

The principle challenge ahead for the Air Toxics Program is the declining budget and the increasing demand for infrastructure development. Effective partnerships with States, local agencies and other stakeholders is needed to overcome these problems Improved methods are also needed for technology transfer through the evolving medium of the internet making strides in improving these methods Mr. Hunt then introduced Bruce Jordan.

Bruce Jordan, Director, Emissions Standards Division (ESD)

Mr. Jordan gave a brief overview of currents efforts in ESD. These include:

- Characterizing the air toxics problem;
- Defining the goal of the air toxics program;
- Tieing all pieces of the Air Toxics Program to a common goal (e.g., MACTs - how do they fit in with other requirements); and,

- Measuring progress in reaching the common goal (i.e., what are the best indicators).

Mr. Jordan stated that data is needed to direct the Air Toxics Program. ESD is currently looking at how to use available funding to meet the four items listed above. One issue related to using the available funding includes how different technical tools relate to each other. For example, in order to prove a model is providing valid results, the results must be compared to actual monitoring data. If monitoring programs can be brought in to validate the models, the results could be used to prioritize activities and funding. He urged the workshop to try to find solutions that are cost effective. Following those remarks, Mr. Hunt provided closing remarks and again welcomed the participants to the workshop.

2.2 Elements of the OAQPS Air Toxics Program

2.2.1 Presentations

MACT - Overview of Statute, Al Wehe, US EPA

Mr. Wehe provided an overview of the Clean Air Act of 1990 air toxics provisions including the history of the 1990 air toxics provisions, the statutory provisions, the basic requirements, and the maximum achievable control technology (MACT) program for reducing emissions of air toxics. This overview was oriented toward reviewing Section 112 of the 1990 Clean Air Act (CAA) in order to provide attendees background for further discussion at the workshop.

In 1990 as Congress reviewed the history of the air toxics program addressed in the Clean Air Act under Section 112, it found that for two decades, efforts to lower these toxic emissions had been stymied by argument, conflict and litigation concerning risk-based analysis and decisions leading to few successful efforts to control exposures to these hazardous pollutants. Between 1970 and 1990 EPA set standards for only seven hazardous air pollutants.

In 1990 Congress replaced this risk-based approach with an approach predicated on the best demonstrated technologies of all sources in a category. It was not because risk considerations were not important that these changes were made (they are still integral elements of the 1990 amendments), but because a reliance on only risk had made rule promulgation nearly impossible. Congress included a risk-based component which calls for assessment of risk remaining after application of performance-based standards and remediation through a risk-based residual risk program.

These standards are known as Maximum Achievable Control Technology (MACT) standards, and Generally Available Control Technology (GACT) standards. In essence, EPA is required to establish control requirements to assure that all major sources of air toxics achieve the level of control already being achieved by the best performing sources in each category. Further, by establishing performance levels rather than mandating particular control methods, Congress ensured that results would prevail over red tape. Congress provided a 10-year schedule in which to promulgate these MACT standards, with certain standards being promulgated in the first two

years, 25 per centum in the first four years, an additional 25 per centum promulgated not later than the seventh year and the remaining 50 per centum not later than the tenth year.

The workshop slides used in Mr. Wehe's presentation provide an outline of the provisions of Section 112, a view of the MACT standards promulgated to date, and an outlook for the future of the MACT program. Further the slides summarize an important tool in MACT standard development, MACT partnerships, which emphasize stakeholder involvement, leveraging the resources, experience, skills, and knowledge of all stakeholders in the program. A description of the MACT Partnerships program is available in the Federal Register (60 FR 16088, dated March 29, 1995).

The just-released *Second Report to Congress on the Status of the Hazardous Air Pollutant Program under the Clean Air Act*, EPA-453/R-96-015, August 1997 provides an up-to-date summary of the Section 112 program. This report will be available through the National Technical Information Service (NTIS); the executive summary and a fact sheet will be available on the OAR policy and guidance website (http://www.epa.gov/ttn/oarpg/rules.html)

Summary of the OAQPS Air Toxics Strategy (OATS), Al Wehe, US EPA

Mr. Wehe continued the presentations with a summary of the OAQPS Air Toxics Strategy (OATS). This strategy is needed because:

- We need a comprehensive vision of how to integrate the various air toxic requirements of the CAA (i.e., fitting them with the criteria programs as best as possible); and,

- We need to improve regulatory and economic efficiency by matching solutions with particular air toxics problems.

The Air Toxics Strategy should.

- Use an air management model to organize the program and its activities;
- Reflect the fact that HAPs have many different kinds and degrees of effects, exposures, and sources; and,

- Build on proactive stakeholder participation.

The impact of the OATS has not yet been defined since OATS is still in draft stage. Specific program elements are being defined (i.e., defining goals of the strategy and how to measure progress).

The Air Toxics Program in OAQPS, Melissa McCullough, US EPA

Ms. McCullough began her presentation with an organizational chart of the OAQPS. This chart is included in Ms. McCullough's presentation handouts in Appendix D of this report.
The four groups within the OAQPS and the purposes of each group are as follows:

- The Emissions Standards Division (ESD), whose purpose is to establish air toxics standards;
- The Air Qualities Strategies and Standards Division (AQSSD), which assesses air toxics;
- The Emissions Monitoring and Analysis Division (EMAD), which measures ambient air, as well as estimates source emissions; and,
- The Information Transfer and Program Integration Division (ITPID), which manages and transfers air pollution and pollution control information and develops and delivers training courses and educational materials.

Ms. McCullough reviewed the purposes of each group and provided examples of the kinds of projects conducted within each group.

Question: Food and drug industries must get approval from the FDA before they release a product. Why not have similar air pollution regulations that require industry to obtain approval beforehand?

Answer: This issue is quite complex and controversial, and focuses on where the burden of proof falls. Whose responsibility is it to prove that a process is safe or unsafe? With the FDA, the burden of proof falls on the industry marketing a drug to have specific exposures for specific effects, and for which they bear responsibility. In air toxics, the issue is much more complex scientifically and already the subject of discussion, especially for environmental groups

2.2.2 Panel Discussion

The panel discussion began with introductions of panel members by Joann Held. Panel members are identified in the Workshop Agenda in Appendix B of this report and on the Attendees List in Appendix C. Panel members agreed prior to the workshop to each provide a short talk on different aspects of the issues defined in the panel issue paper. Tom Rogers was the first presenter. Summaries of the panel presentations follow.

Should Offsite Consequence Analysis of Accidental Releases Be Incorporated into a Permitting Program, Tom Rogers, Florida DEP

Mr. Rogers began his presentation by describing how an offsite consequence analysis (OCA) could be incorporated into a permitting program. There are a number of ways in which such an analysis

could be used. These range from using toxics' concentration levels as an absolute determining factor (i.e., greater than or less than a health-based criteria level) in deciding the permitability of a source (like is done for the criteria pollutants) to using it solely as public information with no effect on the issuance of the permit. Alternatively, the analysis could be considered as a weighted element, in some manner, of a decision to issue a permit. For example, the results of the analysis could be used to force control or work practice requirements or used to develop emergency management planning without being used as a reason to deny permit issuance.

To help determine how an offsite consequence analysis should be used, if at all, Mr. Rogers explained that the more fundamental question of "what are you trying to accomplish" should be addressed. Are you trying to provide complete protection of the general public from any kind of accident; are you trying to reduce risk through better facility design and work practices; are you trying to reduce risk through facility location and waste minimization; or do you simply want better contingency and emergency planning and public information?

Mr. Rogers also addressed the technical tools available for air toxics assessment. He stated that the tools should be consistent with chemical and physical laws and principles. Parameterizations of physical and chemical effects should be based on validated data sets and be peer reviewed, and the air dispersion algorithms should be consistent with those used in the Guideline on Air Quality Models. Data input to these models should be reasonably obtainable and output should correspond to the form of the endpoint criteria being evaluated. The tools need improvement in the areas of emissions characterization and quantification, chemical and physical transformations, multiple compounds analysis, time dependent changes, and less-than-lifetime exposures.

Mr. Rogers continued by listing what he expected to gain from this workshop as follows:

- The knowledge of a suite of models that cover the range of sources and scenarios that toxics modeling may be performed for;
- A better understanding of the tools (models) that are available and what they can and cannot do;
- The knowledge of whether some models are considered "better" than others, based on evaluation studies or physics, that essentially address the same sorts of sources; and
- Better knowledge of what is the best technique at this time for completing a risk assessment analysis.

Question: Should OCA be used in permitting?

Answer: Mr. Rogers stated that, from his perspective:

- Do not use an OCA as an independent means of deciding permit issuance or denial of a permit;

- Use the OCA to force risk reduction measures; and

- Enhance existing contingency or emergency planning processes to address the risk of accidental releases.

Examples of Situations Where Risk is Communicated to the Public, Denis Lohman, Region III

The next panelist, Denis Lohman, provided examples of situations where risk is communicated to the public. Examples included when models are used to determine where to put monitors for landfill monitoring and Superfund Sites.

Emission Inventory Tools for Air Toxics, Lee Page, Region IV

The next panelist, Lee Page, continued by defining the steps involved in the MACT development process. One step in this process is identifying sources emitting HAPs.

Tools that are available for identifying air toxics sources include the following:

- "Compiling air Toxic Emission Inventories," an EPA document that is available on the EPA's Technical Transfer Network (TTN). The TTN is avilable on the web at http://www.epa.gov/ttn;

- Chemical spcific EPA documents (e.g., locating and estimating documents), available on the TNN;

- "Source Identification Procedures for Source Subject to Regulation Under 112d of the Clean Air Act as Amended in 1990," an EPA document that is not yet available on the TTN. It is referred to as the "Source ID Cookbook." Copies should be available from Regional Offices, however, if they are not, contact Lee Page at (404) 562-9131 to request a copy.

Combining Modeling and Inventory Tools, Mike Pokorny, Maryland DEP

The next panelist, Mike Pokorny, provided a brief example of how modeling and inventory tools can be combined. Maryland has developed a tool, named the Air Quality Integrated Management System (AIMS), that integrates modeling, inventories, monitors, etc., to identify the top 30 pollutants with the highest cancer risk in an urban area from all sources (e.g., mobile, area, point, etc.). The AIMS is coded by source category and gives the component of risk for source

categories. The assessment is performed from the individual source risk components. The benefit of this system is that it combines all of the groups together. AIMS also converts to VOC assessment and attainment strategy.

Using Tools for Targeting Sources, Linda Lay, OECA

Linda Lay outlined the organization of the Office of Enforcement and Compliance Assurance (OECA). There are two major Divisions within OECA, the Office of Compliance and the Office of Regulatory Enforcement. The OECA activities on MACT standards include preparing guidance documents, Compliance Assistance Centers and tools, support of rule development, applicability determination support, ADI, enforcement tools, and ATIS support.

Ms. Lay provided a list of compliance assistance tools developed and under development through OECA's Office of Compliance. This list is provided in Ms. Lay's presentation handouts in Appendix D of this report. A brochure is also included which lists contacts for small business compliance assistance centers. These centers help small and medium-sized businesses understand and comply with federal environmental requirements. The Compliance Assistance Centers listed in the brochure are:

- Printing: http://www.pneac.org
- Automotive: 1-888-GRN-LINK, or http://www.ccar-greenlink.org
- Agriculture: http:///es.inel.gov/oeca/ag/aghmpg.html
- Metal Finishing: 1-800-AT-NMFRC, http://www.nmfrc.org
- Access to all Centers: http://es.inel.gov/oeca/mfcac.html

Ms Lay also provided a table that list names and phone numbers of OECA personnel and their various areas of expertise This listing is included in Appendix G of this report.

New Jersey's Risk Assessment Procedures, Joann Held, New Jersey DEP

Ms. Held gave a brief overview of the risk assessment procedures that are completed in New Jersey as a "quick and dirty" way of assessing safety. Alan Dresser provided a detailed summary of these procedures later in the workshop. Ms. Held explained that New Jersey's risk assessment procedure is really a first cut at deciding if the emissions are safe. They perform a pre-model assessment for 50 carcinogens. This smaller list makes the first cut assessment easier. The assessment results in an order of magnitude number to determine risk. New Jersey gave this procedure to industry and it helped to reduce permitting efforts since source emissions requested on the application were reduced.

2.2.3 Group Discussion

The group discussed the issues brought forth in the panel's issue paper. Items included in the paper were refined, and the final version of this paper is included in Section 3.0 of this report. One major discussion point was exposure assessments versus dispersion modeling. The distinction between these two areas includes who is affected in the analysis. Exposure assessment takes people into account in the analysis. Dispersion modeling transports pollutants across land but does not really deal with the people it affects. Also, dispersion models are fairly good at predicting peak concentrations, but not as good at predicting where those concentrations occur. This would be an important issue for applying dispersion model results to exposure assessment.

2.3 Ambient Air Toxics Monitoring and Data Analysis

2.3.1 Presentations

Update of EPA's Compendia of Methods for Monitoring Organic and Inorganic Pollutants in Air, Bill McClenny, US EPA

Dr. McClenny reviewed the EPA's organizational structure and the guidance documents that have been originated by different groups. The revision of the EPA Compendium of Methods for the Determination of Toxic Organic Compounds in the Ambient Air to add three new methods and to update several of the existing methods was then discussed in some detail. All three new methods involve the monitoring of volatile organic compounds in the ambient air: TO-15 addresses the monitoring of the 97 volatile organic compounds listed in the Title III of the Clean Air Act of 1990 by sample collection with canisters and analysis by GC/MS; TO-16 addresses the monitoring of trace gases by FTIR-based open path monitoring; and, TO-17 addresses the use of solid adsorbents and associated analytical equipment for monitoring of toxic VOCs. Both TO-15 and TO-17 present a set of performance criteria that establish the level of performance expected in terms of criteria such as method detection limits, replicate precision, audit accuracy, and data completeness The use of performance-based methods is consistent with the definition provided by the Environmental Monitoring Management Council's (EMMC) of "a monitoring approach that permits the use of appropriate analytical methods that meet preestablished demonstrated method performance standards based on Agency data quality needs." The EPA is moving towards performance-based methods because:

- Procedures for approving modifications to methods create high barriers to new, better, and/or less costly technologies for analysis;
- Specific methods may not give the sensitivity (i.e., 10^{-6} risk levels) needed to meet project Data Quality Objectives (DQOs); and,
- Laboratories are forced into more expensive technology than might otherwise be used.

Dr. McClenny reviewed the EPA Compendium methods that have been or are being revised and indicated that completion of the Compendium in a consolidated volume is in doubt because of retirements and reorganization at the Center for Environmental Research Information (CERI), which was the primary sponsoring agency. Project summaries for the compendia are available in the presentation handouts in Appendix D of this report.

State and Local Participatory Programs, Dave-Paul Dayton, ERG

Mr. Dayton presented information regarding the State and local Participatory Programs on the National Volatile Organic Monitoring Contract. The program supports monitoring programs concerning three distinct components: urban air toxics measurements, speciated non-methane organic compounds (NMOC) (and nonspeciated NMOC), and photochemical assessment monitoring for volatile organics. Each program component provides the following:

- Sampling and analysis support;
- Sampling equipment (UATMP/SNMOC/Carbonyls);
- Site installation and training;
- Site support;
- Central laboratory analysis;
- Quarterly and annual reports; and,
- AIRS-AQMS data entry.

Mr. Dayton reviewed the methods included in the central laboratory analysis and the compounds evaluated. Contacts for this program are:

- Neil Berg, EPA Delivery Order Manager
- Kathy Weant, EPA Project Officer
- Dave-Paul Dayton, ERG Program Manager
- Tim Hanley, ERG Site Coordinator

Details of costing for the programs are provided in Mr. Dayton's presentation handouts in Appendix D of this report.

State and Local Participatory Program: Particulate Monitoring Participatory Program - Saturation Monitoring Repository, Stan Sleva, TRC

Mr. Sleva continued the session by providing a brief overview of the State and local Participatory Program for the Saturation Monitoring Repository. Mr. Sleva's presentation handouts (found in Appendix D of this report) provide a more detailed explanation of the program.

The EPA is encouraging State and local air pollution control agencies to conduct short-term, multi-site ambient air pollutant monitoring studies using saturation monitoring. Saturation monitors are noninterference or nonequivalent sampling methods for measuring particulate matter, carbon monoxide, and NO_x. The samplers are small, portable, and relatively easy to set up and operate. It is helpful to "saturate" a geographical area with the samplers to assess the air quality in areas where high concentrations of pollutants are possible. These monitors help air pollution control agencies in evaluating their ambient air monitoring networks for consistency with the 40 CFR Part 58 air quality surveillance regulations. The Saturation Monitor Repository (SMR) includes a pool of saturation samplers and related equipment which agencies use when it becomes necessary for them to upgrade or borrow saturation sampling equipment.

Mr. Sleva reviewed some past and ongoing studies and project costs. Cost tables are included in Mr. Sleva's presentation handouts. To inquire about a request for services, contact:

Neil Berg (SMR) Project Manager
U. S. Environmental Protection Agency (MD-14)
Research Triangle Park, North Carolina 27711
(919)541-5520

Hurricane Fran Video from the FEMA Burn Site, Neil Berg, US EPA

Mr. Neil Berg provided a videotape describing the sampling procedures and equipment used during the Hurricane Fran debris burn. A map is provided in the presentation handouts to show placement of the sampling equipment. The burn site was used to dispose of wood and debris from Hurricane Fran. Burning and chipping operations were being performed at the site. Testing was being performed for PM_{10}. Additional copies of this video can be obtained from Bill Stancil at (919) 541-2862.

Chemical Mass Balance for Toxic Species (VOC and Particulates), CMB8 Software, Charles Lewis, US EPA

Charles Lewis presented and reviewed the modeling software CMB8. Chemical Mass Balance (CMB) uses source profiles to separate the measured ambient mass concentrations of particulate or VOC into their quantitative source contributions. The U.S. EPA's CMB8 is an updated version of the CMB software for this purpose that has been supported and distributed by the EPA for several years.

The U.S. EPA has tacitly approved CMB as a regulatory planning tool through the Agency's approval of numerous State Implementation Plans which have had a CMB component. Revisions to CMB8 should significantly increase the convenience, efficiency and accuracy of performing receptor modeling by the CMB method. The CMB8 Features:

Windows Environment - 16-bit and 32-bit versions are available for Windows 3.x and Windows 95, respectively.

Species and Source Selection Defaults - the user can specify any one of up to ten sets of fitting species that can be chosen at random by mouse-clicking on a software button.

Input file options - the direct input of ambient and source data files may be done in a variety of formats: blank-delimited ASCII (*.txt), blank-delimited ASCII with columns and rows interchanged (*.car), comma-separated value (*.CSV), xBase (*.dbf), and Lotus123 spreadsheets (*.wks and *.wk1).

Output file options - the output result files can be renamed (both prefix and suffix) and placed in different directories during a session, allowing for a better grouping and identification of results generated during a lengthy session.

Collinearity Treatment - users can select collinearity parameter values directly in CMB8 to use in detecting and handling collinearity problems.

Britt-Leuke Algorithm - the Britt-Leuke algorithm without approximations is used in CMB8 to take account of uncertainty in all variables (e.g., the source compositions as well as ambient concentrations)

CMB8 can be obtained via anonymous ftp for the 16-bit Windows 3.x version at eaf.sage.dri.edu:/cmb80/model/16bit/win3mmdd exe, or for the 32-bit Windows 95 version at eaf.sage.dri edu:/cmb80/model/32bit/wn32mmdd exe, where mmdd is the month (mm) and day (dd) of the version label. The file win3mmdd.exe is a PKZIP self-extracting file that includes the program executable, sample input files, and a tutorial/user's manual.

New Data Analysis Tools for Ambient Air Quality Data, James Hemby, US EPA

Mr. James Hemby reviewed and demonstrated two data analysis tools for ambient air quality data, PAMSDAS and VOCDAT. Examples and screen captures are available in Mr. Hemby's presentation handouts in Appendix D of this report.

VOCDAT is a data analysis tool that performs the following:

- Provides a general platform to display VOC data and to perform QC tasks;
- Import/export AIRS format files;
- Prepares summary of species groups; and,
- Offers options to apply reactivity factors or create weight percent NMHC.

VOCDAT can be obtained via anonymous ftp at ftp.crl.com/users/so/csonomati/outgoing/vocdat. The software files are vocd116a.zip, vocd116b.zip, and vocd117.zip. Demonstration data files are under testdata.zip. A password is required to unzip these program files. Requests for a software password and technical questions should be directed to Sonoma Technology, Inc. at (707) 527-9372.

The data analysis tool PAMSDAS facilitates exploratory PAMS analysis. The capabilities of PAMSDAS include creation of boxplots of VOC species and criteria pollutants, examination of diurnal profiles, development of tables of summary statistics and correlation analyses. The software is currently undergoing significant revision and upgrades. Once PAMSDAS is complete (projected in October 1997), it will be posted on the web and distributed to Regions and States. For additional information on PAMSDAT, contact Mark Schmidt, EPA, at (919) 541-2416 or schmidt.mark@epamail.epa.gov.

Mr. Hemby reviewed the goals and products of the Ambient Air Quality Characterization Project. The goals of this project are to identify, catalogue, and collect ambient air quality data on toxics which are not stored in AIRS and to eventually use these data to assess the air toxics issue. The two major aspects involved in meeting this goal include collecting and analyzing ambient data, and developing and applying indicators. The products of this project include an annual data catalogue and an annual trend/indicator assessment. All State and local agencies which have previously collected ambient air quality toxics data or are currently involved in such measurements are invited to participate in this project. For additional information or to participate in the project,contact James Hemby, EPA at (919) 541-5459 or hemby.james@epamail.epa.gov.

2.3.2 Panel Discussion

Thomas Shoens, Panel Chair, and Peter Kahn reviewed the panel's issue paper with the workshop group. The paper was revised according to group discussion and the final version of the paper is included in this report in Section 3.0. Recommendations made by the panel include:

- Tools - use FTIR monitoring to look at "Hotspots," saturation monitoring, mobile tools for continuous type monitoring, satellite imagery, "Cookbook" approach for VOC data, list of acceptable ambient air level concentrations,

- FTIR may be more beneficial than other methods for doing sampling. Benefits in using FTIR versus canisters or saturation sampling are that they are transportable and provide real-time data.

2.4 Air Toxics Emission Inventories

2.4.1 Presentations

Introduction - National Air Toxics Emissions Inventory, Anne Pope, US EPA

Ms. Pope gave an introduction of the requirements for air toxics inventories to support Section 112, the current status of air toxic inventories, and the needed improvements to air toxic inventories for various Section 112 programs.

Ms. Pope informed the participants that there is no authority in the CAA that requires State agencies to require collection of air toxics emission inventories.

She discussed some consistency problems with the emission inventories. She indicated that a fundamental problem with the inventories is the definition of toxics. The definition of air toxics varies from agency to agency, as well as the type of pollutants submitted. She also explained that all State agencies do not submit the same data. Some States only submit data for MACT or Major Sources, while other States submit data for MACT and Major Sources along with mobile and area sources.

Ms. Pope then presented information on the following: National Toxic Inventory (NTI), Compilation of NTI, Limitations of NTI, Planned Improvements and Data Outputs from NTI. The information is summarized on Ms. Pope's presentation handouts in Appendix D of this report.

Ms. Pope also discussed the list of 40 potential HAPs developed by a team called the Risk Identification Process (RIP). She then gave example data outputs for the 188 HAPs from the 1993 NTI, Version 2.1 All sources combined totaled 4 4 million tons per year (pulled from 1993 NTI, Version 2.1 August 1997) for the 188 HAPs.

Currently, the inventory data allows you to perform analysis for all HAPs in the NTI and look at source categories. For FY 1998, the EPA plans to add facility-specific data such as latitude/longitude and stack heights.

Ms. Pope also indicated that there was a survey mailed out to State and local toxic coordinators from STAPPA/ALAPCO that was due by June 4, 1997. At the time of the workshop, EPA had not received surveys from 50 percent of the States. Ms. Pope stressed that the information from the States is very important for data analysis. The survey was aimed at Residual Risk and Emission Reduction, and without data from the States, the EPA will not have accurate data for analysis.

Emission Inventory Improvement Program (EIIP), Steve Bromberg, US EPA

Mr. Bromberg discussed the emission inventory (EI) procedures and tools. He indicated that the inventories have came along way since 1990 when there was no unanimity. He stated that looking through the issue papers brought back memories of where they were after the first inventory. Since that time, several factors have helped to improve the emission inventory. One of these factors was the development of the Emission Inventory Improvement Plan (EIIP). EIIP is a cooperative effort between State/local agencies, industry and EPA to improve estimates of emissions from various sources. The program was introduced in 1990. In 1993, it was approved and funded by State/local agencies with 105 grant funds. Another factor affecting the emission inventory is the agreement of common terminology (i.e., facility, point or area source). After the first inventory, it was realized exactly what it takes to perform a criteria pollutant inventory.

Mr. Bromberg continued with his presentation of the EIIP process. The EIIP process results in:

- Higher quality inventory data (consistency);
- Empowerment of State/local agencies;
- Cost savings for State/local agencies and industry; and,
- Improved communications and understanding among all inventory groups.

EIIP avoids policy making and research. EIIP teams are concerned with improving data quality because:

- Emission inventories are the foundation of many decisions;
- If mistakes are made early in the process, it will interject errors in downstream calculations;
- Redoing work to address problems is costly and embarrassing; and,
- Unrealistic regulations may result from these errors (also, cannot achieve an emission reduction if emissions are underestimated)

The EIIP membership is a nationwide effort between large and small agencies for standardization and data transfer. The EIIP products include a seven volume series which contains: Planning, Point Sources, Area Sources, Mobile Sources, Biogenic Sources, Quality Assurance and Data Handling and Reporting. Documents can be obtained from the EIIP web page at http://www.epa.gov/oar/oaqps/eiip/.

A preferred method should result in the best estimate and can be accomplished by a typical agency (usually most costly and timely with less uncertainty). An alternative method may be less demanding to accomplish, but may provide a less dependable data set The preferred method is the correct choice when it meets the data users needs. The choice of preferred or alternative method is not a unilateral decision, those who know what the data are going to be used for should be consulted. Mr. Bromberg stated that OAQPS will use EIIP guidance to compile inventories.

Question: Will the States be able to use EIIP in place of AP-42 or along with it?

Answer: EIIP is a cookbook of how to estimate emissions. Usually, there are no emission factors in the EIIP. To estimate emissions, both the EIIP guidance and the AP-42 should be used. First, you should consult the EIIP documents for an answer on the procedures for estimating an emission, and the AP-42 document should be used to select the emission factor.

EIIP has a data transfer prototype pilot test designed to move data from the prototype pilot to an EPA system. The goal is to have agencies transfer data between themselves and EPA.

The prototype takes State/local agencies data systems through the following steps:

State/local Data System⇨Application Interface ⇨EDI Translator (creates a standard data set)⇨X12 Data Set (agency is done)⇨EPA picks up⇨EDI Translator⇨Creates Electronic File⇨EPA Application Interface⇨EPA Data System.

If the prototype works well for EPA and State/local agencies, it will be expanded to industry to transfer data and allow States an easy uniform way of sending data.

Question: Will EPA create an interface with AFS so that States will not have to re-invent an in-house interface like most States previously had to do?

Answer: Yes, but AFS contains only point source data, which is about one third of the HAP data. The EPA is currently looking at the inventory system as a whole from a Federal standpoint. AFS is available, and is not going away anytime in the immediate future.

Mr. Bromberg made the point that, a few years back, the EPA tried to consolidate emission inventory reporting and data requirements. Reporting requirements are scattered throughout the CAA. There were several issues that the EPA could not overcome a few years ago. Since then, the EPA has worked through some of these issues and prepared a consolidated emission inventory draft reporting rule.

Several State/local agencies are collecting toxics data, but State/local agency legislatures have commented that EPA has no authority to require this data collection. Because of their legislatures, several State/local agencies are having difficulty continuing to collect toxics data.

Mr. Bromberg passed out TABLE 1· Proposed Emission Inventory Rulemaking Provisions. This table is included in Appendix D of this report. He stated that the rule will require that every three years State/local agencies generate a toxic inventory report. The rule split the information requirements into thirds. Every year, State/local agencies have to report Major or Significant

sources. Every third year, State/local agencies have to add the remaining sources to the toxic inventory report.

Question: Thresholds for actual or potential emissions?

Answer: Data to be reported under the proposed rule are actual emissions. Reporting thresholds are for actual emissions.

Question: A lot of companies reporting toxic data feel the information is confidential. How do we handle confidential information?

Answer: We do not want any confidential information. This means for toxic inventory reporting you may only get facility level data, sources may request that process level information not be released. Modelers need process level information to do their job, but from an inventory standpoint, the facility level is enough.

Question: What about data uncertainty?

Answer: One of the comments in the issue paper alluded that it was not important Mr. Bromberg feels it is an important issue that has not been addressed. Knowledge of the amount of data uncertainty and having some indication of the quality of data that you obtain is very important. Unfortunately, we have not been given any money to determine quality of data. As more people become aware of the data limitations, we will begin receiving better data.

Question: With the schedule for inventory every three years, are there any plans for a link between meteorological and monitoring data with emissions data?

Answer: Mr Bromberg stated that he was not aware of any plans for this type of link.

Emission Estimation: Techniques and Tools. Guidance and Assistance from the Emission Factor and Inventory Group, Anne Pope, US EPA and Mary Ann Barckhoff, Lockheed Martin.

Ms. Pope began by indicating that, from looking through the issue papers, there was obviously a lack of knowledge of the current tools available through the EPA. All EPA documents, including EIIP documents, guidance documents or Toxic Chemical Release Inventory System (TRIS) data, are available through the Info CHIEF Help Desk. CHIEF stands for the Clearing House of Information for Emission Factors. This number is available for obtaining documents, as well as technical support. The hotline also has resources available for training by the support staff. If training is needed, the help desk staff will go out to State and local agencies and provide onsite training.

There are several tools available for emission estimates. These tools include:

- Continuous Emissions Monitoring (CEM);
- Source Tests;
- Material Balances (for solvent applications); and,
- Emission Factors (AP-42).

Ms. Pope noted that speciation (using the database SPECIATE) is not a recommended EPA method for compiling air toxics or HAP emission inventories. The SPECIATE database was never intended to be used for emission estimation The database should not be used for emission estimation because it was developed as a modeling tool for a very broad class of VOCs (it does not contain a complete list). The second reason is the database only contains approximately 700 profiles, so all of the needed data is not available for emission estimation. Profiles are assigned to other SCCs. For example, an original profile for a smelter may be assigned to all types of smelters. There was no distinction between a smelter used for processing chromium, brass or bronze ore. All smelters were assigned only one profile, which means the correct emissions estimates cannot be obtained when using the SPECIATE database.

Ms. Pope introduced Ms. Mary Ann Barckhoff, who gave a brief overview of EPA's various tools. Ms. Barckhoff described the various EPA Emission Estimation Tools that are currently available as follows:

- FaxCHIEF (AP-42 is loaded on the fax machine)
  Fax: (919) 541-5626 or 0548

- EFIG Web Site (gateway to other sources)
  http://www.epa.gov/oar/oaqps/efig/

- EFIG List Server (receive CHIEF Newsletter via email) subscribe via email to:
  List server@unixmail.rtpnc.epa.gov, type "Subscribe CHIEF Firstname Lastname"

- AirCHIEF CD-ROM (contains EPA reports and databases)
  Call InfoCHIEF for more information (919) 541-5285

- National Emission Trends Viewer CD-ROM (includes EI data from 1985-1995)

- TANKS Version 3.0 (based on the petroleum industry - calculational software to estimate emissions from organic liquid storage tanks)

- FIRE Version 5.1b (Factor Information Retrieval System - EF from AP-42, old AIRS, locating and estimating documents, updated through AP-42 Supplement A&B)

- Info CHIEF Help Desk ***Telephone (919) 541-5285, e-mail address infochief@epamail.epa.gov***

Ms. Pope explained that the AP-42 document is composed of two volumes. Volume I, fifth edition, was completed in 1995. Volume I has been updated since that time with supplements A & B. The update is available online. Volume II, fifth edition, will be available online in August. The AP-42 Background Documents are also available online, through the CHIEF web page. The AP-42 Background document explains the methodology behind the development of the emission factors. Currently, the EPA is creating a link between AP-42 and EIIP guidance, which will make it much easier to search for information. The link will be available in the Fall of 1997 along with the new version of the AirCHIEF CD-ROM.

The predominant new feature of the AirCHIEF CD-ROM (Version 5.0) will be the Adobe Acrobat Format. One of the advantages of the Adobe format is that reader software used to view programs are available through www.adobe.com. The readers are free, but there is a charge for the development software. Also, the new version contains a search engine that will allow you to search the text of the document. The search engine will also allow you to search between chapters in the AP-42 document that the flat format and other databases do not allow.

Due to the overwhelming demand for the CHIEF web page, the dial in version of CHIEF TTN will no longer be available after September 1, 1997. If you have any concerns regarding this, please contact Mr. Ron Myers at (919) 541-5407.

The EPA is currently working on developing a new version of FIRE. It will be a Windows™-based system. The menu items will contain a description of the old codes used. The EPA is looking for user input, so if you have any suggestions, please call the help desk. The help desk will be able to provide the name and number of the person you need to send comments to.

Question: What is the hierarchy of emission factor tools? If I understand correctly, the EIIP guidance was to be used before the AP-42.

Answer: The two are supplemental to each other. There are no point source emission factors in the EIIP guidance, therefore you should use AP-42 for point sources. For area sources, AP-42 contains inadequate emission factors, so you would need to refer to the EIIP guidance. EIIP guidance should be used over the AP-42 for area sources. If the emission factors were adequate, they would not be in the EIIP. AP-42 should be used over the FIRE database, depending on when your version was updated. If you have the latest version of the AP-42, then use that.

For the approaching 1996 emission inventory, the most frequently asked questions were what is the hierarchy and where do I go to find emission factors? Which one do I use? We are going to establish a sequence to walk you through this.

Question: Will there be a link between FIRE and AP-42?

Answer: No. Due to all the different sources and records, it is to difficult to create a link between the two. Hopefully, the EPA will be able to develop a link in the future.

Question: How will we know which source is more recent, in order to determine which one precedes the other?

Answer: Usually, there is a revision date on the web page.

Question: Is it standard practice that you put updates in the Alert section of the web page?

Answer: No. The web page currently does not have an alert section, just a revision date for the document.

Question: Where can the hierarchy sequence for the emission factors be located?

Answer: It is not available yet, but it will be by the end of the year with the 1996 emission inventory. If you would like to keep checking to see when the sequence becomes available, the e-mail address is ***www.epa.gov/oar/oaqps/efig/ei.***

Question: What about draft documents on the web page? Could we use the draft AP-42 for emission factor information?

Answer: The EPA does not recommend using drafts for emission factor information. The drafts are online for comment purposes only, they have not been finalized. If you use the draft documents, do so at your own risk.

Ms. Barckhoff ended with a slide for the Info CHIEF Help Desk. Questions or comments should be directed to (919) 541-5285 or email at ***infochief@epamail.epa.gov***.

2 4.2 Panel Discussion

Mike Fishburn, Panel Chair, presented slides with each of the issue paper topics and explained the panel groups reason for including each comment Mr. Fishburn's presentation handouts are included in this report in Appendix D.

Mr. Fishburn added that there were a lot of comments regarding AIRS. Several panel members felt that it was very important to input data into AIRS for the people who need it. The AIRS area/mobile source module will be replaced with the NET database and arrangements will be made to take care of the acceptance of the AIRS data into the NET database for facilities that have spent a lot of time creating an interface with AIRS.

Comment: There is a need for emission inventory consistency and methodology on a national level, as well as for State and local agencies.

Question: Are you looking for a specific guidance document on how to compile an inventory or a tool?

Answer: Yes and No. EIIP is currently adding toxic emission factors, so there is no need for emission factor guidance, but there is a need for how to and where to go for activity data. Most point sources do not have a specific person responsible for emission inventories, therefore the need exists for guidance and/or a simplified document for someone that does not deal with toxic inventories on a daily basis. There is a need for a reading list on outside source information for State and local agencies, as well as industry.

Comment: There is a need for continuous work on emission factors because they are inadequate when the factors for a particular process or item is not available.

Response: A lot of work on emission factors is inadequate. For example, the Novas study focused primarily on recreational marine vehicles. Outboard usage seems to be declining, while jet ski usage appears to be increasing. Emissions may be offsetting each other or jet ski emissions may be overtaking marine vehicles. There are no emission factors available at this time for jet skis, so there is no way of estimating.

Comment: Hopefully, there will be some guidance and prioritization of pollutants for emission inventories. Some agencies felt it would be nice to have guidance from EPA on which categories to go after and how much time should be spent on emission inventories. If the guidance is only a short list of chemicals and the categories we need to be concerned with, the prioritization is very important. Some agencies are getting everything, including very small numbers, which is very time consuming

Response: Until the EPA gets more data, we can not put the problem in perspective. There needs to be a national effort from both EPA and State and local agencies for standardization.

The final version of the issue paper is included in this report in Section 3.0.

2.5 Dispersion Modeling

2.5.1 Presentations

Air Toxics Modeling, Joe Tikvart, US EPA

Mr. Tikvart began his presentation with an overview of dispersion modeling and air toxics. In the past, the emphasis has been on criteria pollutants. There has been somewhat of an "identity crisis" for air toxics. As this issue is being defined, there is a greater focus in modeling towards air toxics. This promotes a hopeful future as there is emphasis in CAA Title III on risk and the "lessons learned" from criteria pollutants can be used.

Mr. Tikvart listed ideas for discussion for the modeling session of the workshop. These ideas are as follows:

- Areas that need to be addressed in the models for air toxics assessment include similarities to criteria pollutants, dense gas problems (a family of models is needed to address dense gases), chemistry (transformation of pollutants; Gaussian models do not deal well with this), deposition (multi-pathways) problem, and general evaluations (need to know how good a model is).

- Input data - emissions/air quality/meteorological. Obtaining quality data is always a problem.

- Screening Models (Techniques)

- Models - EPA vs. Others - There is no specific program to dictate which model to use.

- Averaging Times

- Sources of Meteorological Data

- Chemical Transformation

- Variable Emission Rates (spikes in emissions)

Mr. Tikvart continued by discussing the current directions of Air Quality Modeling Group (AQMG) Program. The directions listed include:

- National assessment to demonstrate risk reduction to include urban applications and evaluation, and comparisons with national/regional assessments;

- Assessments for individual source categories;

- Outreach (to include workshops, a model clearinghouse, and the SCRAM website); and,

- Assistance to States on Risk Assessments.

Dispersion Modeling of Pollutant Impacts, John Irwin, US EPA

Mr. Irwin began his presentation by listing the goal of his presentation as to provide a basic understanding of the kinds of air dispersion models available and the purposes for which these dispersion models are best used. Many of the EPA dispersion models are available on the SCRAM BBS on the TTN or via internet at http://www.epa.gov/scram001/. Reviews of Eulerian and Lagrangian air dispersion models can be found in Mr. Irwin's summary paper in the presentation handouts in Appendix D.

Mr. Irwin continued by listing considerations for model selection. Questions to be considered in selection include:

- Are we following the dispersing material, or do we watch it go by? (Lagrangian vs. Eulerian, and puff/plume vs. grid);

- Do we allow more than one source? (single vs. multiple sources); and,

- Do we allow more than one source type? (point, area, line, volume).

Basically, the modeling tools are very simple. The usefulness of modeling results depends on how clever you are in the use of these tools. Mr. Irwin provided examples of puff vs. plume models and then reviewed some data to show comparisons of modeling results with observations. Observed data and modeled data do not match exactly In the "real world" (observed) data, there are irregularities that are not simulated by the models.

Assumptions and limitations in Gaussian plume modeling include:

- Plumes go in straight lines;

- Bell-shaped concentration curves exist in the vertical and horizontal planes;

- Wind speed dilutes plumes; and,

- There is enough wind blowing to move the plume downwind (hence, plume models are inappropriate for calm wind conditions).

A factor of 2 between observed vs. estimated concentrations for Gaussian models is considered reasonable, given all the stochastic effects not simulated by standard dispersion models The general trend in modeling seems to slightly overestimate 1-hour concentration maximum concentration values and to slightly underestimate annual concentration values.

Mr. Irwin listed some side topics related to dispersion modeling and provided discussion on each topic. The topics listed are as follows:

Why do things go wrong on estimated vs. actual concentrations?

- Coherent structures (eddies from surface to mixing levels in wind or turbulence field) cause differences in concentrations. As the eddy rolls downwind, it captures the plume, and disperses it.

- Wind directions change.

- It is possible for a plume to split - which may lead to very low concentrations in the center of the plume.

Models simulate the ensemble of many representations of like conditions.

- Uncertainty can only be reduced so far. There is no way of knowing exactly what the wind is going to do.

- Transport directions vs. narrow plumes.

Model evaluations define caveats.

- Comparison data is sparse.

- To validate a model is to confirm that the physics as modeled is indeed happening This is impossible in the atmosphere. Hence, all we can do is evaluate a model. To evaluate a model is to compare modeling results with observations (with no proof that the physics modeled is indeed happening).

- Models produce estimates of what is expected on average. We compare these estimates of average dispersion with observations which contain all the stochastic effects not modeled. We should expect and do find large differences in such comparisons.

Air quality modeling is a skill

- Modeling is the artful use of science. The models themselves are simplistic; it is wise application that is problematic.

Meteorological Data and Electronic Data Transfer, Dennis Atkinson, US EPA

Mr. Atkinson began his presentation with a brief discussion of meteorological data and data processing. Meteorological data is needed for refined modeling. The two types of data needed are surface data and mixing height data. A preprocessor is needed - either PCRAMMET for NWS data or MPRM for on-site data. Mr. Atkinson reviewed formats for a preprocessor.

Current Meteorological Projects Include:

- Revisions to the mixing height algorithm which includes creating two front-end programs to accept surface and upper air CD-ROM data;

- SAMSON CD-Update to include the period 1990 to 1995 that will include Automated Surface Observing System (ASOS) data starting in 1992; and,

- ASOS vs. NWS observer data analysis that will analyze the effects of limited cloud information on dispersion modeling and will compare concentration estimates using NWS observer and ASOS data in ISCST3.

Mr. Atkinson noted that the SCRAM has the latest modeling information available - including models (user's guides), programs (user's guides), guidance documentation, meteorological data, and State/local modeling contacts. This information can be found electronically at www.epa.gov/scram001 or www.epa.gov/ttn.

AERMOD: Source-Specific, Near-Field Dispersion Model, Russ Lee, US EPA

The purpose of Mr. Lee's presentation was to describe the dispersion model AERMOD.

AERMOD is the first product of the AMS/EPA Regulatory Model Improvement Committee (AERMIC). AERMIC was formed with the goal of improving science in applied models.

The model design criteria used for developing AERMOD includes:

- It must be based on up-to-date science;

- It must be simple, yet capture the essence of physical processes;

- It must provide robust concentrations (estimates over a wide range of sources and meteorological conditions);

- It must be easy to update; and,

- It must have reasonable implementation. Inputs to the program should be reasonably available.

Mr. Lee compared AERMOD to the current regulatory model, ISCST3, as follows:

- Both models compute steady-state, near-field impacts;
- ISCST3 assumes Gaussian distribution of the plume in both horizontal and vertical planes, while AERMOD uses a non-Gaussian form when appropriate;
- ISCST3 associates turbulence and dispersion with Pasquill-Gifford stability classes, while AERMOD uses turbulence from modern planetary boundary layer theory and/or from measurements;
- ISCST3 makes no distinction between dispersion from surface and elevated releases, while AERMOD accounts for the differences realistically; and,
- ISCST3 has a discontinuous approach to the treatment of complex terrain while AERMOD uses a more up-to-date continuous approach.

Expectations and future work for AERMIC include:

- Full-featured, updated, applied AERMOD in late 1997;
- Performance evaluation of three or four independent databases;
- Comparison of AERMOD to other applied models; and,
- Future work including urban dispersion, building downwash, wet and dry deposition, non-steady-state, etc.

The evaluation of AERMOD is being completed in two phases. The first is called the developmental evaluation, and is repeated during the development of the model. The second is a final independent evaluation, which will be conducted this fall after AERMOD is finalized. The developmental evaluation included data sets from both surface and elevated releases, rural and urban environments, and flat and complex terrain Although AERMOD is still undergoing revisions, the current version shows less bias than ISCST3.

Question: Does AERMOD handle stagnant conditions?

Answer: Maybe. If conditions hold true from examples studied, it will give closer to observed results than ISCST3 (i.e., the results will be lower than ISCST3).

Source Attribution Modeling for Dioxin, Andy Roth, RAPCA

The purpose of Mr. Roth's presentation was to review a study that was performed for the City of Dayton, Ohio, for dioxins. Dioxin is the term used for any or all of 48 polychlorinated

dibenzodioxins and 87 polychlorinated dibenzofurans. Measurement of dioxin was performed in September 1995 using SW-846 Method 8290.

Six samples were taken at four different sampling sites around Dayton. ISC was used and the predicted concentrations were compared to actual sample measurements. ISC results conflicted with the actual measurements. Possible sources of error include:

- Dioxin emission rate estimates were based on log-normal correlation of dioxin emission rates and ESP temperatures for testing in 1995, 1994, and 1988. If 1988 is not included, the new estimate is ~20% of the model input.

- Perhaps good resolution was not obtained by collecting 24 meteorological data points per model run/sampling period.

- NWS calms protocol does not include winds below 1.54 m/s. These are set equal to 0 m/s. This ignores dispersion during periods of light winds.

An alternative source attribution technique, the Chemical Mass Balance (CMB) Model, was performed to compare results. The result of this comparison was that everything compared - except Sample 5, which was found to include a source afterburner upset that led to the increased emission rates.

Mr. Roth listed two discussion items for the group.

- Receptor modeling techniques may help in dioxin source attribution studies. Source profile library? Mr. Roth stated that, during this study, he was impressed with CMB. This could stand alone from NWS data for short term uses due to the availability of portable met towers.

- ISC should be modified to employ five minute average met data. The availability of ISC source code would be an issue in this modification.

The group discussed a way to "fake out" ISC by giving it five minute data. The user would give it five minute data, ask for a period average, and then, at the bottom, the average would be a 24-hour average.

Practical Problems in Combustion Air Modeling, Dr. Steven Ehlers, US EPA

Dr. Ehlers began his presentation by explaining that the ISCST3 modeling tool requires many parameters and he was unable to find any information available on the sensitivity of modeled results over the range of values presented as defaults for the different values of the parameters. Dr. Ehlers performed a sensitivity analysis of different parameters on the ISCST3 model. The results of Dr. Ehlers' analysis are summarized below. The sensitivity of the model to changes in

the parameter were listed in four categories: severe (>50% difference from baseline Region 6 Protocol results), moderate (10-50%difference), slight (<10% difference), and none.

The analysis results that met Dr. Ehlers' "Severe" criteria are:

- Elevated vs. flat terrain: include terrain <1-2 km; hills taller than stack height only if more than 5 kilometers from stack.
- Rural vs. urban air dispersion coefficient: detailed land use analysis required.
- Surface roughness at application site: EPA-required method, or site-specific justification.
- Watershed size and proximity: use actual watershed area near source; use representative point(s) >10 km away.
- Surface roughness at measurement site: EPA-required value for NWS site
- Scavenging coefficients: isolated events 300%, but rare occurrence in Region VI.

The following parameters met the "Moderate" criteria:

- Anemometer height: underestimates <1 km.
- Particle size distribution and density: require stack test data for particle size and density. This parameter was borderline and was considered close enough to "Severe" to be given special attention at all facilities.

The following parameters met Dr. Ehlers' "Slight" criteria:

- Polar vs. cartesian grid nodes: applicant selects grid.
- Noon-time albedo: specify default values.
- Bowen ratio: specify default values.
- Minimum Monin-Obukhov length: specify default values

The following parameters did not have any impact on the model results:

- Terrain grid file. This is based on the use of the "ELEV" switch in the Control (CO) section and the elevation component in the Receptor Grid files.
- Anthropogenic heat flux.

- Fraction of net radiation absorbed.

New Jersey DEP Risk Assessment Procedures for Minor Sources, Alan Dresser, New Jersey DEP

The purpose of Mr. Dresser's presentation was to explain the risk assessment procedures used in the New Jersey Department of Environmental Protection. Applicability to minor source risk assessment procedures include air permit applications for new or modified sources which emit one or more of 56 specific carcinogens. A list of these carcinogens can be found in Mr. Dresser's presentation handouts in Appendix D of this report.

All sources require a NJDEP Senior Permit Review Engineer to perform a Level I risk assessment. Level I includes calculating ton per year emission rates for each carcinogen, using NJDEP nomographs to obtain long-term ambient concentration of each carcinogen, using NJDEP unit risk factors to obtain cancer risk factors for each carcinogen, and adding incremental risk factors together to obtain the total cancer risk. If the total cancer risk is less than or equal to 1 in a million, the facility passes the assessment. If the risk is greater, then a Level 2 assessment must be performed.

During a Level 2 analysis, the applicants provide information on the sources, NJDEP performs Good Engineering Practice (GEP) stack height analysis with Building Profile Input Program (BPIP), and NJDEP does ISCST3 modeling with 2-3 years of hourly meteorological data. The review is expanded to include 121 carcinogens and 119 noncarcinogens. If the facility fails the parameters provided for a Level 2 assessment (i.e., maximum incremental cancer risk greater than 1 in a million), then the facility is not issued a permit. If the maximum incremental risk is less than or equal to 1 in a million, then the facility passes. If the maximum incremental cancer risk of each carcinogen is 1 in 10,000 to 1 in a million, or the maximum cancer risk is greater than 1 in 100,000, or the cancer risk at any sensitive receptors is greater than 1 in a million, the application goes to a Risk Management Committee

The Risk Management Committee examines the feasibility of better pollution controls or refinement in emission estimates, reducing the proposed hours of operation, modifying stack characteristics for better dispersion (i.e., higher stack height, or change from horizontal to vertical release), or conducting a more refined risk assessment to better define impacts or include other sources at the facility.

2.5.2 Panel Discussion

Mr. Daniel Wise, Panel Chair, led the discussion of the issues presented in the panel issues paper. He stated that the basic need in dispersion modeling is to have more technical guidance and consistency in applying models. Other issues that were discussed during the panel session include:

- AERMOD is not competition for CALPUFF.

- More technical assistance is needed for complex terrain and sparse weather data. CALPUFF can help in these situations. Also, NWS is producing data on winds for every 40 km every 3 hours. The data may be available every hour this year.

2.6 Exposure Assessment Techniques

2.6.1 Presentations

Exposure Modeling: Components, Status, and Uses, Michael Zelenka, NERL

The purpose of Mr. Zelenka's presentation was to provide background on exposure assessment techniques. Mr. Zelenka reviewed the structure of the Office of Research and Development (ORD) and the purpose of each of the four divisions within ORD. The four divisions are the National Exposure Research Laboratory (NERL), the National Health and Environmental Effects Research Lab (NHEERL), the National Risk Management Research Laboratory (NRMRL), and the National Center for Environmental Assessment (NCEA). Mr. Zelenka outlined the role of risk assessment to these groups and defined the focus of each. Presentation handouts can be found in Appendix D of this report.

Mr. Zelenka outlined the steps involved in a risk assessment as follows:

- Hazard Identification - describe the adverse health effects that might occur due to exposure to an environmental contaminant;

- Dose-Response Assessment - determine the toxicity or potency of a contaminant. The dose-response assessment describes the quantitative relationship between the amount of exposure to a contaminant and the extent of injury or disease;

- Exposure Assessment - describe the nature and size of the population exposed and the magnitude and duration of exposure; and,

- Risk Characterization - use the information from the above listed steps to predict the effects of exposure to the contaminant. Estimates are made of the likelihood that a population will experience any of the adverse effects associated with the contaminant, under known or expected conditions of exposure.

Human risk assessment research has evolved to a new approach driven by multimedia legislation, growing recognition of the importance of multi-pathway risk assessments, increased capability to measure multimedia environmental and human exposure metrics, and increased understanding of biokinetics and the use of biological markers of exposure (biomarkers). Mr. Zelenka reviewed the differences between the historic approach to exposure assessment and the evolved approach. The

differences are that, rather than the historic approach of using single factors, the evolved approach considers factors from multiple sources, pathways, routes of exposure, and health endpoints. Risk assessment decisions also now have a multi-media and multi-pollutant focus. Mr. Zelenka reviewed the evolving approaches to several factors involved in exposure assessment, such as exposure pathways, temporal variability at specific locations, etc. Details of these approaches are provided in Mr. Zelenka's presentation handouts in Appendix D of this report.

Human exposure simulation models used at NERL are:

- pNEM/"X" (probabilistic NAAQS Exposure Model for pollutant "X") - simulates the movements of people through zones of varying air quality to approximate the actual exposure patterns of people living in a defined study area;

- HAPEM-MS (Hazardous Air Pollutant Exposure Model for Mobile Sources) - provides long-term (1 year or more) average exposure estimates for pollutants generally attributed to mobile sources; and,

- HAPEM-PS (Hazardous Air Pollutant Exposure Model for Point Sources) - provides annual average estimates of exposures to hazardous air pollutants and resulting cancer incidence for populations residing near point sources.

Mr. Zelenka reviewed comparisons between pNEM and HAPEM in areas such as for indoor sources, residential patterns, and ventilation estimates. These comparisons are listed in the presentation slides in Appendix D.

Mr. Zelenka listed the key elements for exposure model development as:

- Basic research: needed to improve estimates, including those that are modeled, of exposure (e.g., microenvironmental concentrations, activity patterns, dose metrics)

- Improvements to the models;
- More, and better use of GIS;
- Faster and more user friendly models;
- Additional data (measured and derived) and computing platforms that allow the ease and flexibility of performing human exposure research; and,

- Develop a modeling framework so that models that characterize exposure and dose at target sites can be linked, and future exposure models will include the ability to be used as tools for prioritizing the major routes and media of concern.

Microenvironmental Modeling Issues, Dr. Alan Huber, NERL

Dr. Huber began his presentation by stating that the purpose of his presentation was to identify issues with microenvironmental modeling; not to provide any solutions. Microenvironments are the intersection of human presence/activity with a characterizable environment. Our daily activity takes place in a series of microenvironments. Our total exposure is the sum of the exposure from our local microenviroment and the regional environment. The goals of a microenvironment assessment include population-distribution of exposure, special group and/or special microenvironment assessment, effective reduction of exposure, and residual risk and/or relative risk assessment. Model development/application and measurement studies must intersect.

Dr. Huber listed perspectives of models as:

- Regional scale models and ambient air;
- Urban scale models and ambient air; and,
- Local scale (microenvironmental) models - where the exposure begins and ends.

Characteristics used in model selection include pollutant emission sources, chemistry of interest, human activity patterns for exposure, spatial and temporal scales of interest, available meteorology, and numerical methods (i.e., Gaussian plume formulation vs. numerical simulation techniques). Dr. Huber provided examples of exposure modeling activities. Dr. Huber's presentation handouts can be found in Appendix D of this report.

Question: Any research on multiple buildings in urban microenvironments?

Answer: No. Program on regional models. Some research at university level.

Comparing Cumulative Annual Dose Estimates from pNEM to "Literature" Exposure Factors, Thomas McCurdy, NERL

Mr McCurdy began his presentation by reviewing places in the CAA that require exposure assessment There are requirements in the CAA to perform ecosystem health risk and impact assessments. Mr. McCurdy stated that risk assessment procedures are a decision-making process based on science - not science itself.

Mr. McCurdy explained that exposure is the time series of a joint set of air pollution and people-activities at various ventilation rates. Direct data from personal exposure monitors (PEMs) or exposure/intake dose generally are not available, especially for hypothetical scenarios (such as reducing emissions or attaining standards). Therefore, exposure modeling must be undertaken.

Mr. McCurdy listed two general concepts of intake dose and endpoints in exposure assessment as:

- Health impacts, spirometric effects, and symptomatic responses vary greatly with a person's "dose profile." The severity of the effects is a risk assessment issue.

- The major endpoint is the biologically effective dose for organs.

Mr. McCurdy reviewed what constitutes a bad approach to a risk assessment. The bad approach involves making assumptions (i.e., concerning the concentrations of pollutants) throughout the assessment process that leads to false end estimations.

Question: What are the best tools to use at the State and local level?

Answer: pNEM

Real-time Estimation of Polycyclic Aromatic Hydrocarbons, Dr. Nancy Wilson, NERL

The purpose of Dr. Wilson's presentation was to provide overviews of two projects involving monitoring of polycyclic aromatic hydrocarbons (PAH). The monitoring can be performed using either of two instruments manufactured by EcoChem - the PAS 1002i and PAS2000 The instruments perform real-time monitoring of PAH on the surface of fine airborne particles (aerodynamic diameter less than about 1 μm) by ionizing the surface of PAH using ultraviolet light, removing the emitted photoelectrons, and measuring the positive current from the remaining photoionized positive particles. The instruments are not highly precise quantitative instruments. They can best be described as semi-quantitative. The agreement is good between integrated sampling results and the results obtained from the PAS 1002i (the PAS 2000 model was not compared). Dr. Wilson listed some differences in the two instruments. These differences are outlined in her presentation handouts that are in Appendix D of this report.

Dr. Wilson reviewed examples of results obtained using the instruments in collecting real-time values for ambient air. The examples included measurements in a non-smoking household, a smoking household, and the exterior of a veterinarian's office The results showed peaks with a response time of seconds, corresponding to the occupants' PAH-producing activities (for example, smoking in a home or a diesel car driving by the veterinarian's office).

Current activities involving the PAH monitors include:

- Comparing the two instruments to see if the conversion factors are consistent.

- Monitoring total exposure to PAH of preschool children. Studies are including home and day care centers so exposures can be combined to give the total exposure.

The results shown by Dr. Wilson of children's total PAH exposures suggest that studies need to include a multi-media approach, instead of just air, because people's daily activities make a big difference in their exposures.

Minnesota Air Toxics Indexing System, Dr. Greg Pratt, Minnesota PCA

Dr. Pratt began his presentation by explaining a project currently being performed in his office. Minnesota received a grant from EPA to do a measurement and source apportionment of human exposures to toxic air pollutants. This study compares modeling and canister results to results obtained from personal badge monitoring. The study includes 15 VOCs from two inner city neighborhoods and one suburban neighborhood with 20 participants each.

The project involves measuring the personal exposures of individual study participants to the VOCs using personal monitoring badges. Simultaneously, indoor and outdoor concentrations of the same substances will be measured at each participant's home (using badges), in each study neighborhood using canister methodology, and at central sites Additionally, the exposures will be modeled using standard dispersion modeling methods. The hypotheses tested involve comparisons of each of the quantifications of exposure to the "gold standard" of exposure measured on the badge worn by the participant

Dr. Pratt continued with a presentation of an indexing system that was developed in his office. Minnesota implemented a Toxic Air Pollutant Indexing System to rack chemicals by their environmental hazard potential. The system assigns a substance an index number, where the index is the hazard potential found by dividing the potential exposure by the toxicity of the pollutant. To date, 195 pollutants have been indexed and the indexes have ranged over 21 orders of magnitude.

The potential exposure is estimated with Level III Fugacity Model using chemical and physical properties of the substance. The system uses concentrations of the substance estimated in six compartments: air, aquatic biota (fish), terrestrial flora, water, soil, and soil water. Standard toxicity indicators for human health (IRIS2 and HEAST), ecological effects, and other data are used The index values are being used to do the following:

- Set thresholds for reporting requirements (registration, inventory, environmental monitoring, and enhanced emission estimates);
- Set air emission fees using hazard-based fee rates (rather than flat rate);
- Identify persistent and bioaccumulating substances that require further study;
- Refine environmental monitoring goals; and,
- Set priorities for facility review.

2.6.2 Panel Discussion

Ms. Aimee Kennedy, Panel Chair, provided an introduction of panel members and a brief overview of the issue paper for this panel. Panel members provided presentations of certain aspects of the issue paper and the issues were discussed with the workshop group. Ms. Kennedy revised the issue paper, and the final version is included in Section 3.0 of this report. Some general comments made during the panel discussion include:

- Some type of model for use in urban settings would be helpful;
- There is concern that a standardized approach to exposure assessment will stifle State innovation.

2.7 Case Histories of Multi-pathway Modeling Efforts

This section provides summaries of the presentations for this workshop session. There was no panel group for this topic, and, therefore, no issue paper.

The Mercury Study: An Integrated Risk Assessment, Martha Keating, US EPA

The purpose of Ms. Keating's presentation was to describe risk assessment procedures used in a nationwide study of mercury emissions The Clean Air Act as amended in 1990, Section 112(n)(1)(B), required the U.S. Environmental Protection Agency (EPA) to prepare a report to Congress on mercury emissions. A risk assessment was performed to evaluate mercury emissions and a report was prepared for Congress. The assessment was started in 1992, and the report has not yet been released. The purpose of this presentation was to describe the approach which was used to model and characterize the problem, how limitations in the assessment were described, and the lessons learned from applying these tools to a problem that has far-reaching policy implications.

The Mercury Study was designed to integrate a number of different types of information including data on type, sources, and trends in emissions, identification of major pathways of exposure to humans and wildlife, and estimates of control technology efficiencies and costs. The Mercury Study exposure assessment relied on a number of models to predict mercury fate and transport in the atmosphere, watershed, water body and aquatic and terrestrial food chains. The study included electric utilities, municipal waste combustors, and other sources (including area sources).

The study was aimed at answering many questions posed in the beginning of the assessment, which include:

- In considering the sources, pattern, and magnitude of deposition, is there a link between deposition and elevated environmental concentrations?
- What are the adverse effects?

- What are the control technologies available? How much do the controls cost?
- What are the research needs?

The components of the study included:

- Emissions inventory;
- Environmental fate and transport;
- Exposure (numerous exposure pathways were assessed, including wildlife);
- Health effects;
- Risk characterization; and,
- Control technologies and costs.

Each facet of the Mercury Study has it's own set of uncertainties - either due to uncertainties inherent in the approach (e.g., using emission factors for the emissions inventory) or uncertainty related to the models themselves or the parameters used in the models.

Ms. Keating summarized the "lessons learned" from this study as:

- "Science guides, but policy decides " The risk assessment is only one piece of the information needed by the risk manager. Other risk management factors such as economic considerations, technical feasibility, and other non-risk related factors are always part of policy considerations.

- Extensive justification and documentation of model parameters is essential for a "transparent" analyses. The downside is that there is much information for critics to challenge.

- A discussion of uncertainty, even if it is qualitative, is required. Describe the limitations of the assessment. Know your models.

- Sensitivity analyses are useful to test a range of possibilities when there is no one correct answer. Using a range is more defensible than point estimates.

- Use measured data as much as possible to test and corroborate modeled predictions.

- Qualify conclusions, if necessary, with statements about the level of confidence in the results.

The presentation handout in Appendix D provides a more detailed summary of the study.

The Screening Risk Assessment Evaluation for the Proposed Incineration Project at the Anniston Army Depot Chemical Demilitarization Facility, Leigh Bacon, Alabama DEM

The purpose of Ms. Bacon's presentation was to describe a screening risk assessment procedure used in the evaluation of Anniston Army Depot Chemical Demilitarization Facility. Screening risk assessments are comprised of a multi-pathway human health risk assessment (HHRA) and an ecological risk assessment (ERA). The ADEM Air Division did not evaluate impacts for the ERA. HHRAs include estimated risks and hazards from direct exposure through inhalation of emissions and estimated risks and hazards from indirect exposures through soil, water, and food products exposed to emissions depositions.

Ms. Bacon explained that the U.S. Department of Defense currently stores lethal unitary chemical agents (which includes the blister agents HD and HT and the organophosphate nerve agents GB and VX) at the Anniston Army Depot. These agents are stored as bombs, cartridges, mines, projectiles, rockets, and ton containers. The proposed demilitarization of these agents would be achieved through incineration. The HHRA included definition of the study area, definition of the exposed individuals, determination of the concentration of each substance in the environmental media, estimation of the amount of substance each individual is exposed to, and assessment of the toxicity of media concentrations. Methods of exposure evaluated from the incineration include particulate concentrations via air, vapor concentration via air, dry deposition via food and soil, and wet deposition via water and milk products. Emission rates for AAD sources were established using data at the Johnston Atoll Chemical Agent Disposal System (JACADS). Maximum lifetime incinerator/source specific emissions were determined for the chronic assessment. Maximum lifetime term emissions were used for the acute assessment. Air dispersion modeling tools were used to predict the particulate and vapor concentrations for the acute portion of the HHRA. An electronic spreadsheet developed by USACHPPM was used to verify media concentrations for a specific pollutant for a specific exposure scenario. Through dispersion modeling and the use of the electronic spreadsheet, the ADEM Air Division was able to verify media concentrations used in the health effects portion of the SRA. The U.S. Army submitted a SRA for the proposed demilitarization activities at the Anniston Army Depot Ms. Bacon's presentation handouts are included in Appendix D of this report.

2.8 Education and Outreach

2.8.1 Presentations

Training Opportunities in Air Toxics for You Through the Education and Outreach Group, Howard Wright, US EPA

Mr. Wright began his presentation by defining the Education and Outreach Group's (EOG) missions as follows:

- Provide technical air pollution training to primary clients (State and local air agency personnel);

- Promote environmental education to teachers and students, with a focus on K-12; and,

- Enhance outreach activities by forging new partnerships and strengthening existing ones (e.g., small business support, Air Quality Learning Centers, Public Information Officers).

Mr. Wright explained that training needs are assessed through joint needs assessment surveys, a STAPPA/ALAPCO/EPA training committee, course evaluations, and an annual training conference. Ron Townsend explained the need to conduct needs assessment surveys. Needs assessments feed to training priorities, which feed to the Strategic Planning Process. Training ideas can be voiced during the assessment surveys for consideration during the planning process.

Mr. Wright listed ways that training can be provided as:

- Self-instructional materials;
- Classroom courses; and,
- Satellite broadcasts (on the Air Pollution Distance Learning Network (APDLN)).

He then listed several APDLN Broadcasts that are scheduled for the next few months. This type of information, as well as other EOG training information, can be obtained through the following:

- The OAQPS Home Page on the internet;
- The APTI BBS on TTN (dial 919-541-5742);
- The WESTAR Home Page;
- EPA's LAN services menu;
- The APTI 1997 classroom schedule; and,
- State and local site coordinators and training contacts.

Mr. Wright added that an EOG web page will soon be available.

Unified Air Toxics Website, Dr. Nancy Pate, US EPA, ITPID

Dr. Pate began her presentation by defining the purpose of the Unified Air Toxics Website as to provide the general public, federal, State, and local governments and emitting facilities, comprehensive air toxics information (from basic to very technical) in a centralized location on the internet. The website also encourages sharing of information in order to reduce duplication of effort. The website can be accessed at http://www.epa.gov/oar/oaqps/airtox.

The six technical areas either already on the website or soon to be included are:

- Basic Facts;
- EPA Rules and Implementation;
- Pollutants and Sources;
- Technical Resources;
- EPA Programs; and,
- State and Local Agency Programs.

Explanations of these six areas can be found in Dr. Pate's presentation handouts in Appendix D of this report.

2.8.2 Panel Discussion

For the Panel Six discussion, Brian Haugstad reviewed the points made in the issue paper with the group. The panel listed seven basic deficiencies/recommendations to be included in the paper. Examples and discussion regarding each of these issues is provided in Mr. Haugstad's presentation handout in Appendix D of this report. The seven main issues include:

- Training should focus upon the needs of the regulatory agencies implementing the regulations, while clearly understanding who is the target audience.

- Many of the video materials available to States and local agencies are out-of-date.

- Make EPA training and outreach materials more accessible.

- Publications such as quarterly newsletters, fiber-optic television links throughout the state (for state specific education and outreach programs), and informational brochures mailed to regulated facilities to aid in MACT compliance, are helpful in educating regulated facilities.

- Small Business Assistance Groups are often helpful in providing confidential, on-site assistance with regulatory compliance and educational materials to regulated facilities.

- A plain English Guidance Document is needed to instruct agencies on how to effectively collect, analyze, and present data.

- Make training materials and specifically satellite/video training more interactive.

Comment: A plain English guide to the Clean Air Act is available from the Public Assistance Office.

Mr. Haugstad incorporated comments from the discussion. The final version of this paper is included in Section 3.0 of this report.

3.0 Issue Papers

Panel group members worked collectively to develop lists of issues to be addressed during the workshop in each of the workshop areas. The issue papers are structured to be in response to three basic questions. These questions are:

- When are the present technical tools adequate in helping you do your job?
- When are they deficient?
- List possible solutions that might alleviate some of the items on the deficiency list.

The following sections include the final issue papers for each panel. These final papers incorporate discussion and comments made by workshop participants during the workshop.

3.1 Elements of the OAQPS Air Toxics Program, Panel One

What are some suggestions for desirable qualities of toxic tools, in general?

- A whole spectrum of tools is needed, from simple screening tools to sophisticated, complex tools.

- Packages that integrate several tools can make tools easier to use and can address up-front any incompatibility between tools. For example, a combination of tools, such as the Maryland Air Quality Implementation Management System (AIMS), would be helpful in developing an urban air toxics program

- Caution should be used if an attempt is made to force reconciliation between monitored and modeled data.

- Cooperation among various groups with different expertise is often necessary, e.g., EPA, State agencies, city governments, and research facilities Multimedia approaches may also be necessary.

- Ways to communicate risk predicted with these tools should also be available to specialists working with all types of tools.

When are the present technical tools adequate in helping you do your job?

- They are adequate when conducting a screening analysis for a single air toxic contaminant.

- They are adequate when evaluating alternative scenarios for comparative purposes (e.g., cleaning up Superfund sites using a stripper versus other methodologies). These evaluations are good in a relative sense rather than an absolute sense.

When are they deficient?

- They are deficient when less-than-lifetime risk evaluation is required.
- They are deficient when multiple contaminants are involved (cumulative risk analysis for an area).
- They are deficient when source characteristics or emissions are unknown or intermittent.
- They are deficient when they do not address chemical and physical transformations.
- They are deficient when they cannot address time-dependent changes

List possible solutions that might alleviate some of the items on the deficiency list.

- Regional, State, and local agencies are in need of training on which technical tools are available to them, e.g., what is the proper equipment, and the proper use of the tools.
- More validation studies are needed systematically structured to specify characteristics for a range of sources to boost confidence in results of tools especially for more complicated small sources, such as for short stacks, fugitive emissions, etc.
- Prepare materials that can be distributed to small businesses to provide assistance in complying with air, surface and groundwater, wastewater, and waste management regulatory requirements. This is helpful in educating people on air toxics programs.
- It would be helpful to leverage training funding by providing training materials that can be used again in training of other personnel
- An electronic bulletin board system providing written descriptions of real-life solutions to issues would be useful.
- Development of a complete chemical database that includes unit conversions is needed.
- Since there are already so many activities (e.g., Section 112, NESHAPs, MACTs, etc.) going on, a way to mesh together the activities so that work can be performed more efficiently would be helpful.

3.2 Ambient Air Toxics Monitoring and Analysis Data, Panel Two

When are the present technical tools adequate in helping you do your job?

- The guidance documents that are available for performing air pathway analyses at Superfund sites, which could also be used to some extent for non-Superfund activities, are adequate.

- The monitoring data for some toxics are adequate to assess the general trend in toxics levels. They are also adequate for cross-checking estimates of exposure using models for reasonableness.

- Ambient air toxics monitoring tools are available to measure actual ambient levels of specific toxics in those communities and estimate the impacts. The data will allow us to determine which, if any, toxics need to be looked at closer.

- Guidance documents, the Compendium of Methods, and consultation with HQ expert staff have been useful at regional level to the further understanding of the air toxics problem.

- Examples of technical efforts that have worked well are as follows:

- An air toxic sampling effort was initiated with the cooperation of several State and county agencies. Each agency conducts specialized analyses. For example, one agency performs analysis for VOCs via canister sampling/analysis, another performs benzo-a-pyrene (BAP) analyses, and another conducts aldehydes' analyses

- In a recent example, a school was closed due to odor complaints and children and staff getting sick. Through utilizing expert staff, the State's air toxics mobile lab, and regional in-house knowledge, the problem was alleviated through the installation of a permanent sampling location on site and cooperation with the local industries in announcing to the school when upsets occurred.

- There have been successful efforts in initiating air toxics monitoring projects to assist in the multimedia effort to study the problems in communities. Support from the State agency to do the field work helped to get three stations working.

When are they deficient?

- At times, there are State air quality standards or risk-based action limits that are established for particular projects that are much lower than the available method detection limits. Guidance is needed on what to do in these situations.

- Guidance on how to combine available air toxics monitoring and analysis tools into a comprehensive air toxics review is lacking. This guidance should include which monitoring and modeling methods are appropriate in certain situations and how to interpret the monitoring data.

- Emissions data that are temporally or spatially grided to an adequate resolution are also lacking, which makes it difficult to compare ambient versus reported emissions.

- The biggest problem we run into is with the data that is used with the computer software technical tools. An example of a general problem that we have is that the Air Quality Division as a whole has a difficult time collecting and entering accurate data into a single database that everyone can use. We are currently addressing the problems internally through a data management workgroup. An example of a specific problem is that we can use our global positioning system to precisely locate emission sources but the electronic maps that we currently have are not accurate enough to properly represent these source locations.

- Toxics monitoring data are not adequate for developing estimates of exposure in most parts of the country, because there is so little of it and many monitors are located in places where criteria pollutant readings are expected to be high.

- True background monitoring data is needed to evaluate high toxic levels.

- Without consistent health/risk data on air toxics, adequate analysis of the data is difficult.

- The cost of monitoring is high. In addition, most monitoring staff and resources in our state are geared toward criteria pollutants. We typically can only do air toxics monitoring through grants from EPA or by asking the source to pick up the cost for community relation purposes. Typically, we have to rely on past monitoring studies or studies from EPA or other State and local agencies.

Recommendations

- Air toxic pollutants and their impact on communities within urban areas has become an issue that has been getting more attention. Developing a process to address the concerns of the community is needed. This process should include recommendations on appropriate monitoring, modeling, and analysis methods. The following issues could be discussed:

- How do you bring all interested parties/stake holders together to provide information and data that are necessary to address the health concerns of a community?

- How do you develop a plan that fulfills all aspects of the stated objective? The plan could include the following:

  - What are the health or environmental concerns of the community?

  - Is there a high incidence of cancer in the community?

- Can the identified cancer be traced to specific air toxic pollutants?

- What air polluting sources within the community or surrounding communities could be contributing to the specific health problems and is there emissions inventory data available for these sources?

- Should or can inspections be performed at facilities within the community or surrounding communities to obtain information that could be used to link the health problems?

- Could emissions tests be performed at facilities suspected to be emitting contaminants that are significantly impacting ambient air quality and how would this be done?

- With the aid of emissions and air dispersion modeling data what ambient air sampling or monitoring program could be implemented?

- How could the information and data collected be compiled, assessed for data quality, and compared to health standards?

• As local, State, and Federal governments continue to downsize and are asked to do more with less, innovative air toxic monitoring tools and procedures need to be developed.

• Mobile type air toxic monitoring equipment capable of continuously monitoring a wide range of pollutants is needed to identify those sources impacting air quality and characterize what the air quality is within a defined area as it relates community-based health concerns.

• The following are needed to enhance the ability of field personnel to obtain data and information quickly in the field:

• A computer database that can provide aerial photographs. These photographs could be used for evaluating the history of land use at a specific site or industry facility.

Response: There is a database of all aerial photos in the federal government's possession. It is the "Aerial Photography Summary Record System" operated by the USGS in Reston, Va. The phone number is (703) 648-5903.

• A user friendly computer database or cellular phone type system to access information such as: business phone and address directory, health data, meteorological data, emissions inventory data, ambient air data for both criteria and noncriteria pollutants, mapping system capable of overlaying the data described above.

Response: EPA's Envirofacts System, which will soon be completely accessible via the world wide web, may help in resolving this issue.

- Continue to develop FTIR, UVDOAS/open path and laser-based air monitoring technology.

- Guidance is needed on what kinds of requirements may be made in the future so that necessary changes or purchases can be made. Examples of these future requirements are speciate particulate analyses, metals analyses, aldehyde and polar compound analyses. Some of these would require using PM2.5 filters, which are difficult to use due to the size and are also expensive.

Response: There should be some guidance available on fine particulate speciation in the IMPROVE Visibility Transport Monitoring Program.

- A comprehensive federal list of acceptable ambient concentrations for air toxics is needed. **At the Workshop a recommendation was made to change the term, "acceptable ambient concentrations" to a more friendly term. Someone in the group indicated that Region III has an appropriate term.**

- There needs to be an AIRS spatial scale for site-specific monitoring (i.e., neighborhood or city). The scale that is used may not be representative of what the air mass actually is.

- It would be helpful to have training classes of technical tools for FTIR and UVDOAS monitoring. These classes would address identifiable tools and uses, program uses, and where users can go to obtain information.

- Develop and improve remote sensing capabilities, such as satellite imagery, to produce "real-time" flux measurements.

- A comprehensive listing of method detection limits and concentration units are needed to adequately analyze air toxic data.

- Integration of air toxic data into multimedia programs needs to be developed to help evaluate impacts to ecosystems.

- There needs to be an Air Toxics Monitoring Strategy developed.

3.3 Air Toxics Emission Inventories, Panel Three

When are the present technical tools adequate in helping you do your job?

- They are adequate for targeting source categories for toxics analyses.

Response: NO. Source categories have been chosen from experience and background knowledge. Inventories may help in ranking categories.

- The toxic emission inventory data for all source categories are adequate to provide a rough estimate of the relative contribution of various source categories and to assess trends over time.

- They are adequate and helpful in determining rule applicability based on emission level.

When are they deficient?

- We need upgraded tools/software as well as recommended procedures for applying the tools for area, mobile and point sources. The ideal would be to have a reporting system for air emissions that would provide the same details as we now have for criteria pollutants (i.e., stack locations and parameters, etc.).

- The inventories are not as helpful when no uncertainty estimates are included in the inventory. Reliability ratings are somewhat related but are not necessarily enough information. The inventory should provide a quantitative estimate of the uncertainty distribution associated with each chemical and each industry. Such a data set would facilitate Monte Carlo simulations of uncertainty.

- The inventories are not adequate when the base year of the inventory is not coordinated with the available meteorological data. A limited number of meteorological data sets can be produced due to resource constraints.

- The available tools are too poor to develop estimates for mobile source categories that are precise enough to use in comparing the relative impacts of various control strategies, such as fuel reformulation, and on emissions from on highway and nonroad vehicles.

- Speciation profiles in the SPECIATE database are in need of updating for highway vehicles and aircraft. The highway vehicle profiles are in need of improvement, especially for reformulated fuels. These profiles are merely baseline profiles where relative contributions of certain compounds have been adjusted. VOC profiles for diesels are by carbon number rather than specific compounds. Such profiles where contributions of specific compounds are quantified for diesel engines exist and should be incorporated. Newer speciation data

for aircraft engines should be reevaluated and possibly incorporated. There is nothing for nonroad engines in SPECIATE.

- A new toxic emission model for mobile sources, MOBTOX, needs to be developed and guidance provided on how to use the model for State and local government agencies.

- Overall guidance is needed on estimating toxic emissions and uncertainty levels from highway vehicles, nonroad equipment, aircraft, commercial marine engines, and locomotives.

- Once an accounting of HAP emissions has occurred, shouldn't there be some decision-making guidelines concerning the pursuit of evaluating ground level impact? For example, EPA could put the HAPs into "bins" that determine what emission rates of specific HAPs are significant enough to pursue a risk assessment strategy. These bins could also be used to determine what emission levels are significant enough to even include in the accountability portion of an inventory. Do we need to report emissions less than 1 lb (for example) for many of the HAPs? There needs to be some consideration of credibility in regards to the extent that regulatory agencies pursue emissions data. There also needs to be some guidelines for regulatory agencies in this matter in order to eliminate man-hours wasted in data entry and the hard copy forms needed to provide this information to the data entry personnel.

- There may be a need to develop a training program that would include the development of a reading list of references that would provide the requisite background to understand the issues, what inventory work, modeling, and research has been done, what the research needs are, and so on.

- There may be a need to develop specific training programs on how to do a point, area, on-road and nonroad mobile source, and biogenic toxic emissions inventory.

- Since EPA staff has been insistent on the point that the SPECIATE database is not reliable for point source toxic emissions inventories, and should not be used for that purpose, it would be very helpful if EPA could provide speciation profiles that are more appropriate, i.e., either update SPECIATE or provide a separate toxics speciation database.

- There may be a need to develop a consensus-type process, similar to the Emissions Inventory Improvement Program's (EIIP), to compile existing inventory methodologies and/or develop new methodologies. This would help assure that different States and locals used the same steps or procedures in developing toxic emissions estimates.

Response: Few agencies have the resources to become involved in emission factors research. It is anticipated that there will be continued reliance on EPA for research

List possible solutions that might alleviate some of the items on the deficiency list.

- Continue making toxics data (including government and industry data) more accessible and easy to find (internet).

- Encourage good documentation including QA and error estimates.

- Provide some means of dealing with secondarily formed pollutants without running a regional oxidant model. Current tools are not very amenable to doing a good analysis for things like formaldehyde.

Response: There needs to be a policy on handling of "condensibles," air toxics that are solid particulate, air toxics adsorbed on particles, and air toxics that are gases. There should be a distinction between soluble fractions readily absorbed into the body and insoluble fractions. There should be distinctions in inventories between:

TSP - Total Suspended Particulate
PM_{10} - Inhalable particulate

Condensible: Tars, liquid heavy hydrocarbons, naphthalene, etc., that are emitted as liquid drops or vapor and condense in ambient air.

Secondary Particles. Sulfates, nitrates, etc., that are a product of chemical reactions in air. This is mostly a monitoring issue where this fraction should be identified.

Solid Fraction: Insoluble-silica, carbon, silicates.
Soluble-benzene soluble organics, soluble metal compounds, e.g., Pb, Cr, As.
Harmless- salt, sulfates, etc.
Liquid-acid mist.

We need to differentiate in inventories between particles according to origin, composition, and health impacts as well as by size.

- Keep emissions estimation and inventory tools (i.e., emission factor databases) updated and make the updated versions available on a regular basis.

Response: We have previously proposed a "look-up" table in AFS where emission factors that have been used nationwide could be accessed by SCC Code to see what all of the agencies across the country have used to estimate emissions. This would make the most data available to the widest range of users and help achieve nationwide consensus. We should collect information from other nations and incorporate it in the system. They also have some good data and good ideas.

- Do whatever is regulatorily necessary to provide support to existing State air toxics programs. Do this in a hurry before these programs are watered down (or unfunded) due to lobbyists' claims that EPA will be coming forth with their own risk assessment values in the near future and that State programs are duplicative.

- Ensure inventories are compatible with the models likely to utilize the emissions inventories. Meteorological data, deposition data, and inventory data set production should all be coordinated to produce the highest quality coordinated data sets. All three data sets are expensive to generate and can not be performed on a model application by application basis.

OTHER ISSUES:

- There is a need for investigation and resolution of the impact(s) of area source emissions area-wide vs. "hot spots." Is it appropriate to spread emissions over an area (e.g., county-wide) as opposed to looking at the health impacts of a specific location? Is it accurate to apply typical area source type emission factors/ methods based on population or employment rather than doing the detailed type of analysis that might be required for a permit application or a point source inventory?

- There is a need for some way to meaningfully relate health risk assessment and impacts to emissions levels so that emissions data become more meaningful as a consequence (a weighting scheme, screening model?).

- There is a need to tie in with the EPA Consolidated Reporting initiative to clarify what Emissions Inventory responsibilities will be regarding HAPs as opposed to TRI reporting requirements. TRI currently does not collect enough information to perform modeling for health risk assessment.

- There is a need for a model/spreadsheet to apply toxic fractions or speciate on-road and nonroad mobile source emissions and aggregate the emissions of specific toxic chemicals.

- Guidance is needed on inclusion/exclusion of categorically insignificant activities at Title V facilities.

- Activity Data is needed for nonroad mobile sources.

3.4 Dispersion Modeling, Panel Four

When are the present technical tools adequate in helping you do your job?

- EPA guideline dispersion models are powerful, yet easy to use, tools for predicting the ambient impacts of air toxic chemicals for most situations. The two models that are commonly used for predicting air toxics impacts are SCREEN3 and ISCST3.

- ISC3 tends to do a competent job in handling HAPs analyses. Risk assessments comparing modeled concentrations to health-based standards are adequate.

- Receptor modeling is a complimentary tool to ISC3.

- Dispersion models in general are adequate.

When are they deficient?

- The existing guidance on using models specifically designed for hazardous/toxic air releases is not adequate. The use of these models is much more complicated than the use of ISC3 and SCREEN3, especially when quantifying source data. Also, none of the public domain hazardous/toxic refined dispersion models, e.g., ADAM, ALOHA, DEGADIS, HGSYSTEM, SLAB, and AFTOX, are capable of treating multiple sources or more than one set of meteorological conditions in one run. These will become important issues as Section 112(r) programs are implemented.

- There is some concern within the modeling community regarding the accuracy of the available algorithms for modeling downwash caused by nearby structures. The downwash algorithm in EPA's ISC3 and SCREEN3/TSCREEN models is too simplistic and contains a number of unrealistic discontinuities (treatment of plumes just above and below the GEP stack height, the Huber-Snyder/ Schulman-Scire algorithm division point, and the cavity/wake region discontinuity) There is no guideline method for estimating cavity impacts for averaging periods greater than one hour. Regulatory agencies are therefore required to develop their own methods.

- ISCST3 is deficient when determining less than one hour average concentrations from continuous, "steady-state" toxic releases.

- When modeling HAPs, no chemical transformation is assumed. Some of the volatile organic HAPs may be reactive enough to warrant the use of a decay factor in the modeling.

- ISC3 is deficient in simulating valley or channeling effects.

- Regarding deposition modeling

- Calm hours are ignored (which could underestimate the total flux).

- Mercury valence states create difficulty. There is not any good data on this and how it gets deposited.

- For wet deposition, rain out is not considered - only wash out.

- Gas scavenging coefficient and particle size distribution data is limited.

- There is some discontinuity between guidance regarding Superfund sites such as:

- Which receptor height to use to represent the human breathing zone (zero feet versus 3-6 feet);

- What constitutes a secured property line; and,

- Using maximum ground-level concentration versus some statistical analysis instead.

- Guidance for modeling non-point air toxic sources is limited.

List possible solutions that might alleviate some of the items on the deficiency list.

- Develop a guideline method for predicting the impacts of air toxics within building cavities that has the support of the modeling community and that can be used to predict impacts for different averaging periods. A new building downwash algorithm known as PRIME has been developed that addresses most of the technical problems with the ISC3/SCREEN3 downwash algorithms. The PRIME algorithm is now undergoing an independent evaluation. If it performs better than the EPA's current recommended downwash algorithm in this evaluation, it will be recommended as the guideline technique. There are plans to incorporate PRIME in both the ISC3 and CALPUFF models, which will allow for the prediction of long-term impacts using sequential meteorological data. Rhode Island and Texas have developed a computer program that predicts long-term cavity impacts using sequential meteorological data.

- EPA should evaluate each of the HAPs and, where chemical transformation rate is significant, provide guidance on a decay factor for that specific compound.

- Guidance is needed for performing more accurate HAP modeling; for example, characterization of non-point sources.

- Modeling guidance between different EPA offices should be consistent.

- A section on the SCRAM web page for air toxics Frequently Asked Questions (FAQs) is needed.

3.5 Exposure Assessment Techniques, Panel Five

When are the present technical tools adequate in helping you do your job?

- ISC3 modeling coupled with basic inhalation pathway exposure calculations:

- They are adequate when assessing the incremental risk/exposure caused by only one chemical, through the inhalation pathway.

- They are adequate for prioritizing the risk from specific sources by comparing the risk/exposure caused by a chemical at a specific source to another source with the same chemical.

- They are adequate for comparing the risk/exposure caused by one chemical at a specific source before and after compliance.

- HAPEM-MS3 for toxic emissions from mobile sources:

  - Appropriate for estimating annual average human inhalation exposure by hour of the day and season for a population.

  - Appropriate for assessing exposure to toxics that are variable in time or space providing that measured, or modeled, ambient data for that toxic pollutant are available.

  - Adequate when CO can be used as a surrogate for toxics.

- Fugacity Model:

  - Appropriate for assessing concentration of pollutants in different media in order to prioritize HAP list (used by Minnesota to develop their HAP index)

- HEM:

  - Panel members were not as experienced in dealing with this model. Therefore, comments on its adequacy could not be assessed.

  - Interest in learning more about how to apply this model was expressed.

When are they deficient?

- When the exposure to more than one chemical needs to be assessed. The interaction between chemicals is hard to predict.

- When the exposure through multiple pathways need to be assessed. There is no clear guidance on what tools or protocols should be used (expected to be addressed by TRIM).

- When the exposure from multiple sources needs to be assessed. Tools and data are not readily available to determine HAP emissions from all sources in a given area (expected to be addressed by TRIM).

- When the risk assessment results need to be interpreted for use in setting limits or to be communicated to the public.

- How to understand uncertainties.

- How to account for lack of multi-pathway or background data.

- How to enforce limits calculated from risk or exposure assessment results.

List possible solutions that might alleviate some of the items on the deficiency list.

- Provide clear guidance on when Air Toxics Assessments should be conducted.
- Case-by-case MACTs.
- To find the residual risk for existing MACTs to ensure safety.
- Regional air toxics studies.
- Provide clear guidance on who (State, EPA, company) should conduct the exposure assessments (i.e., who has the burden of proof to demonstrate that the limits are protective?).

- Develop a standardized guidance on what should be included in these exposure assessments.

- Multi-pathway vs. inhalation exposure.
- Multiple chemical exposure vs. single chemical exposure.
- Uncertainty analysis (qualitative vs. quantitative).
- Specific modeling techniques or defaults.
- Point source modeling vs. area and mobile sources.

- Provide training for the standardized approach to conducting the Air Toxics Exposure Assessment (instead of standardizing the entire program, a participant recommended developing a web site or bulletin board similar to SCRAM that would have an EPA approved list of exposure models, how and when to use them, EPA expert contacts, and suggested default inputs).

- Provide guidance on how to interpret risk assessment results.
- How to understand uncertainties.
- How to account for lack of multi-pathway or background data.
- How to compare the results to either an absolute incremental risk limit (i.e., 10^{-6}) or a relative risk measurement (i.e., cancer incidents, etc.).

- How to use the results effectively.
- Develop better data to be used in the exposure assessments.
- Toxicity data
- Particle size distributions (will need to require the facilities to do it).
- HAP emissions data from sources to evaluate regional exposure (State will need to help out with this part).

- Software that incorporates exposure routes, toxicity data and GIS and/or population data to evaluate regional exposures (expected to be resolved with TRIM model).

- Biological pharmokinetic data.
- Provide guidance and/or training on how to communicate the risk results.
- Address the following policy questions

    - What role will States play in residual risk determination?

    - What steps (gathering information, training, etc.) do the States need to be doing in order to prepare for their involvement with residual risk?

    - What type of data will be required for the new exposure models, so that the States can start collecting the data if not already available?

    - How will the residual risk program affect States that already have a risk-based air toxics program?

3.6 Education and Outreach, Panel Six

PART ONE:

When are present technical tools adequate in helping you do your job?

1. In providing staff training specific air toxics standards or procedures, and in providing information on general air toxics issues.

2. In providing education, outreach and training to the regulated community. Printed training and outreach materials, and live or taped educational videos are helpful, when provided in a timely manner.

PART TWO:

When are technical tools inadequate?

1. Training often focuses upon general facility operations, and upon pollution control methods. Instead, there should be greater emphasis placed upon regulatory requirements, and the means necessary to regulate these requirements.

2. When training is not provided in a timely basis. This happens frequently.

3. When telecourse speakers provide vague information, and are unable to answer specific questions or details.

4. When communicating risk assessment to the public.

5. When there are no viewing sites equipped to receive satellite courses. When local network sites are not available, otherwise interested participants must either travel to more distant sites, or otherwise not participate

PART THREE:

What recommendations may solve these identified problems?

1. Training should focus upon the needs of the regulatory agencies implementing the regulations, while clearly understanding who is the target audience. Different target audiences have different training needs. (i.e., permit writers vs. compliance staff vs. the public).

Recommendations:

A. EPA should coordinate with STAPPA/ALAPCO and establish an early development stage, that makes greater use of annual and special interest surveys, to more clearly identify target audiences and their training needs.

B. These surveys should include annual updates on State/local toxics expenditures, air toxics monitoring and modeling efforts, emission inventories, exposure assessment efforts, and special studies. A listing of State and local program contacts should also be updated annually.

C. STAPPA/ALAPCO has a listing of State air toxics contacts. State and local agency staff should review these contact lists, to ensure correct staff are listed.

D. Survey the targeted audience well prior to developing the training materials

E. Different State and local regulatory agencies have different goals and training needs. Surveys should identify these differences

F. Survey STAPPA/ALAPCO, EPA Regions, and Trade Associations to determine what type of training is needed, and to specifically identify when the training is most needed.

G. Surveys should include long-term strategic goals and these long-term ideas forwarded to EPA. This will force State and local agencies to actively think and prioritize their training needs long-term.

H. State and local agencies should actively solicit and prioritize their training needs from their identified targeted groups, and this information should be forwarded to EPA.

I. Training goals should be identified for specific regulatory standards.

J. Develop written surveys that may be distributed to State and local agencies, that identifies and prioritizes requisite and required training

K. State and local agencies should conduct their own surveys of the agency staff, to determine their agencies' training needs.

L. Identified training needs could be shared through the use of regional air toxics conference calls.

M. Newly released educational materials should be screened early after receiving it, to insure it is useful for targeted groups

N. States/local programs should be offered the opportunity to participate in the development of educational material.

2. *Many of the video materials available to State and local agencies are out-of-date.*

Recommendations:

A. A quarterly update on all current available EPA training materials should be provided to primary State and local agency air toxics contacts.

B. Primary air toxics coordinators should be contacted directly by APTI, and informed when this information is available on EPA's Unified Web Site.

C. All video and written materials provided by EPA to State and local programs should include dates of publication, and a brief synopsis.

D. The EPA should develop new training materials as soon after State/local surveys are evaluated and significant training needs are identified

E. APTI videos should not be repetitive, but should reflect current policies and procedures.

F. Remember... it is difficult for State and local agency staff to provide industry with training, until State and local program staff first are provided a clear understanding themselves.

3. *Make EPA training and outreach materials more accessible.*

Recommendations:

A. Provide an on-line clearinghouse of all available course materials, including video tapes, training courses, and other training resource materials, by accessing the Unified Air Toxics Web Site.

B. Continually (or quarterly) update course materials on-line, as these materials become available, so that most current training materials are always up-to-date.

C. Separate training materials by discipline or MACT standards, to more easily locate resource materials.

D. The EPA and STAPPA/ALAPCO should contact State and local air toxics staff contacts directly, as opposed to strictly through State/local educational coordinators.

E. Regulatory agencies should solicit input from trade associations and small business assistance groups. Training workshops can then be co-sponsored by all three participating groups.

F. Provide a means whereby training materials already developed by State and local programs may be shared electronically on the Unified Web Site.

G. Provide an easily identified on-line heading (i.e., "air toxics education"), so that on-line browsers may more easily locate educational training materials.

H. Greater publicize the Unified Air Toxics Web Sites. Promote its use among State and local air toxics contacts, and among State and local air directors.

I. For Regional EPA updates, State and local agencies should greater utilize EPA's Regional web sites. Provide regional EPA contacts with recommendations, suggesting how their region may improve their EPA web sites.

J. Make better use of fiber-optic satellite feeds, to involve government agencies, regulated facilities and the general public.

K. To improve training attendance, EPA and State sponsored informational meetings should require minimal long distance travel

L. Class workshops may be improved by supplementing class materials with important instructional video tape materials.

M. In developing effective workshops, descriptive video materials should be included in workshops.

N Use more conference calls. It is cheap and convenient.

O. Workshops are not commonly well attended by the public. Suggestions are needed to improve public participation. Use State/federal advertising and marketing resources?

P. Send important notices to all air toxics contacts, using a list server (i.e., similar to Federal Registrar notices, and Mobile Source e-mailings).

Q. Link other good web sites to the Unified Air Toxics Web Site, for easy access.

R. The Unified Air Toxics Web Site should have a comments section, for agency staff to comment upon education materials, and to make further suggestions.

4. *Publications such as quarterly newsletters, fiber-optic television links throughout the state (for state specific education and outreach programs), and informational brochures mailed to regulated facilities to aid in MACT compliance, are helpful in educating regulated facilities.*

Recommendations:

A. Newsletters may be used to educate and provide all types of compliance standard information to regulated facilities.

B. In order to more effectively solicit comment from the public and from regulated facilities, additional marketing and advertising promotions may be necessary.

C. EPA written materials can be modified and simplified by State/local agencies for State agency instructional purposes (i.e., brochures and newsletters).

D. Publications should be clearly written, in shortened form.

E. Do not include needless language and too great of detail.

F. If materials are too long or detailed, often regulated facilities do not bother reading it, and it is all wasted effort.

G. Use "catchy and colorful graphics" that bring attention to the publication or brochure, and prioritize the ideas that you wish to relay to the reader.

H. In addition to regulator news, newsletters should also include health risk data based upon health studies, that draws the reader further into the article.

I. To reduce duplication of efforts, EPA and State agencies should contact each other when significant communications are forwarded to regulated facilities.

J. Video training should not include extraneous details

5. *Small Business Assistance Groups are often helpful in providing confidential, on-site assistance with regulatory compliance and educational materials to regulated facilities.*

Recommendations:

A. Examples of the nation's most highly effective programs should be summarized and shared nationally.

B. STAPPA/ALAPCO should survey how many small business assistance groups are currently active nationwide. Investigate their effectiveness.

C. Small Business Assistance Programs should be expanded, by increased funding of these sources, and by further sharing of technical ideas between regulated facilities and government agencies.

D Alternatives to directly interacting with government regulatory agencies Regulated facilities often call upon Small Business Assistance Groups, rather than interacting with government agencies. Improved compliance of MACT standards.

6. *A Plain English Guidance Document is needed to instruct agencies on how to effectively collect, analyze, and present data.*

Recommendations:

A. Statistical analysis training is needed

B. More training opportunities need to be provided on the Education and Outreach home page.

C. Risk Assessment More training is needed for Training the Trainers target groups

D. Training materials should use non-technical instruction, whenever possible, to keep training as simple as possible and easy to understand

7. *Make training materials and specifically satellite/video training more interactive.*

Recommendations:

A. Question and answer format.

B. Provide additional MACT standards satellite/ video training. One MACT standard per video.

C. When possible, film on-site at regulated facilities, to demonstrate how to perform required MACT compliance activities.

D. Make video presentations interesting, by using state-of-the-art, color graphics.

4.0 Conclusions

In general, four major themes appeared for discussion during the workshop. These include the strategy of the Air Toxics Program, personnel training, guidance on proper use of the tools, and technical and budgetary resources. A summary of the major themes identified through pre-workshop panel discussion and discussion at the workshop is as follows:

1. An overall strategy for dealing with air toxics issues needs to be developed and technical tools should be designed to fit this strategy.

   - The overall air toxics strategy should include how the various activities within Section 112 relate to each other, such as MACTs, NESHAPs, Urban Air Toxics Program, etc. If these activities can share some of the same data (e.g., inventory and monitoring data), rather than having to recreate these data for each application, duplication of efforts could be reduced and the technical tools can be used more effectively.

   - 'The different technical disciplines need to be made more aware of each other's needs. Air toxics programs should be designed to promote closer working relationships and technical tools should be structured to promote the sharing of air toxics data (i.e., monitoring and inventory data should be provided in a format that can be used in dispersion modeling, which, in turn, should be able to be input easily in exposure models). There is a need for a closer working relationship between exposure modelers and the risk assessors at the Regional and State levels. The exposure modelers are developing algorithms that are scientifically sound, but which may not address the specific questions that need to be answered by the decision-makers at the State and local levels.

2. Training should continue to be recognized as a critical element of the Air Toxics Program.

   - State and local agency personnel need to be advised of the availability of training materials and courses. A clearinghouse of training materials should be accessible to agency personnel and those materials should be kept up-to-date

   - Alternative forms of training, such as internet courses, should be provided for situations where funding is limited and travel cannot be performed.

   - Training materials should be kept as easy to understand as possible. Moreover, training does not mean issuing guidance documents and policy memos, but is a thoughtful process

that involves identifying audiences, developing learning objectives and measurement methods, and determining suitable delivery systems.

- Training must be included as a vital part of the Air Toxics Program and should be built into the rule development process in the early stages. Rule developers must recognize that rule implementation is at least as important, if not more important, than rule promulgation, and training is essential to the implementation.

- Air toxics is recognized as a priority program and the need for additional training materials for this program is recognized. In FY98, additional training, i.e., MACT-specific training, is planned.

3. Guidance on the availability, purpose, and use of air toxics technical tools is needed.

   - On a new or existing website, provide an EPA-approved list of exposure models, how and when to use them, EPA expert contacts, and suggested default inputs.

   - Specific guidance on assessing HAPs is needed, such as guidance on emission inventories for point, area, and mobile sources. The role of the Emission Inventory Improvement Program (EIIP) should be expanded to specifically address HAPs and guidance and tools from State and local agencies should be obtained. For example, a plain English guidance document is needed to instruct agencies on how to effectively collect, analyze, and present data.

   - All publications should be clearly written, in shortened form, and should not include needless language and detail.

4. As Federal, State, and local governments continue to downsize and are asked to do more with less, innovative air toxics monitoring tools and procedures need to be developed.

   - Opportunities, such as this workshop, should be provided for agency personnel to meet each other and develop contacts for various technical issues

   - A contacts list for technical areas within air toxics would be helpful to promote interaction between the various technical disciplines. A list of workshop participants' areas of expertise was developed at the workshop, but it only includes workshop participants. A much more comprehensive list is needed to provide agency personnel with a quick reference for technical questions.

In addition to the general themes that were discussed at the workshop, specific issues within the panel subject areas were identified. The major issues for the panel areas include the following:

- **Monitoring and Data Analysis:** More monitoring data are needed to define the community health concerns caused by air toxic pollutants. In many instances, monitoring has been performed, but the data from the States performing the monitoring is not centrally located and available for analysis. In those cases, the data needs to be compiled for future use. For many pollutants, monitoring has not been previously performed or has not been adequately performed, and additional monitoring is needed.

Sampling and analytical methods should be completed for monitoring pollutants where methods have not been previously available, and outdated methods should be updated. For example, the update of EPA's Compendia of Methods for monitoring organic and inorganic pollutants in air should be completed. These compendia are needed to promote uniformity in monitoring procedures from state to state. The entire revised compendiums should be widely distributed for ease in locating information.

As monitoring methods become available for pollutants not previously monitored, analysis methods and tools must be developed to organize and analyze the data. Projects such as the Ambient Air Quality Characterization Project help to address needs for new analysis tools.

- **Emission Inventories:** The overall need in the emission inventory subject area is for more guidance on including mobile, area, and point sources to provide a complete inventory. Upgraded tools/software are needed, as well as recommended procedures for applying the tools for area, mobile, and point sources. There is a need to review the EPA Consolidated Emission Inventory Reporting initiative to clarify what emission inventory responsibilities will be regarding HAPs as opposed to Toxic Release Inventory (TRI) reporting requirements. The process of meeting inventory reporting requirements needs to be streamlined to reduce the burden of the reporting requirements. Inventories should be consolidated where possible to reduce duplicate data collection and reporting. Overall guidance is needed on:

    - Estimating toxic emissions and uncertainty levels from highway vehicles, nonroad equipment, aircraft, commercial marine engines, and locomotives

    - How to do a point, area, on-road and nonroad mobile sources, and biogenic toxics emissions inventory.

- **Dispersion Modeling:** In general, existing technical tools are adequate, however, more guidance is needed on how to use the tools. Tools are needed to address new issues that result from modeling air toxics. For example, better algorithms are needed to characterize wet deposition, particle/gas partitioning, gas scavenging coefficient and particle size distribution, etc. More technical guidance is needed on using the models to help promote consistency in applying the models.

- **Exposure Assessment:** EPA needs to develop better tools to address exposure assessment needs. Guidance is needed for all personnel on the steps involved in performing exposure assessments. Specific areas that the tools need to consider include:

  - Assessing the exposure through the inhalation pathway versus all routes of exposure;
  - Assessing exposure to humans versus including exposure to animals and plants; and,
  - Assessing exposure in urban settings.

The workshop succeeded in bringing together many technical disciplines to voice opinions on issues relating to areas involving air toxics assessment. Sixteen percent of workshop participants reported that their primary job function is monitoring and data analysis, 32 percent were dispersion modelers, 20 percent perform emission inventory and permitting work, and 32 percent were classified as environmental engineers. The technical disciplines gained information regarding how their work affects work done in other areas. Participants gained knowledge of the many technical tools available to them that may not have known about prior to the workshop. Participants also provided EPA with information by defining their needs for the current tools and for future efforts. On the final day of the workshop, participants completed a workshop evaluation form expressing opinions about the workshop. Participants indicated that the greatest benefit of the workshop was learning who the experts are in various technical areas to help promote interaction between technical disciplines. Participants wanted to learn basic information about all of the disciplines so that they could see how their work fits into the overall air toxics approach. Those speakers presenting new information (e.g., the dispersion model AERMOD) were more helpful because they gave an idea of the current activities and what is coming, relating to air toxics, in the near future. Many comments were received stating that participants were eager to learn more about performing exposure assessments and how EPA plans to approach exposure assessment in the future. They felt that the workshop was helpful in informing personnel of the availability of technical tools. For example, prior to the workshop, panel members developed lists of tools that would be helpful in performing their work. During the workshop, they learned that tools were already available to do many of the things they suggested.

Participants stated that they felt that the workshop was helpful to open lines of communication between States and EPA to help get agency personnel more involved and interested. They felt that the workshop was organized and productive, and was successful in meeting the goals of the workshop. The participants stated that it was helpful to have groups working on developing issues for discussion prior to the workshop. It was suggested that the workshop become an ongoing workshop/training session to help promote interaction between disciplines and to help keep personnel informed of the technical tools that are available to them.

The Workshop Evaluation Forms also allowed participants to make suggestions for future workshops. A summary of the major points identified for consideration in future workshops includes:

- The duration of this workshop (three days) was adequate to address the issues.

- Screen workshop speakers prior to the workshop to ensure that the presentation material is relevant to the purpose of the workshop.

- Provide a complete, good quality copy of the overheads used by presenters. All slides should be provided to participants and the copies of the slides should be readable.

- Hold conference calls with panel members early in the planning process.

- Hold an ice breaker meeting to facilitate participants meeting each other. Some type of activity, other than during workshop hours, would provide for a more informal atmosphere that would promote interaction with other attendees. Ice breakers activities could include a social hour at the hotel the night before the meeting or a ball game.

- Include fewer, but more detailed, presentations in the workshop. Do not use technical jargon in the presentations that most participants will not understand.

- State and local participants want more structure in the panel discussion. The panel discussion during the conference calls prior to the workshop were intended to be a free exchange of ideas relating to the various technical areas. It was suggested that more of a structured approach to these discussions may have been more productive. A list of specific questions for each technical area may have helped to spark discussion.

Appendix A

Letter of Invitation

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

MAR 25 1997

OFFICE OF
AIR QUALITY PLANNING
AND STANDARDS

MEMORANDUM

SUBJECT: Invitation to a National Specialty Workshop on Technical Tools for Air Toxics Assessment

FROM: Joe Touma, Meteorologist JST
Air Quality Modeling Group, EMAD (MD-14)

Dennis Doll, Meteorologist
Air Quality Modeling Group, EMAD (MD-14)

TO: Regional Air Toxics Coordinators (Region I-X)
Regional Modeling Contacts (Region I-X)
Regional Emissions Inventory Contacts (Region I-X)
Regional Toxics Monitoring Contacts (Region I-X)

We have previously explored with you the feasibility of conducting a specialty workshop on technical tools for air toxics assessment. Your response was generally favorable. We are planning on having the Workshop at Research Triangle Park, NC, on June 17-19, 1997. Attendance is open to Regional, State and local agency staff. The workshop is designed for senior staff environmental scientists, engineers, chemists, meteorologists and toxicologists with experience in the topics covered in the workshop.

Attached is a draft agenda for this workshop. In order to plan for a successful workshop, we need full participation from all attendees. The following are some of the parameters:

1. The workshop will be limited to 50 participants. Names will be selected in the order in which they are received; however we will strive to achieve a balance among the Regions, States and local agencies and among those with experience in the topic areas of the workshop.
2. A goal of the workshop is to include reports from the Regional Offices, States and local agencies on internal air toxics initiatives. Attendees are expected to participate in at least one of the following activities: a) as speakers providing Regional, State and local perspectives on either monitoring, emission inventories, modeling or exposure analysis tools; b) as panel members on sessions dealing with these tools; c) as speakers providing case histories of multi pathway analyses efforts, or d) as participants for a focus group, described later. Presenters are responsible

for preparing hard copies of their presentation materials. Panel members are expected to meet at the end of the day to prepare a summary report. Attendees should indicate their preference(s) within 30 days of receipt of this letter, and will be assigned based on their preferences.

3. Once panel members have been identified, several teleconference calls will be scheduled to develop draft issue papers for discussion during the conference. Panel members are expected to coordinate with other experts in their groups on the development of these issue papers.
4. The presentation materials, as well as panel summary reports will be published in workshop proceedings. Certain segments may be video-taped for use in a future APDLN telecast.
5. The workshop will be held in the EPA's Administration Auditorium on 79 Alexander Drive, RTP (see map attached). Attendees are responsible for all travel arrangements and accommodations. A packet containing a list of hotels in the area can be provided. If you wish to car pool locally, please indicate on the registration form and your name will be distributed.
6. The workshop spans three full days (Tuesday, Wednesday and Thursday). In order to have a successful workshop, we ask that all participants commit to staying for the duration of the workshop and plan for traveling on Monday and Friday.
7. An optional one-half day can be arranged for those requesting hands-on computer training on technical tools in using emissions factors to develop emissions inventories with exercises in Air CHIEF and TANKS, or modeling (TSCREEN and ExInter models). In order to assure availability of facilities and course instructors, at least 5 people are needed to enroll in each session.
8. In addition to discussing the issues addressed in this workshop, OAQPS also invites approximately 10 non-federal attendees to participate in a focus group to aid in the evaluation of the national air toxics problem. The purpose of this focus group is to clarify the perspectives of stakeholders on the issue of defining an air toxics problem by addressing such questions as:
   - What characterizes air toxics emissions, ambient concentrations and deposition as "a perceived problem"? Is there a consensus on whether there is one? At what scale?
   - What is an acceptable level of uncertainty in the emission estimates? Ambient measurements? Deposition estimates? Exposure estimates? Health effects data?
   - Given probable action at some level of uncertainty, and the need for reducing uncertainties where possible, for what measures (emissions, health benchmarks, etc) are uncertainties acceptable, and where should efforts/resources be concentrated to reduce uncertainties?

The results of the focus group discussions will, we believe, provide a valuable perspective, given the important issues of data availability and uncertainty. Group discussions will require participation through teleconferencing before the workshop itself. Non-federal attendees interested in participating in this focus group should indicate their interest on the registration form and whether they are interested in meeting in the evening or an optional one-half day session on Friday morning.

Please circulate this invitation to your respective State and local agency contacts. A final agenda including the topics and assigned names will be mailed by April 30. To ensure seating, participants should send their registration forms within 30 days to: Joe Touma or Dennis Doll, USEPA, OAQPS (MD-14), Research Triangle Park, NC 27711. A copy should be sent also to the Regional contact.

If you have any further questions or comments concerning this speciality workshop please contact either of us at:

Joe Touma (919) 541-5381; E-mail: touma.joe@epamail.epa.gov
Dennis Doll (919)541-5693; E-mail:doll.dennis@epamail.epa.gov

Attachment

cc: F. Dimmick (MD-13)
D. Guinnup (MD-14)
B. Hunt (MD-14)
J. Irwin (MD-14)
B. Jordan (MD-13)
D. Misenheimer (MD-14)
D. Mobley (MD-14)
D. Pagano (MD-15)
S. Shaver (MD-15)
J. Tikvart (MD-14)
Workgroup Members

Appendix B

Workshop Agenda

Workshop Agenda

National Specialty Workshop on
Technical Tools for Air Toxics Assessment

June 17-19, 1997
79 Alexander Drive, Administration Bldg. Auditorium,
Research Triangle Park, North Carolina

A workshop on the technical tools developed by OAQPS, Regional Offices, State and local agencies for meeting the goal of the air toxics program: a discussion of issues, initiatives, adequacy, limitations, tool needs and data gaps, and future direction.

Target Audience: Regional Offices, State and Local Agency Technical Personnel

Workshop Size: 50 people

Workshop Mission Statement: Regional and State contacts have expressed an interest in learning about the technical tools required to support many sections of the Clean Air Act regarding the air toxics program so that:

1. They can better support requirements under Title III such as the newly published Risk Management Plans under Section 112(r), residual risk and de-listing requests under MACT rules, the Urban Area Source Study, the Great Waters Studies, etc.
2. They know who are the air toxics topic area experts (office level identification) across EPA, and the States and local agencies in order to obtain rapid assistance.
3. They can better communicate the magnitude of air toxics issues facing the technical analyst and the success in solving air toxic problems.

This interactive workshop includes half-day sessions devoted to Emission Inventories, Dispersion Modeling, Ambient Monitoring and Data Analysis, Exposure Assessment Case Histories, and Education & Outreach as related to supporting the air toxics program. The sessions will be interactive in order to obtain feedback from all attendees, rather than one way OAQPS presentations.

Input from the participants is important to provide direction to air toxics technical needs and to obtain assistance from the State and local agency partners in an era of reduced resources.

Tuesday June 17

7-8 am Workshop Registration

8-9 am Welcome and Announcements, 30 minutes, Joe Touma, Dennis Doll
Introductory Remarks- Bill Hunt, 30 minutes

9 am - 12 noon: Elements of the OAQPS Air Toxics Program

Framing the discussion issues in this segment:

1. *An Overview of Section 112(r), MACT rule, the Urban Air Toxics Study, and the Great Waters Study, etc.*
2. *What technical tools are needed in support of these rules?*
3. *Who are the agency experts in air toxics, how can I get a hold of them?*
4. *Overview of strengths and weaknesses in the technical tools available for doing all adequate technical analysis now and in the future.*

Speakers:

9:00-9:30	*The Clean Air Act Framework for the Air Toxics Regulations. Al Wehe, 30 minutes*
9:30-10:00	*Learn About How EPA Plans to Bring Together the Federal Air Toxics Program (The OATS Report). Al Wehe, 30 minutes*
10:00-10:30	*How Is the Air Toxics Program Structured in OAQPS and Who Has What Functions? Melissa McCullough, 30 minutes*

Panel Discussion: Regional/State/local Perspectives (90 minutes)
Chair: Joann Held (New Jersey)

1. *Tom Rogers (FL): Should Offsite Consequence Analysis of Accidental Releases be Incorporated into a Permitting Program?*
2. *Denis Lohman (Reg 3): Examples of Situations In Which Risk Is Communicated to the Public (e.g. Superfund Remedial Actions; Place-Based Studies; Proposed Permits; and Incident Analysis).*
3. *Lee Page (Reg 4): Emission Inventory Tools: Present and Future*
4. *Mike Pokorny (MD): Combining Modeling & Inventory Tools*
5. *Linda Lay (EPA OECA): Using Tools for Targeting Sources*
6. *Joann Held (NJ): Risk Screening Tools*

12-1: Lunch Break

1 pm- 5 pm: Ambient Air Toxics Monitoring and Data Analysis

Framing the discussion issues in this segment:

1. *Why perform ambient air monitoring for air toxics?*
2. *What are some of the ambient air monitoring methods and costs for air toxics?*
3. *How can I use monitoring data from a subset of air toxic pollutants (such as the PAMS network) in my analyses?*
4. *What ambient air toxics monitoring data are available? Where can I find them? What current summaries and analyses are available?*

Speakers:

1:00-1:30	*Compendium Methods for Monitoring Organic and Inorganic Compounds. Bill McClenny, 30 minutes*
1:30-1:45	*State and Local Participatory Programs: Volatile Organic Toxic Compounds, Including Speciated NMOC, UATMP, Carbonyls, and PAMS. Dave-Paul Dayton, 15 minutes*
1:45-2:00	*Particulate Compounds Including PM10, PM2.5, and Filter Analysis for Toxic Species. Stan Sleva, 15 minutes.*
2:00-2:30	*Video Demonstration of Ambient Sampling and Analytical Techniques for Hurricane Fran Debris Burn Site. Neil Berg, 30 minutes*
2:30-3:00	*Chemical Mass Balance for Toxic Species (VOC, and Particulates). Chuck Lewis, 30 minutes.*
3:15-3:50	*New Data Analysis Tools. James Hemby, 35 min*

Panel Discussion: (45 minutes)

Chair:	*Thomas Shoens (Wayne County)*
Panel Members:	*Peter Kahn (Region 1)*
	Todd Jackson (W. Virginia)
	Victor Guide (Region 3)

5 pm: Adjourn

5-6 pm: Panel members only: Ambient Air Toxics Monitoring and Data Analysis, final summary discussion

Wednesday June 18

8am -12 noon: Air Toxics Emission Inventories

Framing the discussion issues in this segment:

1. *What are potential air toxic pollutants for urban, rural, and mobile sources? What are typical sources, and source categories?*
2. *Are emission factors available for all air toxics pollutants? What do I do for sources that do not have emission factors?*
3. *Where is the information that allows me to compute the total emissions from sources in rural areas, urban areas, mobile sources, fugitive sources, etc.*
4. *Where are the emission tools that I can use? What pollutants do they cover? What is the difference between EPA tools and those from other organizations.*
5. *What are the new procedures to collect and report emissions data?*

Speakers:

8:00-9:00	*Introduction- National Air Toxics Emission Inventory. Anne Pope, 60 minutes*
9:00-10:00	*Emission Inventory Improvement Program (EIIP). Steve Bromberg, 60 minutes*
10:10-11:00	*Emission Estimation: Techniques and Tools. Guidance and Assistance Tools from the Emission Factors and Inventory Group. Anne Pope, Mary Ann Barckhoff, 50 minutes*

Panel Discussion: (70 minutes) *11:00-12:10*

Chair:	*Mike Fishburn (Texas)*
Panel Members:	*Jennifer DeMay (Washington)*
	Bob Ragland (Forsyth County, NC)
	Diane Scher (Tennessee)
	Paul Cocca (EPA OW)
	Richard Cook (EPA OMS)
	Craig Bressan (Lane Regional)
	Brian Haugstad (Iowa)
	Jim Lefik (Allegheny County)
	Mohamed Basher (Allegheny County)

12-1: Lunch Break

1-5 pm: Dispersion Modeling

Framing the discussion issues in this segment:

1. *What dispersion models are appropriate for use in air toxic assessment? What are the advantages and disadvantages of each model?*
2. *What data do I need to run these models?*
3. *What is a screening study and when can I use a screening vs a refined model?*
4. *When do I use EPA models vs other types?*
5. *What is the averaging time to be considered for air toxics?*
6. *Where can I get the meteorological data to run these models?*
7. *Do I need to consider chemical transformation in the dispersion models? If so, are the same models appropriate?*
8. *How do I model sources with variable emission rates?*

Speakers:

1:10-1:25	*Overall Perspective of Air Toxics Modeling Issues-Program Management Issues. Joe Tikvart, 15 minutes*
1:25-2:10	*Introduction to Issues Typically Encountered in Modeling. John Irwin, 45 minutes*
2:10-2:25	*Meteorological Data Needs and Electronic Bulletin Board Systems. Dennis Atkinson, 15 minutes*
2:30-3:00	*AERMOD, the Next Generation Air Dispersion Model. Russ Lee, 45 minutes*
3:00-3:25	*Dioxin CMB Modeling. Andrew Roth (Dayton), 25 minutes*
3:35-3:55	*Practical Problems in Combustion Air Modeling. Steven Ehlers, Region 6, 20 minutes*
4:00-4:15	*New Jersey DEP Risk Assessment Procedures for Minor Sources. Alan Dresser, 15 minutes*

Panel Discussion: (45 minutes) *4:15-5:00*

Chair:	*Daniel Wise (Rhode Island)*
Panel Members:	*Patrick Pakunpanya (Louisiana)*
	Jeffrey Sprague (Illinois)
	Alan Dresser (New Jersey)
	Henry Feingersh (Region 2)
	Samuel Bell (Jefferson County)
	Dom Ruggeri (Texas)
	Steve Kish (Michigan)

5:00 pm: Adjourn

5-6 pm: Panel members only: Air Toxics Emissions Inventories, Dispersion Modeling, final summary discussions

Thursday June 19

8 am -11:30 am: Exposure Assessment Techniques

Framing the discussion issues in this segment:

1. *What are the components of exposure models?*
2. *What types of exposure assessment models are available?*
3. *Can additive exposures be accounted for?*
4. *What is the role of GIS is undertaking exposure and risk assessments?*
5. *Inhalation versus multi-media exposure.*
6. *Addressing uncertainty and variability.*

Speakers:

8:05-8:55	*Exposure modeling: Components, Status, and Uses. Michael Zelenka (NERL), 50 minutes*
8:55-9:30	*Microenvironmental Modeling Issues. Alan Huber (NERL), 35 minutes*
9:30-9:55	*Comparing Cumulative Annual Dose Estimates from pNEM to "Literature" Exposure Factors. Thomas McCurdy (NERL), 25 minutes*
9:55-10:20	*Real-Time Estimation of Polycyclic Aromatic Hydrocarbons. Nancy Wilson (NERL), 25 minutes*
10:20-10:40	*Minnesota Air Toxics Indexing System. Greg Pratt, Minnesota, 20 minutes*

Panel Discussion: (45 minutes) *10:45-11:30*

Chair:	*Aimee Kennedy (W. Virginia)*
Panel Members:	*Jerry Ebersole (Oregon)*
	Jeffrey Hayward (North Carolina)
	Jim Snyder (EPA Region 8)
	Greg Pratt (Minnesota)
	Daniel Gray (Kentucky)

11:30am - 1:30 pm: Case Histories of Multi-pathway Modeling Efforts

12-1: Lunch Break

Framing the discussion issues in this segment:

1. *What recent studies were performed by EPA Headquarters, Regional Offices, and State and local agencies. What are the lessons learned?*
2. *What role did indirect exposure assessments have in the evaluation of hazardous waste incineration and other site-specific assessments in recent years? What are the lessons learned from the WTI incinerator assessment in Region V?*
3. *Examples of visualization techniques to best convey results?*

Speakers:

11:30-12:00 *The Mercury study; an Integrated Risk assessment. Martha Keating, 30 minutes*

1:00-1:30 *The Screening Risk Assessment Evaluation for the Proposed Incineration Project at the Anniston Army Depot Chemical Demilitarization Facility. Leigh Bacon, 30 minutes*

1:30 pm-3:30 pm: Education and Outreach

Framing the discussion issues in this segment:

1. *Availability of EPA training and resource materials, where do I go for more information?*
2. *What are the reference links for information and training?*
3. *Other sources of training?*
4. *Communication/Outreach Tools (e.g. INTERNET, etc.); etc.*
5. *Training Needs in Air Toxics*

Speakers:

1:35-2:25 *Training Opportunities in Air Toxics for You through the Education and Outreach Group. Howard Wright, 50 minutes*

2:25-2:35 *The Unified Air Toxics Web Site. Nancy Pate, 10 minutes*

Panel Discussion: (45 minutes) *2:35-3:20*

Chair: *Brian Haugstad (Iowa)*

Panel Members: *Ellen Morris (Connecticut)*
Samuel Bell (Jefferson County)
Leigh Bacon (Alabama)
Jimmy Johnston (Georgia)

3:20 pm: Summary, next steps

3:30 pm: Workshop Adjournment

Appendix C

Attendance List

NATIONAL SPECIALTY WORKSHOP ON TECHNICAL TOOLS FOR
AIR TOXICS ASSESSMENT

June 17-20, 1997

Name	Agency	Phone	Fax	Email	Panel Number
Angela Andrews	US EPA	919-541-4565			
Dennis Atkinson	US EPA	919-541-0518			
Leigh Bacon	AL DEM	334-271-7861	334-279-3044	lbb@adem.state.al.us	Six
Mary Ann Barckoff	Lockheed Martin				
Mohamed N. Basher	Allegheny County	412-578-8112	412-578-8144	dns@city-net.com	Three
Samuel L. Bell	Jefferson County	205-930-1366	205-939-3019	jcdh@bham.mindspring.com	Four, Six
Neil Berg	US EPA	919-541-5520			
Craig Bressan	LRAPA	541-726-2514	541-726-1205	lrapa@worldnet.att.net	Three
Steve Bromberg	US EPA	919-541-1000			
Charles Buckler	NC DAQ				
Paul Cocca	EPA/OW/OST/SASD	202-260-8614	202-260-9830	cocca.paul@epamail.epa.gov	Three
Richard Cook	EPA OMS	313-741-7827	313-741-7439	cook.rich@epamail.epa.gov	Three
Dave-Paul Dayton	ERG	919-461-1214	919-461-1579	ddayton@erg.com	
Jennifer DeMay	Washington	360-407-6825	360-407-6802	jdem461@ecy.wa.gov	Three
Mark Derf	IN DEM	317-232-8449	317-233-5967	aynos@opn.dem.state.in.us	
Jim Dicke	OAQPS	919-541-0083			
Dennis Doll	US EPA	919-541-5693			

Name	Agency	Phone	Fax	Email	Panel Number
Alan Dresser	NJ DEP	609-633-2675	609-292-7793	adresser@dep.state.nj	Four
Laurel Driver	US EPA	919-541-2859			
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Steven Ehlers	US EPA	214-665-8312	214-665-6762	ehlers.steven@epamail.epa.gov	
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Appendix D

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The Role Of Technical Tools In The Air Toxics Program

National Specialty Workshop on Technical Tools for Air Toxics Assessment

William F. Hunt

June 17, 1997

PURPOSE

- Technical Tools are Designed to Provide the Infrastructure of the Air Toxics Program
- Today, I Will Discuss Our Infrastructure Development Activities, Where We Are Strong, Weak, & Challenges Ahead
- I Will Give You Examples Of Some Success Stories

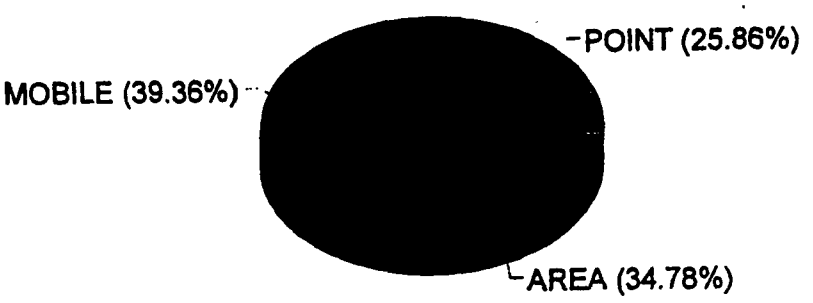
Issues With Air Toxics Infrastructure Development

- No Clear Mandate In CAA For Infrastructure Development
- However, As You Know, This Is Needed To Carry-On Several Mandated Programs: Title V, Urban Air Toxics, Residual Risk, Etc.
- Funding is Limited: We need Consensus and Priorities On Needs
- This Workshop, I Hope Begins Building A Dialogue On All Three Aspects

Emission Inventories & Factors

- National, State & Local Air Toxics Inventories & Emissions Factors Are Being Developed to Meet Various Section 112 Requirements
- Data Gaps Can Not Be Filled Without State & Local Agency Assistance

Total National 188 HAP Emissions (tpy)
by Source Type



Dispersion Modeling

- Some Of The Available Dispersion Modeling Tools Are Still Applicable
- However, New Issues Related To Dense Gases, Particle & Gas Deposition, Atmospheric Chemical Transformations Of Toxic Pollutants Pose New Challenges

Air Monitoring

- Lack Of Technology For Monitoring All Toxic Pollutants
- Inability To Develop QA Procedures
- Expense For Monitoring All Pollutants In All Parts Of The Country
- Consider Requiring State Air Toxics Monitoring Data being Reported to AIRS
- PAMS:
  - Site #2 Is Ideal Platform For Extended Toxic Monitoring

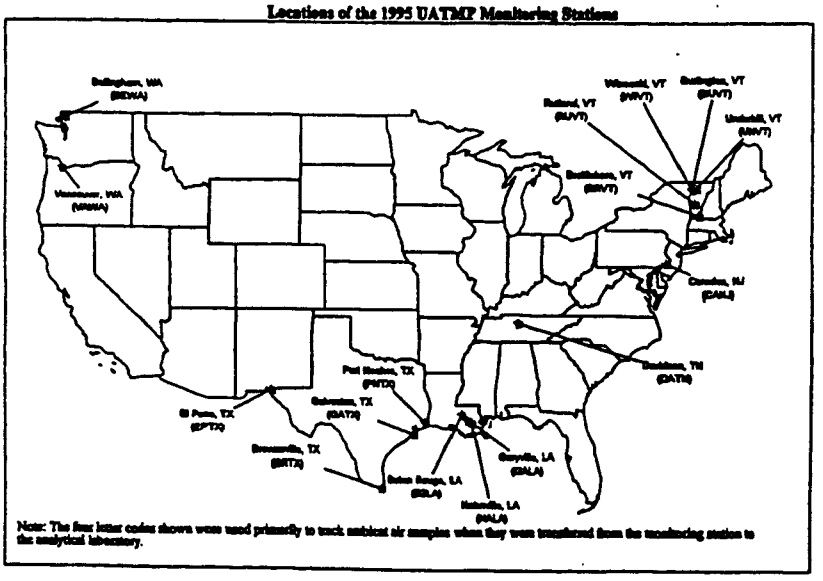
Interpreting Ambient Air Monitoring Data

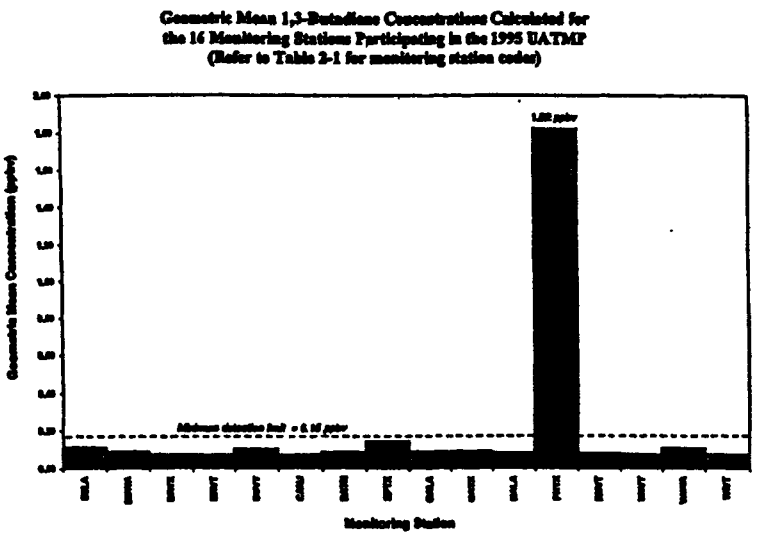
- *An Example from the Urban Air Toxics Program*

- Examples of Data Resources
  - Emission Inventories
  - Fate and transport
  - Historical monitoring data
  - New/current air monitoring results

Example of Spatial Variations 1,3-butadiene

- What can the National UATMP program results say about this compound in urban environments
  - 16 monitoring stations in 1995 UATMP program

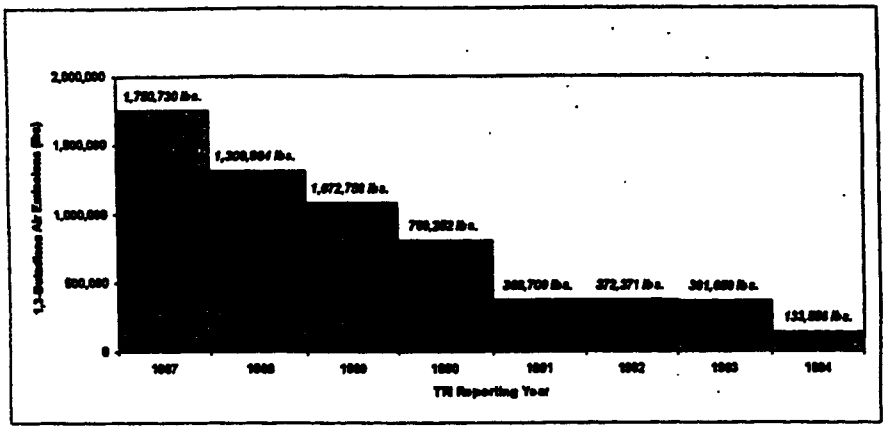




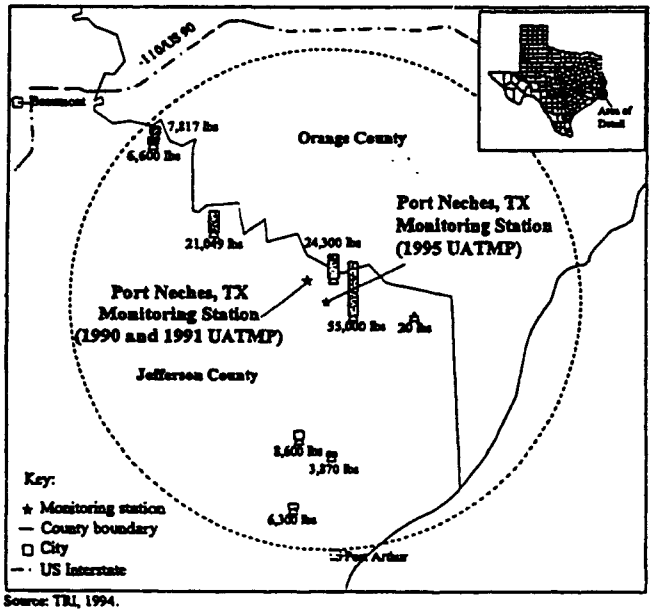
Port Neches, Texas -Example

- ATSDR data indicate Texas and Louisiana as the lead manufacturing states for 1-3 butadiene
- TRI data show nine (9) industrial sources of 1-3 butadiene within 10 miles of the Port Neches, Texas UATMP Site
- TRI data show decreasing trend in emissions data from 1990 to 1995

Total 1,3-Butadiene Air Emissions Reported by Facilities Located within a 10-Mile Radius of the Port Neches Monitoring Station to TRI



Air Emissions of 1,3-Butadiene within a 10-Mile Radius of the Port Neches, Texas (PNTX) Monitoring Station (Emissions Data from TRI Reporting Year 1994)



Source: TRI, 1994.

Port Neches, Texas -Example

- Site Location is critical
  - 1990 and 1991 PNTX data showed
    - much less 1-3 butadiene than 1995 data
  - Why?
    - difference in locations of the PNTX monitoring stations - a major factor

Table 5-1
Geometric Mean 1,3-Butadiene Concentrations Measured at Port Neches, Texas

UATMP Program Year	Geometric Mean 1,3-Butadiene Concentration (ppbv)	Number of Valid Samples Collected
1990	0.39	29
1991	1.11	30
1995	1.82	31

Note: As shown in Figure 5-2, the 1995 UATMP monitoring station in PNTX was at a different location than the 1990 and 1991 UATMP monitoring station.

Air Toxics Indicators & Trends

- Goals:
  - Synthesize Data Collected from Disparate Programs
  - Show National Trends & Patterns
- Challenges:
  - Limited Data Bases
  - No Consensus on Calculating Relative Risk
- Ongoing Work:
  - Government Performance & Results Act--Pilot
  - Developing a Strategy to Measure Progress Towards Reduced Health Risks Resulting from Programs (e.g., MACT)
  - Received Funds to Explore Indicators

Education & Outreach

- Expand Opportunities for Education & Outreach
- Develop Additional Training on Technical Tools for Monitoring, Emissions Inventory, Modeling and Exposure Assessment
- Prepare Training Materials
- Utilize Multi-Media Training Vehicles Such as APDLN Telecourses, Internet, CD-ROM, Classroom Lectures
- Workshops that Bring Multi Disciplines Together to Foster Communication & Information Exchange
- Establish a List of Area Experts to Foster Quicker Communications and Solutions.

Exposure Assessment

- Continue Developing Guidance & Tools to Evaluate Multi-Pathway Human Exposures for Multi-Pollutants
  - Must Expand Scientific Capabilities to Measure Multi-Media Environmental & Human Exposures & Biological Markers of Exposure
- Need to Characterize Residential Multi-Media Exposures:
  - Quantify Contributions From Indoor & Outdoor Sources Including Source-Receptor Relationships
  - Understand Relationship Between Exposure, Dose & Effect

Accomplishments:

- Expanding National Air Toxics Emissions Inventory Data Base
- User Friendly Air Dispersion Models Capable Of Addressing New Concerns
- Several Years Of PAMS Monitoring Data; Easier Ways To Collect Data
- Developing Useful Air Quality Indicators
- Developing Strategy to Measure Effectiveness of Air Toxics Program
- Continuing Research on Exposure Assessment Methodologies
- Expanding Education and Outreach Opportunities

Challenges Ahead

- Declining Budget and Increasing Demand for Infrastructure Development
- Effective Partnership With States, Local Agencies & Other Stakeholders To Improve All Aspects Of Our Work
- Improved Methods For Technology Transfer Through The Evolving Medium Of The Internet

CLEAN AIR ACT
Air Toxics Provisions

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EPA STAPPA/ALAPCO

OUTLINE

- History
- Statutory Provisions
- Basic Requirements
- MACT

History

1970 SECTION 112 PROVISIONS

- Directed EPA to identify air pollutants with hazardous effects and establish standards to prevent any adverse effects "with an ample margin of safety."
- In the first two decades under NESHAPS, EPA set standards for only eight pollutants (most recently benzene in 1989):

Arsenic	Beryllium	Radon
Asbestos	Mercury	Vinyl chloride
Benzene	Radionuclides	

History

EPA's SOLUTION

- For HAPs that are carcinogenic, EPA deemed that there was no safe level of exposure, so to establish standards with "ample margin of safety" was impossible.
- Risk assessment was not formalized in the 1970s, and when standard procedures became available in the 1980s the data contained significant uncertainty.
- EPA began risk assessment studies which take years to complete.

History

THE VINYL CHLORIDE CASE

- EPA and EDF mutually agreed upon a schedule to develop a zero-risk goal in 1977
- EPA took no action for 8 years
- EPA withdrew rule in 1985 citing:
  - High costs for additional VC control
  - No technology could reach zero emissions

History

THE VINYL CHLORIDE CASE (cont'd)

- NRDC sued EPA in 1985
- Court rejected NRDC's position in 1988
- Remanded back to EPA for:
  - Giving too much attention to control technology
  - Not providing an ample margin of safety
  - EPA must:
    1. Determine safe levels without technological or costs concerns
    2. Determine an ample margin of safety (more stringent, but could consider costs)

Statutory Provisions

TITLE III HAZARDOUS AIR POLLUTANTS [CAA Amendments of 1990]

Sec. 301	Hazardous Air Pollutants (Section 112)
Sec. 302	Conforming Amendment (Bookkeeping)
Sec. 303	Risk Assessment and Management Commission
Sec. 304	Chemical Process Safety Management
Sec 305	Solid Waste Combustion (Section 129)
Sec. 306	Ash Management and Disposal

Statutory Provisions

SECTION 112

Sec. 112(a) Definitions
Sec. 112(b) List of Pollutants
Sec. 112(c) List of Source Categories
Sec. 112(d) Emission Standards
Sec. 112(e) Schedule for Standards and Review
Sec. 112(f) Standard to Protect Health and the Environment
Sec. 112(g) Modifications
Sec. 112(h) Work Practice Standards and Other Requirements
Sec. 112(i) Schedule for Compliance
Sec. 112(j) Equivalent Emission Limitation by Permit

Statutory Provisions

SECTION 112 (cont'd)

Sec. 112(k) Area Source Program
Sec. 112(l) State Programs
Sec. 112(m) Atmospheric Deposition to Great Lakes and Coastal Waters
Sec. 112(n) Other Provisions
Sec. 112(o) National Academy of Sciences Study
Sec. 112(p) Mickey Leland Urban Air Toxics Research Center
Sec. 112(q) Savings Provision
Sec. 112(r) Prevention of Accidental Releases
Sec. 112(s) Periodic Report

Basic Requirements

AIR TOXICS PROVISIONS

- Statutory list of 189 HAPs - EPA can delete or add to
- List of categories of industrial facilities emitting substantial quantities of HAPs
- Establish MACT for each category
- Expected 75-90% reduction below existing emission levels
- All standards must be promulgated by Nov. 15, 2000

Basic Requirements

189 HAPs

- List found in Section 112(b)(1)
- Has been corrected since initial publication
- List can be revised through Administrator review, per Section 112(b)(2) (*e.g.*, caprolactum)
- Any person may petition the Administrator to modify the list, per Section 112(b)(3)

Basic Requirements

SECTION 112 SOURCE CATEGORY LIST

- Section 112(c) required list of categories emitting one or more HAP
- EPA published initial list July 16, 1992
  - 166 categories of major sources
  - 8 categories of area sources
- List can be revised per Section 112(c) procedures (*e.g.*, deletion of asbestos processing)
- Urban air toxics study may add more area sources to list

Basic Requirements

MACT

- National Standards
- Case-by-Case Determinations
- Implementation/Delegation

Basic Requirements

RESIDUAL RISK

- Within 8 to 9 years of a MACT standard, residual risks must be assessed and EPA must determine whether more stringent standards are required to provide an "ample margin of safety."
- EPA must consider standards for any carcinogen with $>10^{-4}$ cancer risk

Basic Requirements

ACCIDENTAL RELEASES

- For 100 extremely hazardous air pollutants, facilities must develop a risk management plan to address how to deal with any possible hazards.

Basic Requirements

STUDIES

- Great Waters Study
- Urban Air Toxics Study & Strategy
- NAS Study
- Utility Air Toxics Study
- Mercury Study
- Risk Assessment Study

ALL 4-YEAR MACTs ARE DONE

Clean Air Act -- Section 112 4-Year MACT Standards

MACT Standard	# Source Category	Subpart	Proposal FR Publication & Citation	Promulgation FR Publication & Citation	Initial Compliance Date
Aerospace Industry	1	GG	[illegible]	[illegible]	[illegible]
Asbestos (delisting)	1	–	–	[illegible]	[illegible]
Chromium Electroplating*	6	N	[illegible]	[illegible]	[illegible]
Coke Ovens	1	L	[illegible]	[illegible]	[illegible]
Commercial Sterilizers*	1	O	[illegible]	[illegible]	[illegible]
Ethylene Oxide Chambers*	1	T	[illegible]	[illegible]	[illegible]

ALL 4-YEAR MACTs ARE DONE

Clean Air Act -- Section 112 4-Year MACT Standards

MACT Standard	# Source Category	Subpart	Proposal FR Publication & Citation	Promulgation FR Publication & Citation	Initial Compliance Date
Industrial Cooling Towers	1	Q	[illegible]	[illegible]	[illegible]
Magnetic Tape	1	EE	[illegible]	[illegible]	[illegible]
Marine Vessels	1	Y	[illegible]	[illegible]	[illegible]
Oil-to-Water Treatment	1	DD	[illegible]	[illegible]	[illegible]
Petroleum Refineries	1	CC	[illegible]	[illegible]	[illegible]
Printing/Publishing	1	KK	[illegible]	[illegible]	[illegible]

ALL 4-YEAR MACTs ARE DONE

Clean Air Act -- Section 112 4-Year MACT Standards

MACT Standard	# Source Category	Subpart	Proposal FR Publication & Citation	Promulgation FR Publication & Citation	Initial Compliance Date
Polymers & Resins I Butyl Rubber Epichlorohydrin Elastomers Hypalon (TM) Production Neoprene Production Nitrile Butadiene Rubber Polybutadiene Rubber Polysulfide Rubber Styrene-Butadiene Rubber & Latex	9	U	[illegible]	[illegible]	[illegible]

ALL 4-YEAR MACTs ARE DONE

Clean Air Act -- Section 112 4-Year MACT Standards

MACT Standard	# Source Category	Subpart	Proposal FR Publication & Citation	Promulgation FR Publication & Citation	Initial Compliance Date
Polymers & Resins II Acetal Resin Production Non-Nylon Polyamides Production	3	W	[illegible]	[illegible]	[illegible]

ALL 4-YEAR MACTs ARE DONE

Clean Air Act -- Section 112 4-Year MACT Standards

MACT Standard	# Source Category	Subparts	Proposal FR Publication & Citation	Promulgation FR Publication & Citation	Initial Compliance Date
Polymers & Resins IV -Acrylonitrile-Butadiene-Styrene -Methyl Methacrylate-Acrylonitrile/ Methyl Methacrylate-Butadiene- -Polystyrene Styrene Acrylonitrile Polyethylene Terephthalate	4	JJJ	[illegible]	[illegible]	[illegible]

ALL 4-YEAR MACTs ARE DONE

Clean Air Act -- Section 112 4-Year MACT Standards

MACT Standard	# Source Category	Subparts	Proposal FR Publication & Citation	Promulgation FR Publication & Citation	Initial Compliance Date
Secondary Lead Smelters	1	X	[illegible]	[illegible]	[illegible]
Stationary MACT	1	II	[illegible]	[illegible]	[illegible]
Stage I Gasoline Marketing	1	R	[illegible]	[illegible]	[illegible]
Wood Furniture	1	JJ	[illegible]	[illegible]	[illegible]

[illegible]

MACT

MACT PROGRAM - What Does The Future Hold?

- Budget reductions in 1993, 1994, 1995 and 1996
- Work slowed on most NESHAP due in 1997
- Need to address potential "Permit Hammers"
- Potential budget stability in 1997 and 1998

MACT

MACT PARTNERSHIP - The Basic Approach

- UPFRONT planning and working with all parties
- LEVERAGE resources / experiences / skills / knowledge
  - State and Local Regulators/Permit Specialist
  - Industry and Environmentalists
- CONSENSUS-based standards development

MACT

MAXIMUM ACHIEVABLE CONTROL TECHNOLOGY

- Section 112(d)
- Section 112(g)
- Section 112(j)

MACT

NATIONAL STANDARDS

- Section 112(d)
  - For new sources, best controlled similar source
  - For existing sources, the average emission limitation achieved by the best performing 12 percent (at least)
  - Additional reductions based on costs and non air quality impacts

MACT

CASE-BY-CASE MACT

- Section 112(j) - the "permit hammer" provisions
  - Occurs when MACT standard is late by 18 months after due date
  - Permit contains case-by-case MACT
- Section 112(g) - sources with increases in HAP emissions
  - Changed operations
  - Offset and de minimis allowances (not currently operational)

COMPLIANCE HAS BEGUN FOR 2-YEAR MACTs

Clean Air Act -- Section 112 2-Year MACT Standards

MACT Standard	Source Category	Subparts	Statutory Date	Proposed FR Publication & Citation	Promulgated FR Publication & Citation	Initial Compliance Date
Dry Cleaning*	5	M	[illegible]	[illegible]	[illegible]	[illegible]
Hazardous Organic NESHAP	1	F,G,H,I	[illegible]	[illegible]	[illegible]	[illegible]

Dry Cleaning
* [illegible]

SUMMARY

- Air toxics program is driven by CAA
- Many MACTs are being developed
- Traditional reg development is too expensive and permit hammers may fall
- MACT partnerships is one answer

SUMMARY OF OAQPS AIR TOXICS STRATEGY (OATS)

A MID COURSE ADJUSTMENT THAT

- Organizes the program around a management model
- Remembers - HAPs differ
- Works based on building consensus

June, 1997

WHY IS EPA DEVELOPING THIS STRATEGY?

to protect the public health and environment

- we need a comprehensive vision of how to integrate the various air toxics requirements of the CAA (fitting them with the criteria programs as best as possible)
- we need to improve regulatory and economic efficiency by matching solutions with particular air toxics problems

Summary of Draft OATS

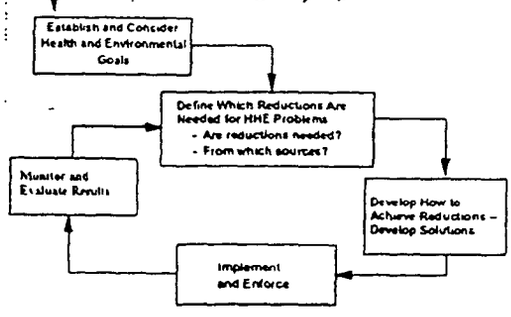
OVERVIEW OF STRATEGY

The Air Toxics Program Should ...

- Use an air management model to organize the program and its activities
- Reflect the fact that HAPs have many different kinds and degrees of effects, exposures, and sources
- Build on proactive stakeholder participation

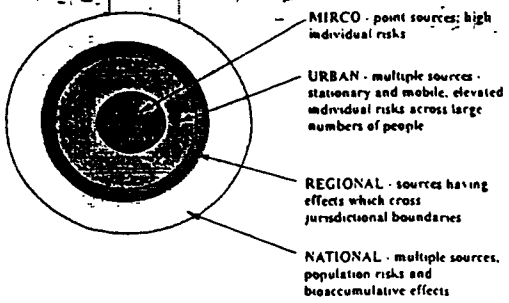
Summary of Draft OATS

A Model for the Air Toxics Program



Summary of Draft OATS

The Air Toxic Problem Varies – By Scales



Summary of Draft OATS

WHY PARTNERSHIPS?

- Uncertainty in science and information
- Need for consensus based decision making
- Availability of skills, knowledge and abilities -- plenty of leverage opportunities
- Upfront plans to address stakeholder interests

HOW DOES OATS BUILD ON CAA?

- A credible air toxics program must set goals and have a strong information base to measure progress in the overall success of the program.
- The evolving air toxics program should prioritize its efforts such that the most hazardous pollutants and problems are dealt with first and best.
- The air toxics program should continue to use the MACT approach as its cornerstone with residual risk standards used in a very focused manner. We need to reduce the need for residual risk standards

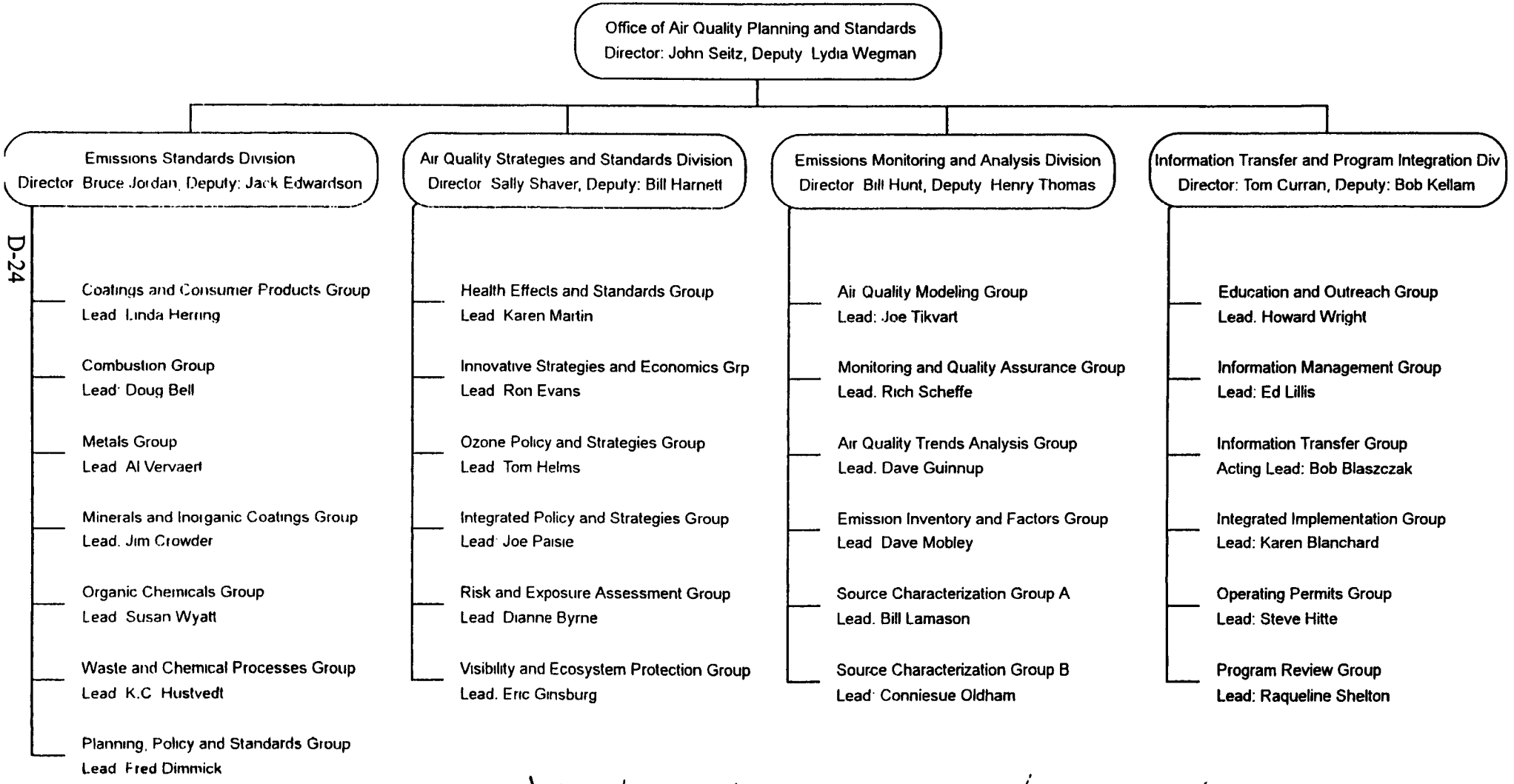
OATS' IMPACT

- OATS report is still in a draft stage
- Elements of OATS plan are in progress
  - Can we describe the problem?
  - What are the goals of the program?
  - How can progress be measured?

The Air Toxics Program in OAQPS

Who Does What From Where on Air Toxics?

The Office of Air Quality Planning and Standards



OAQPS Website: http://www.epa.gov/oar/oaqps/

ESD Establishes Air Toxics Standards

- Establishes national emissions standards and manages Federal Programs for controls of air toxics from stationary sources
- Develops new source performance standards; control techniques guidelines; standards for hazardous wastes under RCRA; and guidance for implementing standards at the State and local level
- Develops strategies and policies for regulatory programs, including co-controls for HAPs and criteria pollutants

Examples of ESD Air Toxics Projects

- Development of MACT standards
- Air Toxics long term goals and strategy
- Characterization of the Air Toxics Problem
- Innovative approaches, e.g. Generic MACT and the Consolidated Air Rule

AQSSD Assesses Air Toxics

- ✓ Develops national and geographically focused strategies and programs based on assessment of effects, exposure, risk, and economics
- ✓ Provides expertise for health and environmental effects, exposure and risk assessement
- ✓ Responsible for special studies
- ✓ Provides expertise in benefits assessment, economics and regulatory impact

Examples of AQSSD Air Toxics Projects

- Mercury, Great Waters and Utility studies
- Urban Area Source Program and strategy development
- Risk Identification Project and development of Residual Risk program
- Toxics Contingent Valuation Project

EMAD Measures and Estimates

- Develops and assists in using air models, as well as emission factors and inventories
- Develops methods and assists in measurement of ambient air, as well as source emissions
- Analyzes air quality data and documents progress
- Source of technical expertise on measurement and estimation methods

Examples of EMAD Air Toxics Projects

- National Toxics Inventory
- Ambient Air Quality Data Catalogue and Analysis
- Urban Air Toxics Monitoring Program
- Workshop on Technical Tools for Air Toxics

ITPID 's Stock in Trade is Information

- Manages and transfers air pollution, and pollution control, information
- Manages information transfer systems
- Develops and delivers training courses and educational materials on technical and management aspects of air pollution control
- Manages the integration of air toxics programs under section 112 with operating permits programs

Examples of ITPID Air Toxics Projects

- MACT implementation strategy development
- Air Toxics Health Effects Summary
- Annual Air Toxics Implementation Working Meeting and Air Toxics Workshop
- Air Toxics informational video

Should Offsite Consequence Analysis of Accidental Releases Be Incorporated Into A Permitting Program?

Florida Department of Environmental Protection

And, If So . . . How?

- To meet specific criteria (in the sense of a standard) and used to decide permit issuance
- As a weighted element of the decision to issue a permit, but not have to meet specific criteria

Florida Department of Environmental Protection

And, If So . . . How? (cont.)

- Used to force control or work practice requirements, the degree to which is based on the severity of the OCA results
- Used for emergency planning or public information only
- Not required as part of a permit application

Florida Department of Environmental Protection

What Are You Trying To Accomplish?

- Complete protection of the general public from any kind of accident
- Complete protection of the general public from most accidents (risk levels)
- Better protection of the general public from any kind of accident

Florida Department of Environmental Protection

What Are Trying To Accomplish? (cont.)

- Reduction of risk through facility design and work practices
- Reduction of risk through facility location and waste minimization
- Better contingency and emergency planning
- Public right to know (information)

Florida Department of Environmental Protection

Analysis Tools Are Important

- What are the capabilities of the tools available to support what you are trying to accomplish?
- How good do the tools have to be to be usuable in a permitting program?

Florida Department of Environmental Protection

Public Health Criteria Data Is Important

- Is the quality of the health and risk information sufficient to support what you are trying to accomplish?
- How do we reconcile the different uncertainties among the tools and the public health data used in an OCA?

Florida Department of Environmental Protection

Regulatory (Political) Questions?

- Should we be "permitting" accidents?
- What is not being done through 112(r), MACT, NESHAPS, or other programs that we believe need to be accomplished in a permit program OCA requirement?
- Who is not covered by an existing program, but should be?

Florida Department of Environmental Protection

What Should We Expect From the Tools?

- Consistent with chemical and physical laws and principles.
- Parameterizations of physical and chemical effects should be based on validated data sets and be peer-reviewed.
- The air dispersion algorithms should be consistent with those used in the Guideline for Air Quality Models.

Florida Department of Environmental Protection

What Should We Expect From the Tools? (cont.)

- Data input used in the models should be reasonably available.
- Output data should correspond to the form of the endpoint criteria being evaluated.

Florida Department of Environmental Protection

Weaknesses of Current Tools

- Emissions characterization and quantification.
- Chemical and physical transformations.
- Multiple compounds analysis.
- Time dependent changes.
- Less than lifetime exposure

Florida Department of Environmental Protection

Workshop Expectations

- The knowledge of a suite of models that cover the range of sources and scenarios that toxics modeling may be performed for.
- A better understanding of the tools (models) that are available and what they can and cannot do. What situations and substances are each applicable?

Florida Department of Environmental Protection

Workshop Expectations

- The knowledge of whether some models. are considered "better" than others, based on evaluation studies or physics, that essentially address the same sorts of sources.
- Better knowledge of what is the best technique at this time for completing risk assessment analysis?

Florida Department of Environmental Protection

Workshop Expectations

- The development of a complete chemical database that contains all of the chemical and physical characteristics that are used in any of the tools. This includes a units conversion program since every model uses different units.

Florida Department of Environmental Protection

U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF ENFORCEMENT AND COMPLIANCE ASSURANCE
OFFICE OF COMPLIANCE

LIST OF COMPLIANCE ASSISTANCE TOOLS DEVELOPED AND UNDER DEVELOPMENT

SECTOR FACILITY- INDEXING PROJECT

- The Manufacturing Branch initiated the Sector Facility Indexing Project. This Project is a pilot data integration effort that synthesizes environmental records from several data sources into a system that allows facility-level and sector analysis. The Project focuses on five major industries: petroleum refining, iron and steel, primary non-ferrous metals, pulp mills, and automobile assembly. Using national databases, the Project provides the following information for each of the 699 facilities within the five industry categories: name, location, permits held under major statutory programs, compliance history, self-reported pollutant releases under TRI, the relative toxicity of chemicals released, toxicity-weighted pollutant releases, a description of the population surrounding the facility, and the actual production or production capacity. Contact: Mike Barrett 202-564-7019 or Maria Eisemann at 202-564-7016.

SECTOR NOTEBOOKS

- In October 1995, the Office of Compliance published 18 Sector Notebooks. Each notebook contains: a national industry summary, description of the industrial process, a waste release profile, pollution prevention opportunities, a summary of statutes and regulations, a compliance and enforcement profile, a list of compliance activities , and a directory of contacts. During the first year of availability, approximately 45,000 copies were distributed. More than 25,000 copies were requested and distributed by OC to other Federal, state and local government offices; more than 14,000 copies were downloaded from EPA's Internet site, Enviroene; more than 5,000 copies were sold by the Government Printing Office to requestors in the private sector; and over 100 countries requested and received full sets of 18 notebooks. Contact: Seth Heminway 564-7017.

- Based upon the success of this project, OC is developing eight new notebooks for release in FY 1997. They address the following industry sectors: power generation, federal facilities, transportation, plastics and synthetic resins, pharmaceuticals, textiles, shipbuilding and foundries.

DRY CLEANING

Tools Currently Available:

1. ***Plain English Guide for Perc Dry Cleaners: A Step by Step Approach to Understanding Federal Environmental Regulations***--This document assists owners and operators of dry cleaning shops in understanding and complying with federal air, hazardous waste, and wastewater regulations. The Korean and the Spanish versions of the Plain English Guide will be available in February 1997. Contact Joyce Chandler 564-7073.

2. ***Multimedia Inspection Guidance*** - This document assists field personnel in State, local, and EPA Regional offices to conduct multimedia inspections and compliance assessments of dry cleaners. A multi-media inspection checklist is included in the Guidance for on-site visits. Contact Joyce Chandler 564-7073.

3. ***Compliance Strategy*** - The Strategy assists State, local, and EPA Regional officials by providing multimedia information on the requirements applicable to the dry cleaning industry. It contains a comprehensive list of EPA products relating to dry cleaners. In addition, it discusses techniques and agency policies designed to promote compliance assistance. Contact Joyce Chandler 564-7073.

4. ***Compendium of Education Materials*** - This is a searchable database of existing educational environmental materials and activities for dry cleaners. It may be used by Regions, States and other entities providing compliance assistance, as well as by members of the dry cleaning community. Contact Joyce Chandler 564-7073.

5. ***Generic Dry Cleaning Equipment Owner's Manual*** - Proper maintenance and operation of equipment can be one of the first and easiest steps to help achieve compliance and undertake pollution prevention. The Office of Air and Radiation developed this manual for dry cleaners with older machines who could not obtain the manufacturer's instructions for their specific equipment. Contact George Smith at 919-541-1549

6. ***Profile for the Dry Cleaning Industry*** - This sector notebook provides information of general interest regarding environmental issues associated with the dry cleaning industrial sector. To order call US Government Information at 202-512-1800. Order number 055-000-00512-5.

7. ***NESHAP Regulation Translations*** - Since a significant percentage of the dry cleaning community does not speak English as its first language, the NESHAP for Perc Dry Cleaners was translated into Korean, French, Chinese, Vietnamese and Spanish. Contact Joyce Chandler 564-7073.

Tools/Activities Under Development:

1. ***Virginia Partnering Project*:** This project is a partnership between the State and the drycleaning industry in Virginia. The project will prepare and provide documentation to improve compliance in the state and undertake pilot projects to determine most effective methods to improve compliance for drycleaners. The project will also provide support during implementation of new regulatory requirements. Contact: Joyce Chandler 564-7073.

PRINTING

Tools Currently Available:

1. ***Printers National Environmental Assistance Center***. This Center is a partnership between industry and state environmental experts to create an environmental assistance center for the printing industry, which comprehensively addresses the environmental compliance needs of small printers, plus provides information on how to achieve compliance by reducing waste and emissions. The intent of this telecommunications-based Center is to work in collaboration with printing trade associations and other printing industry experts, regulators and technical assistance providers to develop and deliver environmental resources for printers. The Center can be found at Internet: http://www.hazard.uiuc.edu/pneac/pneac.html.

2. ***Multimedia Compliance/Pollution Prevention Assessment Guidance for Lithographic Printing Facilities.*** This guidance helps Regions and States determine the compliance status of printing facilities and identify ways to bring them into compliance and go beyond compliance. This document highlights opportunities to implement pollution prevention and innovation technology. Furthermore, the document can be provided to the printing community for conducting self-assessments/self-audits and can be valuable in assisting printers to develop methods to incorporate pollution prevention into their everyday practices. The guidance was pilot tested at several printing facilities in the State of Washington. This product supports the Division's work in the printing sector, and it also accomplishes several items that are important to OC. First, it provides a *sector based* assessment guidance in a *multimedia* format. Second, it assists both regulatory agencies and individual printers audit printing operations; and third, it provides pollution prevention information to printers. Contact: Doug Jamieson 202-564-7041

Tools/Activities Under Development:

1. ***Partnering Project with Maryland.*** To partner with State and printing industry in Maryland. Prepare and provide documentation and pilot projects to improve compliance with printers. To pilot the use of customer demands as an incentive for printers to come into compliance and adopt pollution prevention methods.

INDUSTRIAL ORGANIC CHEMICAL MANUFACTURING

Tools Currently Available:

1. ***Joint EPA/CMA/SOCMA/API Subpart CC Rule Compliance Assistance Tool*:** The compliance assistance tools being developed in partnership with industry are a compliance assistance manual, training module and self-audit checklist for use by the regulated community and inspectors. The Subpart CC Rule requires control of organic emissions from tanks, containers, impoundments and miscellaneous units. Contact Walt Derieux 564-7067.

2. ***Process-Based Self-Assessment Tool for the Organic Chemical Industry*:** This tool has been developed primarily for small to medium-sized facilities in the organic chemical manufacturing industry. It will be an effective tool for environmental control officers, managers, and other facilities personnel in developing and implementing a strategy to identify and track waste streams associated with a particular, or group of, units, production operations and the associated waste stream treatment or disposal operation that may impact facilities' environmental compliance. Contact Jeff KenKnight 564-7044

3. ***Chemical Industry Baseline Report* (1990-1994):** The purpose of the baseline report is to provide a general profile of the chemical industry and to present a 5-year base period reference point of its compliance history. The report presents an overview of compliance trends and status by analyzing enforcement-related data for industries that are classified under the 2800 series of the SIC system. Contact Walt Derieux 564-7067

4. ***EPA/CMA Root Cause Analysis***: A joint EPA/CMA project, to understand underlying factors that contributed to noncompliance and to find assistance tools, regulatory reform and management recommendations to promote and improve compliance. Contact Sally Sasnett 564-7074.

5. ***Chemical Compliance Assistance Center***: The center, in part, will support the states and local agencies by providing one-stop location for accessing federal regulatory, compliance and technical assistance information. Contact: Emily Chow 202-563-7071.

6. ***CCSMD EnviroSenSe Homepage***: A free public integrated environmental information system to provide information on pollution prevention, innovative technology and compliance assistance. Internet address http://es.inel.gov/oeca/ccsmd.html

7. ***Sector Notebook "Profile of the Organic Chemical Industry"***: EPA published in September 1995 a sector notebook (EPA/310-R-95-012) on the organic chemical industry that included general industry information (economic and geographic), a description of industrial processes, pollution outputs, pollution prevention opportunities, Federal statutory and regulatory framework, compliance history and a description of partnerships that have been formed between regulatory

agencies, the regulated community and the public. Order from US Government Information 202-512-1800 Order #055-000-00515-0.

8. ***Hazardous Organic NESHAP Compliance Assistance Tool:*** This tool will address the hazardous organic NESHAP (HON) rule. This rule under 40 CFR part 63 sets the Maximum Achievable Control Technology standards applicable to the portion of the organic chemical industry that is the synthetic organic chemical manufacturing industry. Contact Marcia Mia 564-7042.

Tools Under Development:

1. ***Corporate Executive Guide to Facility Environmental Management.*** Designed for small business owners, this document will help in planning for a comprehensive management program. Contact Rich Satterfield 564-2456.

2. ***Catalogue of Industry Environmental Compliance/Management Documents***: A joint compendium of compliance, technical and other resources. Contact Rich Satterfield 564-2456.

3. ***Protocol for Conducting Environmental Audits***: A guide for small and medium sized business on how to conduct compliance and management audits. Contact Rich Satterfield 564-2456.

4. ***Chemical Industry State Root Cause Analysis.*** To understand underlying factors that contributed to noncompliance in state enforcement actions and to find assistance tools, regulatory reform and management recommendations to promote and improve compliance. Contact Reggie Cheatham 564-2425.

FOOD AND KINDRED PRODUCTS

Tools Under Development:

1. ***Compliance Guidance.*** This project will develop a multi-media compliance guidance for small businesses in the food and kindred products fields. Contact: Becky Barclay at (202) 564-7063 or barclay.rebecca@epamail.epa.gov.

AGRICULTURAL PRACTICES

Tools Currently Available:

1. The Agriculture Compliance Assistance Center is operational and providing outreach, fact sheets, compliance assistance and liaison activities to the agricultural community on sector requirements An Internet-available home page is currently on line. The Agriculture Compliance

Assistance Center relies heavily on existing providers of agricultural information. Internet address: es.inel.gov/oeca/ag/aghmpg. html.

2. ***The Agricultural Issues Forum Conference Call*** is held monthly by the Ag Center. Each call provides a link between Regions to discuss agriculture sector compliance/enforcement issues and to communicate what is going on in the Regions.

3. ***"Major Existing Laws and Programs that Could Affect Producers of Agricultural Commodities"*** was issued in September of 1996 by the Ag Branch. It is being made available on the Internet. This document provides a succinct, general description of EPA's requirements that may impact farms and is intended as a guide to EPA's requirements. The Internet version will be cross linked to specific information on requirements. Internet address: es.inel.gov/oeca/ag/aghmpg. html

4. ***A CAFO compliance/enforcement strategy*** is currently under development and a draft is expected to be available in the Spring of 1997. This strategy will provide guidance on performance expectations (see the CAFO MOA guidance.) OECA will sponsor a national meeting for CAFO compliance. Contact: Al Havinga 202-564-4147.

5. ***The Agriculture and Ecosystems Division has entered into an Interagency Agreement (IAG) with USDA-Cooperative State Research, Education, and Extension Service.*** The activities being funded in FY 97 under the Interagency Agreement will further the development and dissemination of compliance assistance information to the agricultural community, which can serve as national models. The following grants have been selected:

> **Delaware**--This project will develop a plain-language guide book that describes EPA regulations which impact agriculture.
>
> **Cornell**--This project will identify agricultural water quality impacts in a watershed; assess local perceptions of regulatory criteria; and develop outreach materials on compliance. The project will be utilized as a national model for community based ag/urban interface issues. The watershed selected will include operations subject to NPDES permit requirements for Concentrated Animal Feeding Operations (CAFOs).
>
> **Kentucky**--This project will assess the educational needs of small and minority farmers regarding EPA issues and regulations. A small and minority farmer's handbook and one-on-one Extension educational programs will be developed.
>
> **Missouri**--This project will address air quality requirements affecting farmers and agribusiness. The project will develop a broad-based educational program on air quality issues such as the storage and handling of grain, fugitive emissions, volatilization, burning, and air-stream opacity. Information relating to uncontrolled air quality at animal

operations and safety issues associated with air quality at agricultural operations will also be covered. Contact: Ginah Mortensen: 913-551-7864.

Tools Under Development:

1. CAFO Inspector Guidance/Self-Auditing Handbook: Guidance on identifying the need for permit, compliance with permit, compliance with "no-discharge program," and implementation of best management practices. Usable by farmers. Contact: Al Havinga 202-564-4147.

AUTO SERVICE AND REPAIR

Tools Currently Available:

1. The Automotive Compliance Assistance Center - GreenLink. Contact Everett Bishop (202) 564-7032. Managed by the Coordinating Committee for Automotive Repair (CCAR) a consortium of 40+ automotive affiliates representing a wide range of interests within the auto service industry. Greenlink provides a toll-free phone number with fax-back capability, a private voice box for the user to leave an anonymous question which in turn will provide a private answer to the caller within four days, or human interaction with a CCAR representative. For those users with Internet capability, GreenLink has a web site, Internet capability, Greenlink has a web site, Internet address, http://www.ccar-greenlink.org. Their phone number is 1-888-GRN-LINK . Both of these systems provide a repository of compliance requirements, information and assistance providers available to automotive shop owners and technicians.

Tools Available This Year:

1. Consolidated Environmental Screening Checklist w/Support Documentation. Contact: Julie Tankersley (202) 564-7002. A one page screening checklist with the major environmental regulatory requirements associated with this industry. A support booklet will be available with the checklist to assist users in "how to use" the checklist and including more information for each requirement, and where to seek further assistance.

2. Educational Modules for Shop Owners and Technicians. Contact: Everett Bishop (202) 564-7032. A series of environmental educational modules which identifies the major activities associated with auto repair and service. The modules will discuss the historical nature of the regulation, the regulation and all that is involved with it, health and safety issues associated with the activity, pollution prevention opportunities and how to get more information if the user has more detailed questions.

ELECTRONICS AND COMPUTERS

Tools Currently Available:

1. Printed Wiring Board Compliance Assistance Center. OC in with partners to be determined will be opening a compliance assistance center for Printed Wiring Board Manufacturers that will serve as a "one-stop" source of information for federal regulations and pollution prevention practices. The Center will include a "walk through a plant" feature in which users can click on parts of the manufacturing process and find out the applicable regulatory requirements and potential pollution prevention and control means for compliance. Contact: Keith Brown 202-564-7124.

2. Electronic Database. Developed an electronic database of almost 1,000 Federal and State of Texas environmental recordkeeping and reporting requirements that may apply to manufacturers in the computer and electronics industry. These basic requirements were further refined to include information at the data element level, and the database includes over 8,000 reported data elements. This project will be expanded to enable businesses to query the database and determine their regulatory responsibilities. Contact: Keith Brown 202-564-7124.

WOOD PRESERVING

Tools Currently Available:

1. Wood Preserving RCRA Compliance Guide. This guide was designed to provide both industry and inspectors with a "plain English" summary of the applicable statutory and regulatory requirements, general information on the industry and the processes used, and the geographic distribution of the industry. Contact: Seth Hemingway 202-564-7017

METAL FINISHING

Tools Currently Available:

1. The National Metal Finishing Resource Center. The Office of Compliance in conjunction with the Department of Commerce and the metal finishing industry, established this virtual compliance assistance center which opened in October of 1996. The purpose of the Center is to provide industry with "one-stop" shopping for federal environmental regulatory, compliance and pollution prevention information.

CLEAN AIR ACT APPLICABILITY DETERMINATIONS

Tools Currently Available:

1. The Office of Compliance updated the Clean Air Act Applicability Determination Index (ADI) to include 325 new determinations and expanded it to include the MACT program. The ADI is a computerized, menu-driven compilation of all policy and technical determinations issued pursuant to the Clean Air Act in the following categories: asbestos, CFC's, NESHAP, NSPS, woodstoves and Part 63 MACT standards. Within each category, users can search by date, subpart, references, and string word searches. The compilation is currently available on the Agency's Technology Transfer Network, which receives an average of 1,200 calls per month on the Index. Contact Belinda Breidenbach 202-564-7019.

CFCS

Tools Currently Available:

1. Section 608 Compliance Assistance Pilot Project. Through this effort, an overview of the amendments to the 608 requirements, training module, and self-audit checklist were developed. These compliance assistance tools were made available to the public through CMA and the Stratospheric Ozone Information Hotline. Contact: Dawn Banks at 202-564-7034.

SHIP BUILDING

To be available this year:

1. Compliance Guide: In conjunction with the Office of Air and Radiation, OC will produce a guidebook to complying with the NESHAP for Shipbuilding and Ship Repair standard. Contact: Suzanne Childress 202-564-7018.

2. Ship Building Sector Notebook: In-depth profile of demographics, compliance profile, economic trends, p2 opportunities. Contact: Suzanne Childress 202-564-7018.

TEXTILES

To be available this year:

1. Textiles Sector Notebook: In-depth profile of demographics, compliance profile, economic trends, p2 opportunities. Contact: Brenda Briedenbach 202-564-7019

TRANSPORTATION

Tools Currently Available:

1. "Fuel for Thought...How to Reduce Wastes at Your Shop" brochure (Sept. 1996) (Contact: Elson Lim (202) 564-7006). A brief multimedia guide for shop owners and technicians of vehicle maintenance repair shops on how to environmentally manage and minimize their wastes and how to prevent pollution.

Compliance Tools To Be Available This Year:

1. Environmental Compliance Checklist. A concise screening checklist similar to Auto Checklist will be developed for railroad industry. Contact: Virginia Lathrop (202) 564-7057.

2. Sector Notebook for Rail, Truck and Pipelines and 3. Sector Notebook for Air Transport, Ship and Barge. These sector notebooks will be developed and completed this year. Contact: Virginia Lathrop (202) 564-7057.

4. Report on Consolidated Emergency Plans. Compilation of how states, cities and industry have used innovative approaches for integrated and consolidated emergency plans. Contact: Virginia Lathrop (202) 564-7057.

5. The Transportation Environmental Compliance Center. A joint effort between DOT and EPA to develop the Center is underway with a target completion date in the Fall. Contact: Virginia Lathrop (202) 564-7057.

6. Rural Electric Compliance Guidance Document. Compliance guidance manual to assist Rural Electric Cooperatives. The manual will be completed in FY 1997. Contact: Chris Oh (202) 564-7004.

NATIONAL AGRICULTURE COMPLIANCE ASSISTANCE CENTER

The Ag Center provides information to help producers of agricultural commodities and their supporting businesses meet their environmental requirements, prevent pollution before it occurs, and reduce costs by identifying flexible, common-sense ways to achieve compliance.

Communications efforts are directed primarily at agricultural information providers — including federal and state agencies, land grant universities, trade associations, industry representatives, product and service providers, farm worker associations, environmental advocacy groups, and the agricultural press and trade journals — who ultimately convey information to agricultural farmers and farmworkers.

The Ag Center is coordinated from EPA's Kansas City Regional Office, giving it direct access to a large segment of the agricultural community and first-hand information on factors that affect the compliance of producers and agribusinesses.

COMPLIANCE ASSISTANCE CENTERS:

- Printing: http://www.pneac.org
- Automotive: 1-888-GRN-LINK (476-5465) http://www.ccar-greenlink.org
- Agriculture: http://es.inel.gov/oeca/ag/aghmpg.html
- Metal Finishing: 1-800-AT-NMFRC http://www.nmfrc.org
- Access to all Centers: http://es.inel.gov/oeca/mfcac.html

PRINTERS NATIONAL ENVIRONMENTAL ASSISTANCE CENTER

PNEAC addresses the environmental compliance needs of small printers and provides information on how to achieve compliance by reducing waste and emissions. Information is provided through a World Wide Web site, satellite training, "best-in-class" pollution prevention videoconferences, and two listservs or "chat rooms": PRINTECH, designed for technical printing issues, and PRINTREG, which focuses on environmental laws and regulations affecting the printing industry.

PNEAC is operated by the University of Wisconsin-Extension, Solid & Hazardous Waste Education Center, and the Waste Management and Resource Center of the Illinois Department of Natural Resources, with the collaboration of 12 industry associations, nonprofits, and government agencies.

"THROUGH PNEAC'S MATERIALS EXCHANGE, I WAS ABLE TO CLAIM 80 ROLLS OF MOISTURE BARRIER KRAFT WRAP TO USE AS A PROTECTIVE UNDERLAYMENT FOR FINISHED PRINTED MATERIAL LOADED ONTO (OFTEN DAMP) PALLETS."
—JEFF ADRIAN, JOHN ROBERTS CO.

NEW CENTERS IN 1997/98:

Four new centers will be established in 1997/98. EPA is seeking partners in the private sector to jointly plan and operate the following centers:

- **Transportation:** Contact Virginia Lathrop at 202-564-7057.
- **Printed Wiring Board Manufacturers:** Contact Keith Brown at 202-564-7124.
- **Small Chemical Manufacturers:** Contact Emily Chow at 202-564-7071.
- **Local Governments:** Contact John Dombrowski at 202-564-7036.

SMALL BUSINESS COMPLIANCE Assistance CENTERS

Small Business Compliance Assistance Centers

Small Business Compliance Assistance Centers represent an innovative approach to help small and medium-sized businesses nationwide better understand and comply with federal environmental requirements.

Developed by EPA's Office of Compliance, each center focuses on a particular industry and is operated in partnership with industry, academic institutions, environmental groups, and other federal and state agencies. The goal is to help the hundreds of thousands of small businesses across America:

- Identify the specific federal environmental regulations that apply to their own line of business.
- Take appropriate steps to improve their compliance with environmental regulations.
- Consider pollution prevention approaches and environmental improvements that will bring profits and savings to the company.

The centers also provide state and local officials with easy-to-access information on federal rules and pollution prevention technologies.

Each Compliance Assistance Center provides some or all of the following services via the Internet and toll-free telephone:

- Easy access to federal regulations, interpretations, and guidance
- Compliance tools and process-specific training
- Information exchange through "chat rooms" and conferences
- Databases of technologies and pollution prevention ideas

Four Compliance Assistance Centers are already up and running, and four more are on the way.

GreenLink™ — The Automotive Compliance Information Assistance Center

GreenLink™ provides compliance assistance to the automotive service industry, primarily owners and technicians of auto body and repair shops, but also automotive trade associations, automotive educators and students, and new car dealer service departments.

Operated by CCAR, the Coordinating Committee for Automotive Repair, a consortium of 38 industry affiliates, GreenLink™ provides information on compliance requirements, technologies, and activities that can reduce pollution. Also available from GreenLink™ are several tools:

- Consolidated multi-media checklists that can be used by shop owners as a self-assessment tool, or by state inspectors as a building block to design their own multi-media checklists.
- Environmental curriculum modules that walk shop owners and technicians through statutes, regulations, and health and environmental issues for each auto service activity.

"We use CCAR information very regularly in our automotive program..." —Joe Sequin

National Metal Finishing Resource Center

The NMFRC is designed as the most comprehensive and substantive environmental compliance, technical assistance, and pollution prevention information source available to the metal finishing industry. The center's Internet Web site offers information in convenient and user-friendly forms. Users can, for example:

- Search the NMFRC technical databases for abstracts, full-text articles, and reports.
- Find summaries of environmental, safety, and health regulations.
- Download, read, and print full-text regulations.
- Get listed in the Vendor Directory, or search the directory for over 300 suppliers of metal finishing equipment and services.
- Enter the NMFRC On-Line Conferences: read messages, post a question, give an opinion.
- Find metal finishing shops in specific geographic locations.
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Research and Development EPA-625/R-96/010a February 1997

EPA

Project Summary

Compendium of Methods for the Determination of Inorganic Compounds in Ambient Air

This Project Summary is the announcement of the availability of a collection of methods for measurement of inorganic pollutants of interest in ambient air. These methods have been prepared to provide regional, state and local environmental regulatory agencies and other users with step-by-step sampling and analysis procedures for the determination of selected inorganic pollutants in ambient air. The methods comprise the *Compendium of Methods for the Determination of Inorganic Compounds in Ambient Air*, which is intended to assist those persons responsible for sampling and analysis of ambient inorganic pollutants.

Determination of pollutants in ambient air is a complex task, primarily because of the wide variety of compounds of interest coupled with the lack of standardized sampling and analysis procedures. Many inorganic compounds can be sampled and analyzed by several techniques, often with different interferences and detection limitations. This Compendium contains a set of 17 methods (in 5 categories) presented in a standardized format, with a variety of applicable sampling methods and various analytical techniques for specific classes of inorganic pollutants, as appropriate to their ambient levels and potential interferences. Consequently, this treatment allows flexibility in selecting alternatives to complement the user's background and laboratory capability. These methods may be modified from time to time as advancements are made.

This Project Summary was developed by EPA's Center for Environmental Research Information (CERI), National Risk Management Research Laboratory (NRMRL), Office of Research and Development (ORD), U.S. EPA, Cincinnati, OH, with assistance from the ORD's National Exposure Research Laboratory (NERL) at Research Triangle Park, NC. Its purpose is to announce key findings of the research project, which is fully documented in a separate report of the same title (see Project Report ordering information on the last page).

Introduction

The Clean Air Act Amendments of 1990 (CAAA of 1990) have significantly increased the responsibilities of both federal and state agency programs for evaluating and maintaining air pollutant emissions compliance. In turn, this increased responsibility has generated a need for more personnel trained to interpret, enforce, and respond to regulatory initiatives. Consequently, the Agency has restructured its technology transfer program to more effectively provide technical assistance in the form of publication of technical documents, presentations and workshops, and development of tools to assist Agency personnel in keeping their skills up-to-date so that they may efficiently cope with the many changes evolving in new programs, equipment, sampling and analytical methodology, and available enforcement tools.

Limited guidance has been available to state and local agencies or to other organizations concerned with the determination of inorganic pollutant concentrations in ambient air. As a result, state and local agencies and others responding to air pollution problems have had to develop their own monitoring strategies, including selection of monitoring methods, sampling plan design, and specific procedures for sampling, analysis, logistics, calibration and quality control. For the most part, these procedures were based on professional judgments rather than adherence to any documented uniform guidelines. Many governmental agencies and professional or research organizations have developed ambient air monitoring methods and procedures, mostly to respond to specialized needs. But these methods and procedures have, *in general,* been neither standardized nor readily available to other agencies involved with ambient air monitoring for various pollutants.

To meet these needs, EPA's ORD, through CERI and NERL has supported technology transfer programs involving standardized, peer reviewed monitoring methods for regulatory and industrial personnel via publications of a series of methods Compendia. Other Compendia in this series, reflecting EPA's commitment to technology transfer, are:

- *Compendium of Methods for the Determination of Toxic Organic Compounds in Ambient Air,* EPA 600/4-89-017, June 1988.
- *Compendium of Methods for the Determination of Air Pollutants in Indoor Air,* EPA 600/4-90-010, April 1990.
- *Compendium of Methods for the Determination of Toxic Organic Compounds in Ambient Air, Second Edition,* EPA 625/R-96/010b, February 1997.

These Compendia have historically assisted Federal, State, and local regulatory personnel in developing and maintaining necessary expertise and up-to-date technology involving sampling and analysis of both indoor and organic hazardous air pollutants (HAPs). The objective of this project was to develop and standardize methods for measuring inorganic pollutants of interest in ambient air and publish them in this *Compendium of Methods for the Determination of Inorganic Compounds in Ambient Air.* This fourth Compendium adds much needed methods for measurement of inorganic pollutants in ambient air to the series.

Consistent with past practices, the Compendium methods are provided as guidance only in appropriate monitoring situations. In particular, these methods are not intended to be used as specific regulatory guidance for measurement or monitoring purposes and are offered with no endorsement for suitability or recommendation for any specific application; rather, this is merely to document the methods and to make them more widely available.

Structure and Content of the Inorganic Compendium

This Compendium has been prepared to provide regional, state and local environmental regulatory agencies, as well as other interested parties, with specific guidance on the determination of selected inorganic compounds and pollutants in ambient air. A visual guide to the organization of the Inorganic Compendium is illustrated in Figure 1, while Table 1 lists the 17 methods which comprise the 5 chapters of the Compendium. The 17 methods have been compiled from the best elements of methods developed or used by various research or monitoring organizations. They are presented in a standardized format, and each one has been extensively reviewed by several technical experts having expertise in the methodology presented.

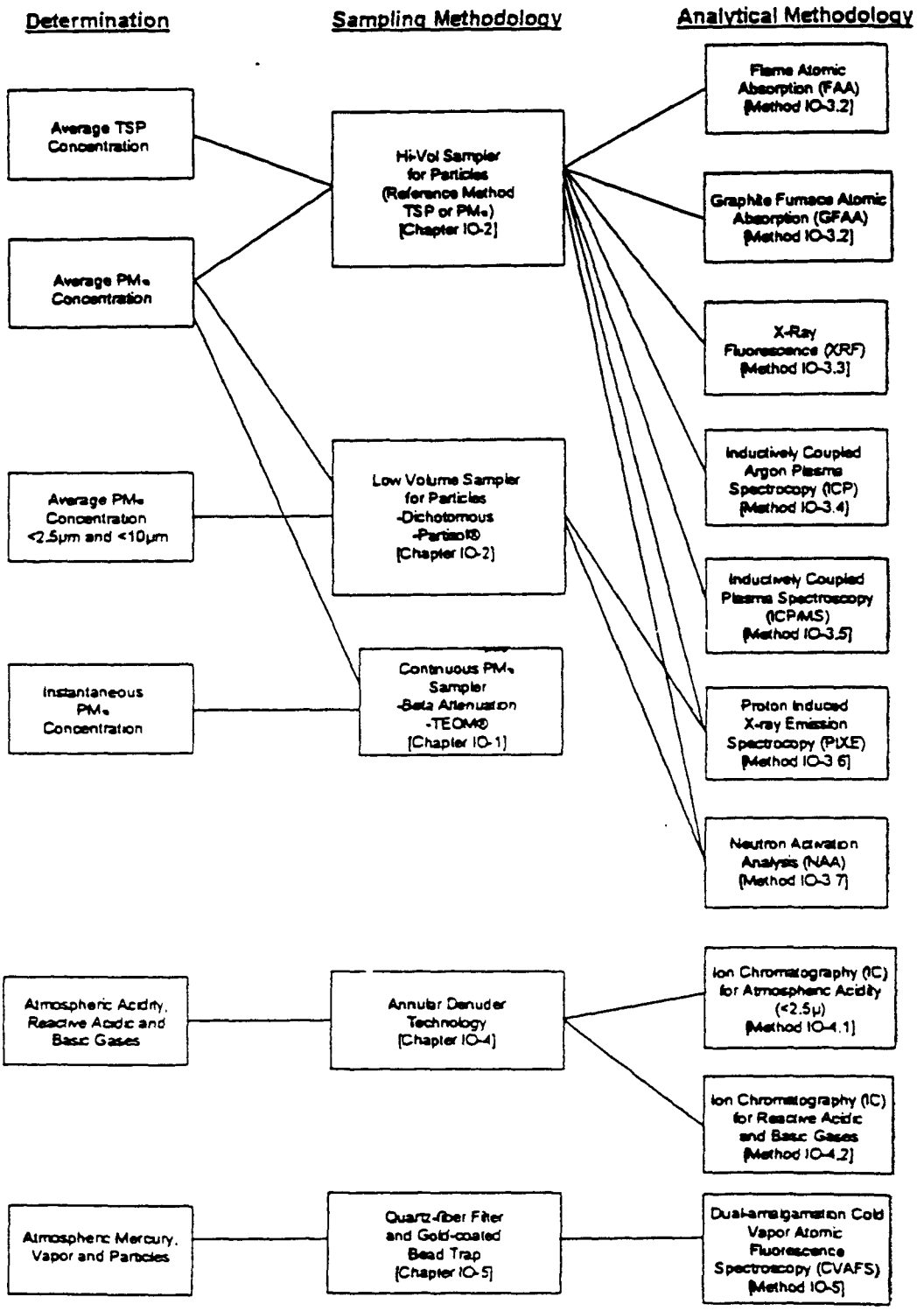


Figure 1. A visual guide to the organization of the Inorganic Compendium.

Table 1. Methods in the Inorganic Compendium

Chapter IO-1 Continuous Measurement of PM_{10} Suspended Particulate Matter (SPM) in Ambient Air

Method IO-1.1	Determination of PM_{10} in Ambient Air Using the Graseby Continuous Beta Attenuation Monitor
Method IO-1.2	Determination of PM_{10} in Ambient Air Using the Thermo Environmental Inc. (formerly Wedding and Associates) Continuous Beta Attenuation Monitor.
Method IO-1.3	Determination of PM_{10} in Ambient Air Using a Continuous Rupprecht and Patashnick (R&P) TEOM® Particle Monitor

Chapter IO-2 Integrated Sampling of Suspended Particulate Matter (SPM) In Ambient Air

Method IO-2.1	Sampling of Ambient Air for Total Suspended Particulate Matter (SPM) and PM_{10} Using High Volume (HV) Sampler
Method IO-2.2	Sampling of Ambient Air for PM_{10} Using a Graseby Dichotomous Sampler
Method IO-2.3	Sampling of Ambient Air for PM_{10} Concentration Using the Rupprecht and Patashnick (R&P) Low Volume Partisol® Sampler
Method IO-2.4	Calculations for Standard Volume

Chapter IO-3 Chemical Species Analysis of Filter-Collected Suspended Particulate Matter

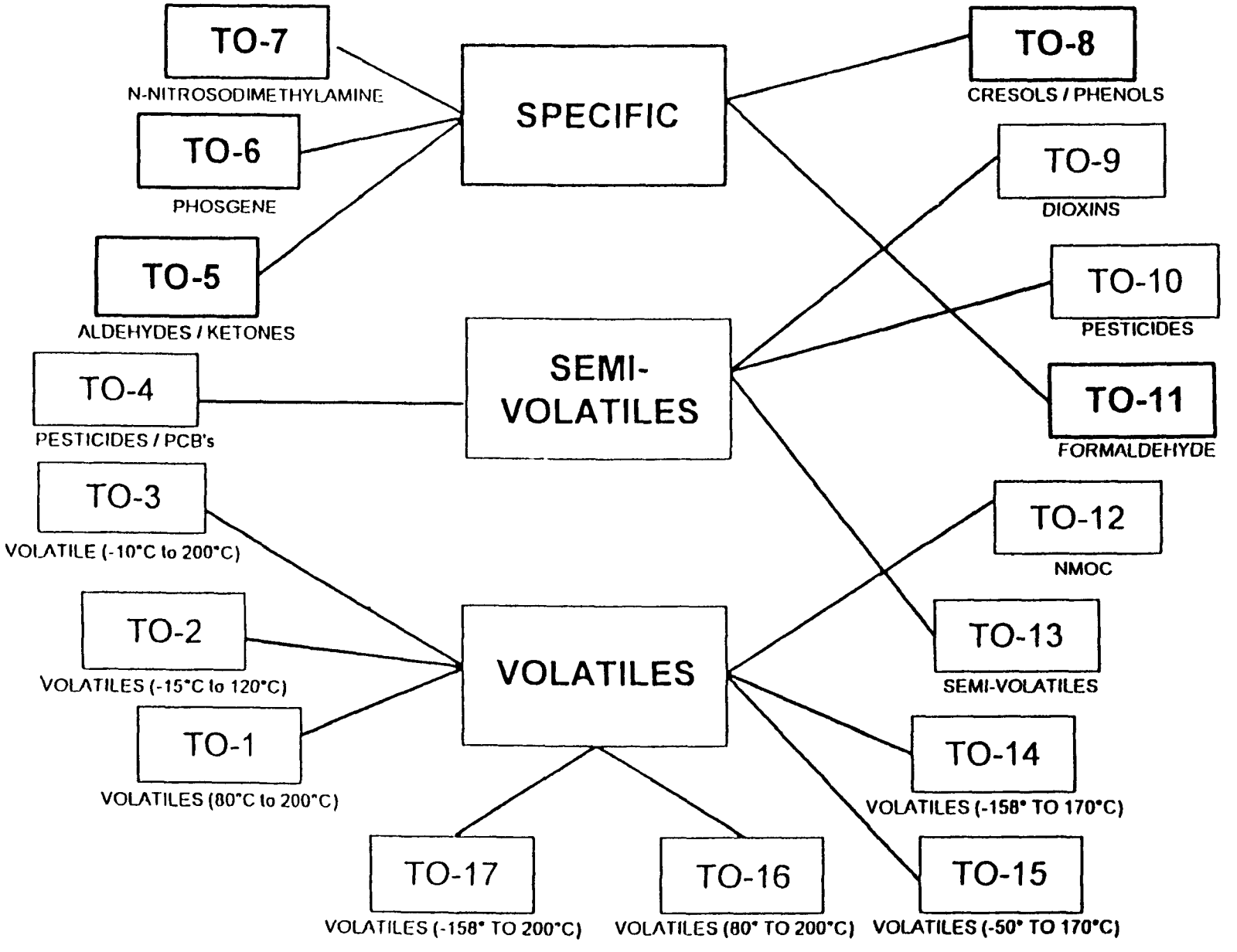
Method IO-3.1	Selection, Preparation and Extraction of Filter Material
Method IO-3.2	Determination of Metals in Ambient Particulate Matter Using Atomic Absorption (AA) Spectrometry
Method IO-3.3	Determination of Metals in Ambient Particulate Matter Using X-Ray Fluorescence (XRF) Spectrometry
Method IO-3.4	Determination of Metals in Ambient Particulate Matter Using Inductively Coupled Plasma (ICP) Spectrometry
Method IO-3.5	Determination of Metals in Ambient Particulate Matter Using Inductively Coupled Plasma/Mass Spectrometry (ICP/MS)
Method IO-3.6	Determination of Metals in Ambient Particulate Matter Using Proton Induced X-Ray Emission (PIXE) Spectroscopy
Method IO-3.7	Determination of Metals in Ambient Particulate Matter Using Neutron Activation Analysis (NAA) Gamma Spectrometry

Chapter IO-4 Determination of Reactive Acidic and Basic Gases and Strong Acidity of Atmospheric Fine Particles in Ambient Air Using the Annual Denuder Technology

Method IO-4.1	Determination of the Strong Acidity of Atmospheric Fine Particles ($<2.5\mu m$)
Method IO-4.2	Determination of Reactive Acidic and Basic Gases and Strong Acidity of Atmospheric Fine Particles

Chapter IO-5 Sampling and Analysis for Atmospheric Mercury

Method IO-5.1	Sampling and Analysis for Vapor and Particle Phase Mercury in Ambient Air Utilizing Cold Vapor Atomic Fluorescence Spectrometry (CVAFS)


TO-7
N-NITROSODIMETHYLAMINE
TO-6
PHOSGENE
TO-5
ALDEHYDES / KETONES
SPECIFIC
TO-8
CRESOLS / PHENOLS
TO-9
DIOXINS
TO-10
PESTICIDES
TO-11
FORMALDEHYDE
TO-4
PESTICIDES / PCB's
SEMI-VOLATILES
TO-3
VOLATILE (-10°C to 200°C)
TO-2
VOLATILES (-15°C to 120°C)
TO-1
VOLATILES (80°C to 200°C)
VOLATILES
TO-12
NMOC
TO-13
SEMI-VOLATILES
TO-14
VOLATILES (-158° TO 170°C)
TO-15
VOLATILES (-50° TO 170°C)
TO-16
VOLATILES (80° TO 200°C)
TO-17
VOLATILES (-158° TO 200°C)

EPA/625/R-96/010b

Compendium of Methods for the Determination of Toxic Organic Compounds in Ambient Air

Second Edition

Compendium Method TO-16

Long-Path Open-Path Fourier Transform Infrared Monitoring Of Atmospheric Gases

Center for Environmental Research Information
Office of Research and Development
U.S. Environmental Protection Agency
Cincinnati, OH 45268

January 1997

Method TO-16
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DISCLAIMER

This Compendium has been subjected to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

METHOD TO-16

Long-Path Open-Path Fourier Transform Infrared Monitoring Of Atmospheric Gases

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METHOD TO-16

Long-Path Open-Path Fourier Transform Infrared Monitoring Of Atmospheric Gases

1. Scope

1.1 Fourier transform infrared (FT-IR) spectroscopy used for open-path monitoring of atmospheric gases is undergoing a vigorous development and growth period. Until now the developmental effort and the most of the data acquisition have been performed by highly trained individuals experienced in the fields of instrument development and spectroscopy. In the future, operators trained at the technician level will be required to perform the operation routinely. This method is intended to address that need. Specifically, the method is intended to allow trained technicians to acquire data in a standardized way and to process that data to obtain atmospheric gas concentrations. The primary intent is that the results will be obtained in a consistent fashion.

1.2 This method is intended for the use of an FT-IR system that acquires data using a long, open air path and does not require the acquisition of a sample for subsequent analysis. The system produces data that is a time sequence of the path-averaged atmospheric concentrations of various gases. Because the FT-IR can potentially measure the concentration of a large number of atmospheric gases, this method does not address the requirements for measuring a particular gas or a set of gases. Rather, it is intended to be a generalized method.

1.3 The method is intended to be instrument independent in that it discusses the processing of spectra so that gas concentrations can be obtained. The primary geometric configurations of FT-IR instruments that are commercially available are the monostatic configuration and the bistatic configuration. These configurations are shown schematically in Figures 1 and 2. This method can be used to process data from either of these types. It is assumed that the FT-IR is under computer control and that the controlling software will allow the manipulation of the spectra. This method is specifically designed to process spectra that will be analyzed by the commonly called classical least-squares technique. If the classical least-squares technique is to be used, the spectra must be processed in a specific way, and this document describes the steps of that processing. Although there are other ways to analyze the spectra, such as partial least squares, iterative least squares, spectral subtraction, principal component analysis, and peak height and peak area calculations, the use of these techniques requires that the spectra be processed in a different way than is described here. While some of the procedures given here are applicable to the other analysis techniques, this method addresses only the classical least-squares technique.

1.4 The method is not intended as a tutorial for the use of the computer software or the instruments themselves. Inclusion of this type of explanation would make this document excessively long. When certain features from the software packages are called for, it is assumed that the user has read or can read the appropriate description in the specific manual. As far as the instruments are concerned, it is assumed that the operator has participated in instrument training provided by the specific instrument manufacturer and that this training has been sufficient to enable the operator to produce spectra and to save them on a disk.

1.5 Since this method in this document is considered to be a set of operational procedures, the document does not contain an in-depth explanation about the origin or the rationale for the inclusion of particular steps. For a more complete and rigorous discussion of the FT-IR technique, the user of this method is referred to EPA's *FT-IR Open-Path Monitoring Guidance Document* (1).

1.6 The intent of this document is to provide the operator with stepwise procedures producing concentration data from spectra taken with an FT-IR. To accomplish this, items such as background spectra, water vapor reference spectra, and stray light are discussed. In keeping with the concept of a procedure, these quantities must be specified directly. However, the entire area of FT-IR remote sensing of the atmosphere is undergoing rapid change, and parts of these procedures will without doubt need revision in the future. Throughout this document the user must keep in mind that for each procedure in the TO-16 method there may be other equally valid procedures that are currently being used that are not described here.

1.7 Finally, a statement about computer automation of these procedures is in order here. The method does not address the problem of automation directly and implies that an operator is available to perform the individual steps. Some operational software packages already exist that incorporate many of these routines in an automatic way. It is felt that each procedure potentially can be automated, but the steps listed here are those that need to be incorporated in any automated procedure.

2. Summary of Method

2.1 For the purpose of this document the operation of an FT-IR remote sensor is divided into two parts. The first is initial data acquisition after the system has been set up by the manufacturer and the second is what is considered to be routine data acquisition. The first of these data acquisition periods is intended to produce data that will form the basis of a quality assurance data set. The second is devoted to the production of time sequences of atmospheric gas concentration data.

2.2 There are several items that need to be determined before the FT-IR system can be put into routine service. These items have been selected to determine how the system is functioning initially and include the shortest path length that will saturate the detector, the ambient black body radiation level for the bistatic configuration, the stray light inside the instrument for the monostatic configuration, and the return intensity as a function of distance. Beyond these steps there is a survey set of data that should be acquired. Data from this survey set will form the basis of the routinely monitored quality control checks for the instrument.

2.3 In addition to the FT-IR data it is required that the ambient temperature and the relative humidity be monitored on a continuous basis so that the water vapor concentration as a function of time can be determined. It is to be clearly understood that relative humidity measurements alone are not relevant to this operation but the amount of water is. These data should be acquired at the site where the FT-IR data is taken. Use of data taken at airports miles away is not appropriate.

2.4 The initial step in the procedure for determining the concentration data for various gases is the production of a set of interferograms, and it should be the interferograms that are saved as the primary data. The various procedures given in Section 8 of this document use the single beam spectrum that is created from the interferogram. A single beam spectrum taken with a monostatic system over a 414-m

path length is illustrated in Figure 3. Various atmospheric constituents as well as a stray light component are pointed out. However, it is the interferograms that are considered the most important data. If they are not saved they cannot accurately be reproduced by simply performing the inverse Fourier transform. Once a set of target gases has been selected, the wave number regions to be used in the analysis are chosen. For the monostatic instrument geometry, the stray light component must next be subtracted from each single beam spectrum. For the bistatic case, the black body radiation spectrum must be subtracted from each single beam spectrum. One spectrum from this set is then chosen to be the background, or I_0, spectrum, and this can be turned into a synthetic background spectrum. A second spectrum is then used to create a water vapor reference spectrum, and all the remaining spectra are then converted to absorbance spectra. All the spectra to be analyzed are then checked for wave number shifts. Finally, the absorbance spectra are analyzed by the classical least-squares technique.

2.5 It is suggested that, if possible, twice each day a short cell filled with a known quantity of gas should be inserted in the infrared beam, and four spectra should then be recorded. The instrument must be operating in exactly the same manner as it is when it is routinely acquiring data but this time with the cell. These spectra are analyzed in the same way as all other spectra, but for the particular gas in the cell. This data is then added to the appropriate control charts. No exact procedure for using this cell and no specifications for the cell are provided at this time within this document. Not all the instruments that are commercially available can accommodate a cell, and many gases cannot be easily used in such a cell.

2.6 A subset of each day's spectra is then selected and the following two items are determined: the root mean square (RMS) noise in three wave number regions and the return beam intensity at two wave numbers. The range of water vapor concentrations over the time period during which the subset of data was taken is calculated. These data are also then added to the appropriate control charts.

2.7 The remainder of the data can then be checked as described in Section 8 and then against the data quality objectives provided by the monitoring program.

3. Significance

3.1 VOCs enter the atmosphere from a variety of sources, including petroleum refineries, synthetic organic chemical plants, natural gas processing plants, and automobile exhaust. Many of these VOCs are acutely toxic; therefore, their determination in ambient air is necessary to assess human health impacts.

3.2 The environmental impacts from the release of airborne VOCs is a topic of great interest among air pollution scientists. It is important that measurement methods be developed to accurately assess the impact of airborne chemical emissions on the environment. Until now, traditional air sampling/analytical techniques (i.e., solid adsorbents, treated canisters, portable gas chromatographs, etc.) have been used to characterize emission impacts of airborne toxic chemicals in the environment.

3.3 The method of trace gas monitoring using FT-IR-based, long-path, open-path systems has a number of advantages that are significant over traditional methods. Some of these advantages are related to the path monitoring aspect of this method which, by its very nature, distinguishes the method from all point monitoring methods. The main advantages of these systems are the following:

- Integrity of the sample is assured since no sampling actually occurs.
- Multi-gas analysis is possible with a single field spectrum.
- Path-integrated pollutant concentrations are obtained.
- Spatial survey monitoring of industrial facilities is possible if scanning optics are used.
- Coadding of spectra to improve detection capabilities is easily performed.
- Rapid temporal scanning of line-of-sight or multiple lines-of-sight is possible.
- Monitoring of otherwise inaccessible areas is possible.

3.4 Applications include the monitoring of atmospheric gases along the perimeters of industrial facilities or, from an elevated, centrally located platform, monitoring over the industrial facility to infrared sources or retroreflectors placed along the facility edge. Other applications include monitoring (1) at hazardous waste sites during remediation or removal operations to provide warnings of high concentrations and to verify that back-to-work conditions have been achieved; (2) in response to accidental chemical spills or releases; (3) in workplace environments to develop concentration profiles at the worker level; and (4) in the ambient air for some compounds. It is theoretically applicable to the measurement of all gaseous compounds that exhibit absorption spectra in the mid-infrared region of the electromagnetic spectrum.

3.5 Significant advances have been made in recent years to develop the FT-IR systems into practical remote sensing tools, particularly in the understanding of the importance of water vapor interference associated with FT-IR methodology. As indicated in this method, the generation of a background spectrum for a given measurement and the generation of water vapor spectra to account to water vapor interference in mid-infrared measurements are features of the FT-IR measurement technique that deserve more attention. The significance of Compendium Method TO-16 is that it is the first such method to address all the features that are required to make a field measurement using FT-IR-based systems. As such, it provides a guide to field measurement as well as a basis for improvement and further consideration.

3.6 The ultimate significance of remote sensing with FT-IR systems is a matter of cost effectiveness and of technological advances. Technological advances are required in at least two important areas: (1) the improvement in the characteristics of the instrumentation itself and (2) the development of "intelligent" software. The software is required to improve the means for short-term adjustment of background and water vapor spectra to account for the continual variation of ambient conditions that can adversely affect the accuracy and precision of FT-IR based systems.

4. Applicable Documents

4.1 ASTM Standards

- Method D1356 *Definition of Terms Relating to Atmospheric Sampling and Analysis.*

4.2 EPA Documents

- *Technical Assistance Document for Sampling and Analysis of Toxic Organic Compounds in Ambient Air*, U. S. Environmental Protection Agency, EPA-600/4-83-027, June 1983.
- *Quality Assurance Handbook for Air Pollution Measurement Systems*, U. S. Environmental Protection Agency, EPA-600/R-94-038b, May 1994.
- *Open-Path Monitoring Guidance Document*, U. S. Environmental Protection Agency, EPA 600/4-96-040, April 1996.

5. Definitions

[Note: This section contains a portion of the glossary of terms from the guidance document (1) for remote sensing that is applicable to Compendium Method TO-16. When possible, definitions of terms have been drawn from authoritative texts or manuscripts in the fields of remote sensing, air pollution monitoring, spectroscopy, optics, and analytical chemistry. In some cases, general definitions have been augmented or streamlined to be more specific to long-path, open-path monitoring applications and to Compendium Method TO-16. These definitions were intended to remain scientifically rigorous and still be generally applicable to the variety of FT-IR open-path remote-sensing issues that must be addressed by the operator.]

5.1 **Absorbance**—the negative logarithm of the transmission. $A = -\ln(I/I_0)$, where I is the transmitted intensity of the light and I_0 is the incident intensity. Generally, the logarithm to the base 10 is used, although the quantity I really diminishes exponentially with A.

5.2 **Apodization**—a mathematical transformation carried out on data received from an interferometer to alter the instrument's response function. There are various types of transformation; the most common are boxcar, triangular, Happ-Genzel, and Beer-Norton functions.

5.3 **Background Spectrum**—1. With all other conditions being equal, that spectrum taken in the absence of the particular absorbing species of interest. 2. Strictly, that radiant intensity incident on the front plane of the absorbing medium. 3. A spectrum obtained from the ambient black body radiation entering the system. This background must be considered in FT-IR systems, in which the IR beam is not modulated before it is transmitted along the path. For FT-IR systems that do not use a separate source of infrared energy, the background is the source of infrared energy.

5.4 **Beer's Law**—Beer's law states that the intensity of a monochromatic plane wave incident on an absorbing medium of constant thickness diminishes exponentially with the number of absorbers in the beam. Strictly speaking, Beer's law holds only if the following conditions are met: perfectly monochromatic radiation, no scattering, a beam that is strictly collimated, negligible pressure-broadening effects (2,3).

5.5 **Bistatic System**—a system in which the receiver is some distance from the transmitter. This term is actually taken from the field of radar technology. For remote sensing, this implies that the light source and the detector are separated and are at the ends of the monitoring path.

5.6 Fourier Transform—a mathematical transform that allows an aperiodic function to be expressed as an integral sum over a continuous range of frequencies (4). The Fourier transform of the interferogram produced by the Michelson interferometer in an FT-IR is the intensity as a function of frequency.

5.7 FT-IR—an abbreviation for "Fourier transform infrared." A spectroscopic instrument using the infrared portion of the electromagnetic spectrum. The working component of this system is a Michelson interferometer. To obtain the absorption spectrum as a function of frequency, a Fourier transform of the output of the interferometer must be performed. A brief overview of the FT-IR is provided in *FT-IR Theory* (5). An in-depth description of the FT-IR can be found in *Fourier Transform Infrared Spectrometry* (6).

5.8 Intensity—the radiant power per unit solid angle. When the term "spectral intensity" is used, the units are watts per steradian per nanometer. In most spectroscopic literature, the term "intensity" is used to describe the power in a collimated beam of light in terms of power per unit area per unit wavelength.

5.9 Interference—the physical effects of superimposing two or more light waves. The principle of superposition states that the total amplitude of the electromagnetic disturbance at a point is the vector sum of the individual electromagnetic components incident there. For a two-component system of collinear beams of the same amplitude, the mathematical description of the result of addition is given by $I(p) = 2I_0(1 + \cos[A])$, where I_0 is the intensity of either beam, and A is the phase difference of the two components. The cosine term is called the "interference term" (7,8). See also "Spectral Interference."

5.10 Interferogram—the effects of interference that are detected and recorded by an interferometer; the output of an FT-IR and the primary data that is collected and stored (6,8).

5.11 Interferometer—any of several kinds of instruments used to produce interference effects. The Michelson interferometer used in FT-IR instruments is the most famous of a class of interferometers that produce interference by the division of an amplitude (9).

5.12 Light—strictly, light is defined as that portion of the electromagnetic spectrum that causes the sensation of vision. It extends from about 25,000 cm^{-1} to about 14,300 cm^{-1} (4).

5.13 Minimum Detection Limit—the minimum concentration of a compound that can be detected by an instrument with a given statistical probability. Usually the detection limit is given as 3 times the standard deviation of the noise in the system. In this case, the minimum concentration can be detected with a probability of 99.7% (10,11).

5.14 Monitoring path—the actual path in space over which the pollutant concentration is measured and averaged.

5.15 Monostatic System—a system with the source and the receiver at the same end of the path. For FT-IR systems, the beam is generally returned by a retroreflector.

5.16 Reference Spectra—spectra of the absorbance versus wave number for a pure sample of a set of gases. The spectra are obtained under controlled conditions of pressure and temperature and with known concentrations. For most instruments, the pure sample is pressure-broadened with nitrogen so that the

spectra are representative of atmospherically broadened lines. These spectra are used for obtaining the unknown concentrations of gases in ambient air samples.

5.17 Relative **Absorption Strength**—a term used exclusively in Compendium Method TO-16 to describe the relation of absorption due to interfering species to the absorption of the target gas.

5.18 **Resolution**—the minimum separation that two spectral features can have and still, in some manner, be distinguished from one another. A commonly used requirement for two spectral features to be considered just resolved is the Raleigh criterion. This states that two features are just resolved when the maximum intensity of one falls at the first minimum of the other (5,6). This definition of resolution and the Raleigh criterion are also valid for the FT-IR, although there is another definition in common use for this technique. This definition states that the minimum separation in wave numbers of two spectral features that can be resolved is the reciprocal of the maximum optical path difference (in centimeters) of the two interferometer mirrors employed.

5.19 **Retroreflector**—the CIE (Commission Internationale de l'Eclairage) defines retroreflection as "radiation returned in directions close to the direction from which it came, this property being maintained over wide variations of the direction of the incident radiation." Retroreflector devices come in a variety of forms and have many uses. The one commonly described by workers in remote sensing uses total internal reflection from three mutually perpendicular surfaces. This kind of retroreflector is usually called a corner cube or prismatic retroreflector (12).

5.20 **RMS Noise**—this quantity is actually the statistical quantity rms deviation. In Compendium Method TO-16 the rms noise (deviation) is calculated by using a least squares fit to the baseline. Because of this calculation, the rms noise in Compendium Method TO-16 uses the quantity N-2 in the denominator rather than N-1 as normally described.

5.21 **Single Beam Spectrum**—that spectrum which results from performing the Fourier transform on the interferogram. It is not a transmission spectrum. The term "single beam" is a holdover from older instruments that were double beam instruments.

5.22 **Source**—the device that supplies the electromagnetic energy for the various instruments used to measure atmospheric gases. These generally are a Nernst glower or globar for the infrared region or a xenon arc lamp for the ultraviolet region.

5.23 **Spectral Intensity**—see Section 5.8.

5.24 **Spectral Interference**—when the absorbance features from two or more gases cover the same wave number regions, the gases are said to exhibit spectral interference. Water vapor produces the strongest spectral interference for infrared spectroscopic instruments that take atmospheric data.

5.25 **Synthetic Background**—a spectrum that is made from a field spectrum by choosing points along the baseline and connecting them with a high-order polynomial or short, straight lines. The synthetic background is then used to find the absorbance spectrum.

5.26 **Wave Number**—the number of waves per centimeter. This term has units of reciprocal centimeters (cm^{-1}).

6. Apparatus and System Requirements

6.1 Summary

6.1.1 Compendium Method TO-16 is a procedure that deals with how spectra taken with an FT-IR are to be processed in order to obtain various atmospheric gas concentrations. General requirements for FT-IR instrumentation is being prepared by a committee of L'Organisation Internationale de Metrologie Legale (OIML) and will be available in the very near future.

6.1.2 The instrument requirements listed here are limited to those that will define a rudimentary but operational system. The requirements are delineated into three categories: those of the FT-IR sensor itself (see Section 6.2), the computer associated with it (see Section 6.3), and the software that allows for data analysis (see Section 6.4).

6.2 FT-IR Sensor Requirements

6.2.1 The system should be capable of making spectral absorption measurements along an open air optical path.

6.2.2 The system can be either of the monostatic or the bistatic geometry.

6.2.3 The system must be able to produce and save an interferogram and a single beam spectrum.

6.2.4 The system must be able to operate with a resolution of at least 1 cm^{-1} over the mid-infrared region (700–4200 cm^{-1}).

6.2.5 The system must be capable of acquiring data by co-adding individual interferogram scans in one-scan increments. As a minimum, the system must be able to acquire data from a one-scan interferogram to an interferogram made up of sufficient co-added scans so that at least 5-min concentration averages can be obtained.

6.2.6 The system must be able to perform the mathematical procedure of Fourier transformation on the interferogram, thereby producing a so-called single beam spectrum. The transform can be performed as part of post-acquisition processing or in quasi-real time. If performed in quasi-real time the process of transformation should not add significantly to the data acquisition time.

6.2.7 Although there is no agreed upon procedure for the use of a gas cell with these systems, the system may have provisions for installing an ancillary gas cell in the optical beam. If that is the case, the installation must allow for the entire beam to pass through the cell. The cell can be of any of several designs: short, either single or double pass; multi-pass capable of producing a relatively long optical path; or a multi-chambered cell with the individual chambers interconnected and in parallel with one another.

6.3 Computer Requirements

6.3.1 The computer must be capable of acquiring data in the form of interferograms with sufficient speed so that the system is able to operate in quasi-real time.

6.3.2 The computer must have provisions for storing of the data acquired in one 24-h period. The storage must accommodate the interferograms.

6.3.3 The computer must have sufficient RAM to operate the controlling software and the data manipulation software.

6.4 Software Requirements

6.4.1 The software must have provisions for manipulating the spectra so that all the individual procedures listed here can be accomplished.

6.4.2 The software must be able to perform the analysis for concentration using classical least squares.

7. Materials and Supplies

7.1 Only a small number of materials are required in addition to the basic instrument for this method. However, the basic instrument operation may have specific material requirements such as liquid nitrogen or nitrogen, etc. A listing of any specific instrument's requirement for material must be obtained from the manufacturer.

7.2 A set of gases may have to be purchased in order to acquire spectra with a cell. This set of gases is intended to allow the operator to determine the precision and accuracy of the data obtained from the field spectra, but at the present time no procedure using a cell has been developed. The specific gases required are dependent on the particular monitoring program. If necessary, the gases can be purchased as pure gases, which are then diluted with nitrogen for use, or they can be a mixture of gases that are properly mixed at purchase. The dilution step can be quite cumbersome and it is recommended that appropriate mixtures of gas be acquired directly whenever possible. The required concentrations of the gases are dependent on the anticipated concentration of the target gas in the atmosphere and the ratio of the actual path length used to the length of the cell. Many applications will require that these gases be purchased with certifications traceable to the National Institute of Standards and Technology.

7.3 The only other material that may be required is a set of screens of varying mesh that will be used when determining whether the system is responding linearly. This screening can be regular aluminum window screen or made of other opaque metallic materials. The size of the mesh is not really important, but the screen should be large enough to cover the entire beam. The mesh itself should be chosen so as to change the transmitted intensity by an easily measured amount (on the order of 25% or more). The screen must not be made of any plastic materials as they transmit infrared energy. This in itself is not a problem but the plastic materials introduce absorbance at specific wave numbers and may not provide the desired result.

8. Standard Procedures for Processing of Infrared Spectra

8.1 Summary

The specific procedures that are required to produce atmospheric gas concentration data are included in this section. They start with the general operations procedure that describes how the other individual procedures should follow one another.

8.2 Suggested Order of Generation of FT-IR Concentration Data

8.2.1 This section provides the FT-IR operator with a systematic approach to the generation of FT-IR concentration data. These procedures are recommended for operators with little experience with FT-IR operation. As the operator gains more experience with the production of FT-IR concentration data, he may want to reorder the sequence of events to better fit his experimental schedule.

8.2.2 Assumptions

8.2.2.1 Compendium Method TO-16, in general, does not describe the general planning that is necessary to conduct a field program. It is felt that each data acquisition program is different and all programs cannot be covered in depth with a single procedure. For example, the time for acquiring a single spectrum can vary from a single scan of a few seconds up to a half hour. The actual time required for any one program is dependent on that program and therefore is not discussed further in this procedure. Much of the planning for the acquisition of data is connected to the generation of a detailed quality assurance/quality control (QA/QC) program plan, and this method is not considered to be such a plan. Section 9 presents individual items that should be addressed as a minimal quality assurance effort. The procedures in Section 8 cover only the production of concentration data.

8.2.2.2 It is also assumed that water vapor concentration data for the data acquisition period is available. This method does not discuss how to acquire that data, however. The water vapor concentration data is used for post-analysis review and for some of the QA/QC checks.

8.2.2.3 From this point on, it is assumed that the individual spectra have already been acquired. It is assumed that the interferograms have been converted to single beam spectra. It is further assumed that no other data manipulation has occurred.

8.2.3 The suggested order for the production of concentration data utilizing FT-IR is given below.

- Selection of wave number regions for analysis in the presence of interfering species (see Section 8.3).
- Generation of a background spectrum (see Section 8.4).
- Production of a water vapor reference spectrum (see Section 8.5).
- Subtraction of stray light or black body radiation (see Section 8.6).
- Generation of an absorbance spectrum (see Section 8.7).
- Correction for spectral shifts (see Section 8.8).
- Analysis of field spectra for concentration (see Section 8.9).
- Post-analysis review of the data (see Section 8.10).

8.3 Selection of Wave Number Regions for Analysis in the Presence of Interfering Species

8.3.1 Purpose. This section instructs the operator on how to select the wave number regions that are to be used in the analysis of field spectra. This section includes the process of working with interfering species because the absorbance spectrum of any one particular gas frequently overlaps with

the absorbance of another species. This section also provides the operator with a measure of the strength of the interference.

8.3.2 Assumptions. One of the most important requirements when utilizing classical least squares as an analysis technique is the identification of all possible compounds whose absorption spectrum can interfere with the absorption feature being analyzed. It is therefore imperative that the operator has as complete knowledge as he can of the compounds that are expected to be present during the measurement period. The assumption made here is not only that this knowledge exists but that reference spectra for all the potentially present compounds also exist. The operator should be aware that absorption spectra from unexpected chemical compounds may appear during the data acquisition phase and that these must be accounted for in the analysis for the most accurate data.

8.3.3 Additional Sections Referenced. Section 9.2 is referenced in this section.

8.3.4 Methodology. While FT-IR spectra can in fact be acquired before it is known exactly what wave number region to use for any particular gas in the analysis, this is never a good idea. If on-line analysis is a requirement then the wave number regions must be selected first.

When starting, the operator must be aware that this is likely to be an iterative procedure and some wave number regions may be rejected in the process. The selected wave number region can be quite narrow, but there are some dangers in selecting a very narrow region. It is best if the operator at first selects the entire absorbing band structure, using the end points as the 1% absorbance values relative to the peak. If narrowing the wave number region becomes necessary, the operator should be aware that the selected wave number region should always encompass the largest possible range in absorbance.

This procedure starts by an examination of the absorption spectrum of the target gas and selection of the absorption feature that has the highest absorption coefficient and is outside the strong absorption regions of water vapor and carbon dioxide. The wave number region to use is the region that is covered by the entire peak under study. It is not necessary to include any wave number region whose relative absorbance is less than 1% of the peak. The absorption coefficient is calculated and the expected absorbance is calculated by using the anticipated concentration at the site. This absorbance is compared to the noise equivalent absorbance obtained from Section 9.2. If the expected absorbance is not 3 times higher than the noise equivalent absorbance, then that wave number region should be rejected. It is likely that if the anticipated absorbance does not meet this criterion then measurement of that particular gas will have to be rejected because the remaining absorption coefficients will be too small.

If that test is passed the procedure continues. The absorption features of all the other gases known to be present at the measurement site are then compared to the target gas for possible interferences. If the total interference is thought to be too strong, the wave number region is rejected and the process is started over with a different absorption feature. If all of the features in the target gas are rejected, the gas concentration cannot be measured by FT-IR.

To calculate the absorption coefficient for any particular feature, the operator must measure the absorbance of the feature being used at the peak of the feature. This is done by using the reference spectrum. Then by using the expression $\alpha = A/cl$ the absorption coefficient α is determined. The A in this expression is the peak absorbance measured from the reference spectrum, and the cl is the concentration-path length product also obtained from the reference spectrum.

Once α is obtained, an estimate of the peak absorbance can be made as follows. Use the expression $A = \alpha cl$, where the c is the anticipated concentration at the site and l is the anticipated path length. The

c and the l used here must have the same units (e.g., ppm, meters) as the reference spectra. The calculated A is then the anticipated peak absorbance at the site.

To judge whether a particular gas is a possible interfering species, a comparison of the absorption features must be made. This is initially done by simply comparing the spectra of all the other compounds known to be present at the site with the absorption feature under study. If any overlap between the two spectra exists the gas must be considered an interfering species.

To judge the strength of any interfering species the absorption coefficients of the interfering species must be calculated as above and an estimate of the anticipated absorbance at the measuring site made. In measuring the correct absorbance to use for the interfering species, the operator should use the highest absorbance of the interfering species spectrum within the overlapping wave number region. Note that the actual peak absorbance of the interfering gas may very well fall outside the overlap region. The absorption coefficient and the anticipated absorbance at the site for the interfering species is then determined exactly as described above. Then the fractional overlap of the spectra must be determined and the estimated impact on the actual measurement is made.

To determine the fractional overlap, measure the wave number region of the overlap in the spectra and then divide that by the entire wave number region selected for the target gas. The measurement should be made by using the 1% relative absorbance wave numbers of the interfering species.

To estimate the strength of the overlapping absorbing feature, multiply the fractional overlap of the interfering species by the anticipated absorbance at the site (for the interfering species). Then divide that product by the anticipated absorbance at the site for the target gas. The total interfering strength is then the sum of all the strengths for the individual interfering species.

The classical least squares technique is a very powerful tool for analysis and can determine the presence of very small quantities of gas in the presence of a fairly large interference. While no hard rule can be given, the operator should be concerned and at least attempt to find another wave number region if the total strength of the interfering species is more than 5 times the anticipated absorption of the target gas at the site.

If the operator rejects the wave number region, then the process is repeated with the next highest absorption coefficient and so on until a suitable wave number region is found. The operator is advised to record a table of these wave number regions in a permanent notebook for the specific gases that he is working with. It is likely that these calculations will have to be done only once for any particular target gas.

8.3.5 Procedure

8.3.5.1 Examine the reference spectrum of the target gas and select the absorbance feature with the highest absorbance that is outside the strong absorbance of water and carbon dioxide.

8.3.5.2 Record the wave number region using the relative 1% absorbance peaks as the end points.

8.3.5.3 Calculate the absorption coefficient α using the peak absorbance.

8.3.5.4 Calculate the anticipated absorbance at the field site using the α from Section 8.3.5.3, the concentration anticipated at the field site, and the path length anticipated at the field site.

8.3.5.5 Compare the result of Section 8.3.5.5 with 3 times the RMS noise calculated from Section 9.2.

8.3.5.6 Compare the absorbance spectra of all the gases known to be present in the atmosphere at the site. Record any overlaps with the selected region.

8.3.5.7 Calculate the following.

8.3.5.7.1 The absorption coefficient α of the interfering species using the peak absorbance in the overlap region.

8.3.5.7.2 The fractional overlap.

8.3.5.7.3 The anticipated strength of the interfering species.

8.3.5.7.4 The sum of the interfering strengths.

8.3.5.8 Accept or reject the wave number region.

8.3.5.9 If necessary repeat Sections 8.3.5.1 through 8.3.5.8 with the next highest absorbance peak.

8.4 Generation of a Background Spectrum

8.4.1 Purpose

8.4.1.1 This section instructs the operator on how to generate a background spectrum that can then be used as I_0 in Beer's law. A background spectrum can be generated by several methods. These methods are (a) the upwind background, (b) the cross-path background, (c) the zero target gas background, and (d) the synthetic background. The first three backgrounds are generally used with no further processing, but the synthetic background has to be made. Each is briefly discussed below.

8.4.1.2 Since the synthetic background is the only one that requires computer processing, it is the one for which the actual steps are given in this procedure.

8.4.2 Assumptions

8.4.2.1 The wave number regions for the analysis have previously been chosen.

8.4.2.2 Field spectra have been acquired, and one of them is to be used for a synthetic background.

8.4.2.3 Software is available that allows a synthetic background to be made.

8.4.3 Additional Sections Referenced. No other sections are referenced.

8.4.4 Methodology. In the derivation of Beer's law, one calculates how much the intensity of the infrared source diminishes as the energy traverses an absorbing medium. To calculate the concentration of the gas, the operator must compare the initial intensity obtained in the absence of the target gas with the measured intensity obtained when the target gas is present. This initial intensity is called the background, and it is the response of the instrument to the infrared source in the absence of any absorbance due to the target gas. A variety of phenomena are responsible for the shape of the background curve. A number of these phenomena are related to the instrument, but the predominant atmospheric process that shapes the background is the absorbance due to water vapor.

If any absorbance due to the target gas remains in the background, the absolute values of the gas concentration cannot be measured. In this case, only values relative to the concentration in the background will be obtained.

The upwind background is one that is predominantly used at smaller sites, where it is fairly simple to move the system from one side to another. Once the wind direction is known, the system is set up so that the path is along the upwind side and a spectrum that is to be used as a background is acquired. This procedure is normally done twice a day (morning and evening), and these spectra are generally used as backgrounds with no further processing.

The argument is made that an upwind background will contain only target gas concentrations from upwind sources. The remaining downwind field spectra will then give correct values from gases at the site alone. While this is a valid argument, it is not a very strong argument for the use of an upwind spectrum, and any variability in the upwind sources may erroneously be interpreted as variability of the target gas concentration at the site itself. Also to be noted when using such a spectrum is that it may not be valid for the entire time period the operator intends. As the water vapor concentration changes, the curvature of the baseline in the spectra changes also. This will give rise to high error bars (as calculated from classical least squares) and to variability in the target gas concentration that follows that of water. When that occurs, this background (or any background) may no longer be valid.

The cross-path background is taken with an optical path placed along one side of the site and with the wind velocity parallel to it. This background is generally used when the geometry of the site allows it, and it supposedly has no target gas concentration. This type of background may also pose some unwanted problems. If the wind is very light, then the gases from the site can indeed diffuse into the optical path. Target gas concentrations from elsewhere may be present, and interpretation may present the same problems described above.

Some researchers have obtained a background spectrum by simply waiting long enough for the gas concentration to go to zero. This method will not work for gases that are always present in the atmosphere, such as methane or carbon monoxide. This procedure may be used if there is sufficient time in the program for the waiting period and if real-time analysis is not an immediate requirement, but it is not clear whether the water vapor concentration will be in a satisfactory range. Also, the operator should not expect any one background to remain valid for more than a few days, and then a new background must be obtained.

If the measurement program merely requires a "yes" or "no" response to the question of whether a compound is present, then any spectrum that is taken may possibly be used for a background. If possible, the operator should use a spectrum that has a minimum of the target gas, but that is not necessary if the analysis software allows negative numbers. (Note that it is the difference of the concentration in the two spectra that will be measured.)

If, however, the absolute values of the concentration of the target gas in the optical path are required by the measurement program and no applicable spectrum can be found that is void of the target gas absorption, a synthetic background must be used. A synthetic background is one that is made from a single beam field spectrum, and it may have some of the target gas in it. Once a field spectrum has been selected, a new baseline is made to replace all the absorbance features in the wave number region used for analysis with a new curve that resembles the instrument baseline as closely as possible. This new baseline is made by connecting the data points along the original baseline with straight line segments, or by some other appropriate fitting procedure, thereby removing any absorbance features. The difficulty with this method is knowing where the baseline actually is. No points within any absorbance feature of the original spectrum can be used. A portion of a field spectrum and the synthetic background made from it by connecting the data points with very short straight line segments is illustrated in Figure 4. The original field spectrum has absorption lines due to water vapor in it.

Selecting the points for the baseline for a synthetic background may be quite difficult when large wave number regions are used or when the curvature of the baseline is high. This is a problem with the wave number region used for the analysis of ozone, for example.

8.4.5 Procedure

8.4.5.1 From the set of available spectra, select one spectrum by using the following criteria.

8.4.5.1.1 The target compound concentration should be near a minimum.

8.4.5.1.2 The interfering species concentration should be at a minimum.

8.4.5.1.3 The vapor pressure concentration should be in the mid range of water vapor concentrations during the period for which the background is to be used.

8.4.5.1.4 The return intensity at 987 cm^{-1}, 2520 cm^{-1}, and 4400 cm^{-1} should be normal for this instrument and for the particular path length used.

8.4.5.2 Once the candidate spectrum has been selected, use the available software to create a synthetic background.

8.5 Production of a Water Vapor Reference Spectrum

8.5.1 Purpose. This section instructs the FT-IR operator on how to create a water vapor reference spectrum from a single beam field spectrum. Absorption due to water vapor represents an interference to the spectral region of the target gas, and these interferences must be accounted for in whatever analysis routines that are finally used. Water vapor presents the predominant absorption features in the spectra acquired by the FT-IR, and the operator can expect it to interfere with the target gas spectrum. It is essentially impossible to create a water vapor reference spectrum in the laboratory by using a cell because the concentrations required are not normally attainable, and measuring the amount of water vapor in the cell is very difficult. Therefore, the water vapor reference spectrum has to be made from the acquired field spectra. Fairly large changes in the atmospheric concentrations of water vapor can occur rapidly, and that generally implies that a new water vapor reference spectrum has to be created.

8.5.2 Assumptions

8.5.2.1 The wave number regions for the analysis of the remaining spectra have previously been chosen.

8.5.2.2 Field spectra have been acquired, and one of them is to be used for a water vapor reference spectrum.

8.5.3 Additional Sections Referenced. Activities and evaluations performed in Section 8.4 are referred to in this section.

8.5.4 Methodology. The first step in the process of creating a water vapor reference is the selection of a single beam spectrum from the set available. The selection is based on a number of criteria. During the process, any absorbance due to the target gas must be subtracted from the water vapor reference. This can be done in a number of ways, but until the operator gains some familiarity with the FT-IR analysis process, it is best to do this by starting with a spectrum that contains a reasonable amount of the target gas and any other interfering species. In this way it may be possible for the operator to see the absorbance feature and do the subtraction interactively. Otherwise, the concentration of the target gas needs to be measured by using an analysis routine and then subtracted by using the library reference spectrum.

There is also some argument that can be made to specifically acquire a spectrum with a large number of scans and to use that as a water vapor reference spectrum. The large number of scans ostensibly gives a smaller noise value. This argument is not generally true with the FT-IR systems because the calculated RMS noise is not usually generated by the system electrical noise. The majority of the calculated RMS noise seems rather to be the result of slight changes in the water vapor concentration and other atmospheric constituents from one spectrum to the other.

From the set of available spectra, one spectrum must be selected by using the following criteria.

- The target compound concentration should not be near a minimum. As the operator gains more experience at creating a water vapor reference he may want to minimize the target gas absorption if possible.

- The interfering species concentrations should not be near minima.

- The vapor pressure concentration should be in the mid range of water vapor concentrations during the period for which this particular water vapor reference spectrum is to be used. It should be remembered that many of the water vapor lines may be saturated as far as the instrument response is concerned. That implies that the time period that can be covered with any one water vapor spectrum must be carefully chosen. However, at the present time no explicit guidance concerning the length of time that a single water vapor reference is valid can be given. Perhaps the best advice is to compare the curvature of the baselines of the single beam spectra. If that is changing rapidly, a new water vapor reference spectrum may have to made.

- The return intensity at 987 cm^{-1}, 2520 cm^{-1}, and 4400 cm^{-1} should be normal for this instrument and for the particular path length used. Any spectrum that has been acquired in foggy or rainy conditions should not be used.

The last criterion is included as a check to determine that the instrument is operating correctly.

Once the candidate spectrum has been chosen, it must be turned into an absorption spectrum by using the background spectrum created in Section 8.4.

The new water vapor absorbance spectrum must now be analyzed for the presence of absorbance due to the target gas. To accomplish this, the normal analysis procedure can be used if an older version of the water vapor reference spectrum already exists. It is likely that using the older water vapor reference will result in somewhat higher error bars from the analysis. At the present time this can be ignored. The results of this analysis should be zero, but it can give a positive result if there is an absorbance due to the target gas in the newly created water vapor reference. If a positive value exists then that amount of the target gas must be subtracted from the water vapor reference spectrum. The exact procedure to use for the subtraction process will depend on the software that the operator has.

If no other water vapor reference exists, the following procedure must be used. A set of 15 pairs of spectra must be acquired with the FT-IR. They should be taken so that no time elapses between them. They should be acquired with the same number of scans and the same resolution as the newly created water vapor reference spectrum. The individual 15 pairs are used to create 15 absorbance spectra. These spectra should not contain any of the target compound absorbance because they have been taken back-to-back, and it is hoped that each will contain the same amount of the target gas absorption. These spectra must then be analyzed for the target compound by using the newly created water vapor reference.

The average value of the results of this analysis should be zero. If it is not but some positive or negative bias exists, some amount of the target compound absorbance is still in the water vapor reference spectrum.

There are two possibilities to consider if a bias exists. The first is that the baseline of the newly created water vapor reference is not quite correct, and the second is that some of the target compound must be subtracted from the newly created reference spectrum. (This can give rise to either a negative or a positive bias.) At the present time no procedure exists to correct for curvature of the baseline. If the operator decides that baseline curvature is the primary problem, then there is little that he can do to correct the problem.

If a bias exists that is not from a baseline curvature then the operator must subtract some of the target gas from the newly created water vapor reference. If an interactive software mode for subtraction exists, the subtraction can be done in an interactive mode using the target gas reference spectrum as the subtrahend. If an interactive software mode is not available, the target gas reference can be used as follows. The target gas reference spectrum can be multiplied by an appropriate factor and the result subtracted from the newly created water vapor reference. The path length at which the water vapor reference spectrum was acquired is known and the target gas concentration is known in parts per million from the analysis above. The reference spectrum absorbance is given in terms of parts per million meters. So the operator must divide the absorbance of the spectrum by the path length in meters and by the ratio of the concentrations (reference/calculated). The resulting spectrum can then be subtracted from the created water vapor reference.

Repeat the analysis procedure and this process until the target gas concentration is zero.

8.5.5 Procedure

8.5.5.1 Select the single beam spectrum that is to be used for a water vapor reference using the criteria listed above.

8.5.5.2 Create an absorbance spectrum using the appropriate background spectrum.

8.5.5.3 Analyze the newly created water vapor reference for the target gas.

8.5.5.4 If necessary, subtract the proper amount of the target gas absorption from the water vapor reference.

8.5.5.5 Reanalyze the water vapor spectrum.

8.5.5.6 Repeat Sections 8.5.5.3 through 8.5.5.5 until the target gas concentration is zero.

8.6 Subtraction of Stray Light or Black Body Radiation

8.6.1 Purpose. This section instructs the operator how to subtract the stray light or black body radiation measured by the instrument from the field spectra. This procedure can be used by operators using either the monostatic or the bistatic instrument configurations. The subtraction for either configuration is performed by using single beam spectra.

8.6.2 Assumptions. Assumptions. For both the stray light component and the black body radiation component measurement the instrument must be operating at its equilibrium conditions. That is, the FT-IR must have been allowed to warm up. As long as the operating conditions are not changing rapidly, the spectra should be acquired by using a large number of scans so as to provide a good signal-to-noise ratio. Since these spectra have to be subtracted from the field spectra, noise will be added to the analysis, and a longer acquisition time minimizes the electrical noise. Acquiring data for up to one half hour is satisfactory. Not much is gained in the signal-to-noise ratio by acquisition times longer than that.

8.6.3 Additional Sections Referenced. No other sections are referenced.

8.6.4 Methodology. The procedure for subtracting stray light is primarily to be used for the removal of a spurious signal from FT-IR instruments using the monostatic configuration with a second beam splitter. While it is possible to have scattered light that gives rise to unwanted signals in instruments

using the other geometric configurations, this component is very difficult to measure and is considered to be a difficulty that the manufacturer has to deal with. This type of stray light subtraction will not be discussed further in this method. Instrument manufacturers strive to have the stray light as small as possible compared to the intensity returning from the retroreflector, but to remove it all can be a formidable task, and it should therefore be measured and subtracted. It is fairly simple to show mathematically that, whatever percentage of the return intensity the stray light intensity represents, that percent error will be carried through to the final result in the analysis. The presence of stray light can sometimes be detected visually in the single beam spectrum as is shown in Figure 3. Therefore, it has to be subtracted from the spectra if the errors in the data are to be minimized. The intent of the specific program may indicate it is not necessary to subtract the stray light spectrum from the field spectra; an example is when only the identification of compounds is necessary.

Once the stray light intensity is known and measured it should not change unless some component of the optical system is changed or reoriented. Therefore, the stray light spectral subtraction can easily become part of the routine analysis. Since the stray light component is generated inside the instrument, its intensity is not path-length dependent. This means that the stray light will change its intensity relative to the return intensity as the path length changes. It can easily be measured by simply slewing the instrument away from the retroreflector and acquiring a spectrum.

The need to subtract the black body radiation arises only in bistatic systems that have an unmodulated source at one end of the physical path. It is convenient to think that the black body radiation comes from the fact that the field of view of the receiving telescope is larger than the angle that the infrared source subtends; therefore, the instrument allows the infrared energy from the surroundings into the system. This is only partially true, and if the instrument is at the same temperature as the surroundings, the black body radiation can be thought of as coming entirely from the instrument enclosure. That is because all black body radiators at the same temperature radiate the same amount of energy per unit area. Therefore, the easiest way to measure the black body spectrum is to turn the source off and then acquire a spectrum.

There is an additional problem with the black body radiation curve that occurs when the instrument is pointed at the sky. When this situation occurs it is very likely that there will be an emission spectrum superimposed on the black body curve. The emission spectrum arises from several atmospheric gases and is quite variable. Even the smallest amount of cloud cover will dramatically change the intensity of this spectrum. That fact makes it almost impossible to subtract the emission spectrum totally. It is advisable to avoid pointing the instrument so that it has the sky in the field of view. If that cannot be avoided, the operator should be aware that higher than normal errors can occur in the data in the region below about 1050 cm^{-1}.

Small changes in the ambient temperature (10 ^{o}K) are not thought to be significant in the black body radiation, and thus one spectrum should be usable for an extended period. These spectra should be subtracted from the field spectra after the single beam spectra have been obtained. If the interferograms are subtracted and the single beam is then calculated, a different result is obtained. The reason for that is not fully understood at this time.

8.6.5 Procedure

8.6.5.1 Measure the stray light in the instrument by slewing the instrument off the retroreflector.

8.6.5.2 Subtract this spectrum from each single beam field spectrum before proceeding with the analysis.

8.6.5.3 Measure the black body radiation spectrum by turning the source off.

8.6.5.4 Subtract this spectrum from each single beam field spectrum before proceeding with the analysis.

8.7 Generation of an Absorbance Spectrum

8.7.1 Purpose. This section instructs the operator on how to generate an absorbance spectrum from the field spectra and an appropriately chosen background spectrum.

8.7.2 Assumptions. The following assumptions are made.

8.7.2.1 An appropriate background spectrum is available.

8.7.2.2 All the field spectra have been converted to single beam spectra.

8.7.2.3 All the field spectra have been corrected for stray light and the black body radiation if necessary.

8.7.3 Additional Sections Referenced. No other sections are referenced.

8.7.4 Methodology. Beer's law is the underlying physical law that governs the way the least squares analysis is performed. Mathematically, Beer's law is written as $I(\nu) = I_0(\nu)\exp(-\alpha CL)$. In order to calculate C, the concentration of the gas in the atmosphere, one must divide by I_0 and take the logarithm of the result. That gives $\ln(I_0/I) = \alpha CL$. The spectrum described by the term $\ln(I_0/I)$ is called the absorbance spectrum. The FT-IR analysis is actually done by using the logarithm to the base 10, but this is normally transparent to the operator.

All software packages that are available for least squares analysis allow the generation of an absorbance spectrum. The operator is generally asked to supply the background spectrum, but then the process is mathematically performed by the computer. It is important to understand that some correction may be necessary to the field spectra before they are converted to absorbance spectra.

8.7.5 Procedure. Use the available software to create the absorbance spectra.

8.8 Correction for Spectral Shifts

8.8.1 Purpose. This section instructs the operator on how to align two spectra so as to minimize the errors involved with spectral shifts.

8.8.2 Assumptions. The field spectra have been acquired and are in the single beam format. A water vapor reference that is to be used for analysis is available. A background spectrum has been prepared and is available for use. In order to check for a shift between the field spectrum and the reference spectrum, an absorbance spectrum must be used if the reference spectrum is an absorbance spectrum.

8.8.3 Additional Sections Referenced. No other sections are referenced.

8.8.4 Methodology. There are three ways that a spectral shift will affect the FT-IR data analysis. The first is when a spectral shift between the field absorbance spectrum and the water vapor reference spectrum exists. The second is when a spectral shift between the field absorbance spectrum and the library reference spectrum for the target gas exists. The third is when a nonsynthetic background is used and a spectral shift exists between the background and the field spectra. A spectral shift compared to the instrument may also be noticed when new reference spectra are purchased or produced on an instrument

other than the one used for data acquisition. The first two of these comparisons are done using absorbance spectra, but the third must be done with single beam spectra.

When a synthetic background is used, any spectral shift between the field spectrum (single beam) and the background spectrum (single beam) is irrelevant. That is because the synthetic background generation process does away with all spectral features of interest.

A question arises as to what sort of a shift is really important to the analysis. Some researchers discuss this in terms of absolute quantity of wave numbers. This is not really satisfactory because then apparently small shifts are important for some spectral features while at other times they are not. If a Gaussian shape is used to describe the absorption line shape, then it is possible to show mathematically that when the absorption feature of interest shifts by about 10% of the line width (FWHH), a 5% error occurs in the least-squares analysis. If a Lorentzian line is used to describe the actual line shape, the shift can be about 15% of the line width (FWHH) before a 5% error occurs when least-squares analysis is used. Experimentally, if a 5% error is acceptable, it is only seldom that line shifts will be important. However, if a 1% error is all that is allowed by data quality objectives, then the same calculations show that a 0.5% shift (FWHH) of the line is all that can be tolerated. This really implies that wave number shifts will probably not be important when broad absorption features (such as presented by ozone) are used but will be crucial for narrow absorption features (such as presented by carbon monoxide). The predominant spectral feature in the FT-IR open path field spectra is water vapor, and the pressure-broadened lines of water have a line width (FWHH) of about 0.2 cm^{-1}. Since water is the predominant feature, the errors produced by the classical least-squares technique will be primarily caused by how well water is handled in the analysis. That means that water vapor must always be checked for shifts.

Experience has shown that when a spectral shift occurs, the magnitude of the shift is different in the C–H (2900–3000 cm^{-1}) stretch region than it is in the fingerprint region. This implies that all line shifts are caused by some change in the interferometer and/or the system optics. If that is truly the case, then the shift is linear in wave number, and a linear correction must be applied when the correction is made throughout the field spectrum. Some computer software automatically identifies a wave number shift and then shifts the entire spectrum by the proper amount. If that software is available it should be used.

The best place to determine whether a shift has occurred is in the low-wavelength or high-wave-number end (in the region of the C–H stretch) of the spectrum. It may also be possible to automatically determine during the acquisition phase whether a shift has occurred and then shift each individual spectrum as it is being acquired. To do that, some known spectral feature present in every spectrum must exist. Thus it may be possible to select some water vapor line that is present in all the spectra covering a particular time period and compare all the spectra with that particular line. A shift of that kind guarantees that all the field spectra are aligned one to the other but does not automatically guarantee that the field spectra and the reference spectra will be aligned. At any rate, at the present time no such line has been agreed upon, and it may not be possible to select a single line for all occasions.

If shifting software is not available, two problems are presented to the operator. The first is how to recognize a shift and the second is how to correct for it over the entire wave number region.

Recognizing that a shift has occurred can be facilitated by subtracting one spectrum from another. If a small (less than the line width) shift has occurred, the difference will appear as an "S"-shaped curve. This kind of curve is closely related to the first derivative of the line shape if the shift is small.

Determining the absolute magnitude of the shift can be a difficult task, and no simple mathematical relation exists between the features of the S-shaped curve and the magnitude of the shift. At the present time, the best estimate of the magnitude of the shift is obtained from measuring the difference of the peak positions of the two lines. However, this is best done on spectra that have been interpolated to increase the number of data points. Or, if the operator so chooses, he may zero fill the interferogram by a factor of 2 or 4 in order to increase the number of data points.

Since the correction for a shifted spectrum is most likely linear in wave number, the shift must be done in steps if appropriate software is not available. A shift between the individual library reference spectra and the field absorbance spectra can be overcome because the library spectra can be individually shifted. It may also be possible (depending on the software available) to rename the water vapor reference spectrum so that there are two or three of them, each with its own shift, and then do all the analysis simultaneously. The same procedure can be used to overcome a shift between the field spectra and the background spectrum when a synthetic background is not used. However, if the shift is small (less than the data point spacing) but significant, then all the spectra may have to be interpolated or zero filled to correct for the shift.

8.8.5 Procedure (applicable when shifting software is not available).

8.8.5.1 Subtract the two spectra and examine the residual for an S-shaped curve. Do the background and the field spectra first because these have to be done with single beam spectra.

8.8.5.2 Determine the magnitude of the shift by comparing the peaks of the individual lines.

8.8.5.3 Shift one spectrum with respect to the other. This will have to be done in the target gas analysis regions and may have to be done several times.

8.8.5.4 Create absorbance spectra from the field spectra and the background and repeat Sections 8.8.5.1 through 8.8.5.3.

8.8.5.5 Perform a correction for shift to the water vapor reference spectrum, the reference spectrum, and the background if necessary. The field spectra should not be shifted, as this requires the most time.

8.9 Analysis of the Field Spectra for Concentration

8.9.1 Purpose. This section instructs the user on the procedures used for the analysis of FT-IR absorbance spectra in order to produce gas concentration values.

8.9.2 Assumptions. The spectra have been converted to absorbance spectra and all changes and corrections listed in the above sections have been made to them. A set of reference (library) spectra that includes the target gas, the interfering gases, and a water vapor reference is available for use. A software package that is capable of performing least squares analysis on the spectra is available.

8.9.3 Additional Sections Referenced. No other sections are referenced.

8.9.4 Methodology. There are a number of ways to analyze the spectra in order to obtain concentration data. These include peak height or peak area analysis, spectral subtraction, partial least squares, iterative least squares, principal component analysis, etc. While these methods are all usable, this procedure uses classical least squares as described mathematically by Haaland and Easterling (13). The use of classical least squares requires that the spectra be prepared in a specific way for the analysis to work efficiently and effectively. Thus the majority of Compendium Method TO-16 is concerned with preparation of the spectra.

It is likely that, when the other techniques cited above are used, the data will have to be prepared in a different manner. Under those conditions the steps of this procedure that deal with spectral preparation are not usable.

Whatever software is available to perform the classical least-squares technique, it must be able to perform the analysis of a single target gas in the presence of interfering species. It is only seldom that the range of wave numbers used for the analyses will be free of absorbances due to interfering species. This is particularly true of water, and the analysis routines must be able to perform a multiple linear regression of the field spectra.

There are a number of software packages that are in use that perform classical least-squares analysis of the spectra. These all have somewhat different user interfaces and operating conditions, but in all cases the mathematical algorithms are transparent to the user. Therefore, the software packages are not described in detail here. Since the classical least-squares analysis is a multiple linear regression, it must have certain items available for it to function. The items that are common to all available analysis packages include the target gas reference spectrum, the background (or I_0) spectrum, the water vapor reference spectrum, and whatever interfering gas reference spectra are necessary. Most software packages are, however, only available with the FT-IR instrument itself. The primary concern for this procedure is that the analysis itself follows the classical least squares described mathematically by Haaland and Easterling (13).

8.9.5 Procedure. The individual steps in this section are dependent on the specific software available to the operator. Since the individual packages are not described here, the specific steps required for any one package are not either.

8.10 Post-Analysis Review of the Data

8.10.1 Purpose. The purpose of this section is to provide the operator with a way to check the data for possible problems. This procedure primarily makes use of plotted data in the form of the concentration of one gas plotted against the other and of time sequence plots. There is one statistical determination that can be used to determine if correlations exist between pairs of data. The primary tool used here is for the operator to look for trends in the data where none should exist. The specific tests of the data are described below.

8.10.2 Assumptions. The only assumption is that all of the spectra have been analyzed by use of the least-squares analysis software.

8.10.3 Additional Sections Referenced. No other sections are referenced.

8.10.4 Methodology. The operator should make several plots of the concentration data. The first should be a set of plots of target gas concentration versus time. These plots should be examined for any expected trends in time. For example, ozone in rural areas generally follows a diurnal pattern with a minimum at about 0600 hours and a maximum at about 1500 hours. The concentration values should not go negative to any great extent; although around zero concentration the values may go slightly negative, the average value over time should be zero. Suppression of negative values should never be done in the analysis because then a zero average can never be achieved. If values go negative with time in a regular fashion, then something is amiss with the data. The most likely case is that there is a small remaining absorbance due to the target gas in the water vapor reference spectrum. If the concentration values are much higher than the anticipated values, there may also be a problem with the water vapor reference spectrum. In this case there may have been too much of the target gas absorbance subtracted

from the water vapor reference. If that is so, the water vapor reference should be fixed and then the data reanalyzed.

Plots should be made of the target gas concentration versus the water vapor. If the variability of the target gas and the water vapor are correlated and this is not expected, the water vapor reference spectrum must, in most cases, be corrected.

The next step is to plot the concentration values of those gases whose concentrations are expected to be correlated. This includes any gases that are derived from the same source. If the variability of these gases is not correlated, the data must be carefully examined for the cause. There are no good guidelines to judge what is causing that problem, but a nonlinear response of the instrument for one of the gases is a possibility. If that is suspected, the operator must carefully examine the QA data for possible clues.

Another check of the instrument can be made by analyzing the spectra for N_2O. Nitrous oxide is present naturally in the atmosphere with a concentration very close to 300 ppb. The variability in this concentration should be less than $\pm 10\%$. If this is not the case then all the data must be suspect. Another gas that is always present in the atmosphere is methane. The variability of methane can be fairly large, particularly in the proximity of landfills. That means it is somewhat more difficult to use as a quality check of the data but it can still be used. The value of the atmospheric concentration of methane should never fall to less than about 1.7 ppm.

If the FT-IR instrument is a bistatic one and there is any possibility that the instrument was admitting energy from the sky when the black body radiation measurement was made, there might be a problem with the observed detection limits. If that occurs, it is possible that the analysis is flawed because of emission spectra in the black body radiation.

Another check for the quality of the data can be obtained by examining the errors calculated by the least-squares analysis routine. If there is an abrupt change in the relative error and no obvious reason such as an abrupt change in the water vapor concentration, it may be that a new interfering species, not accounted for in the analysis, has been measured.

Once these checks have been made on the data, the operator must follow the data quality checks that have been written for the specific program that is being studied.

8.10.5 Procedure.

8.10.5.1 Plot the data as a function of time and check for unexpected trends.

8.10.5.2 Plot the target gas data concentration as a function of water and determine if the variability is correlated.

8.10.5.3 Determine whether N_2O and CH_4 have been correctly measured.

8.10.5.4 Determine whether correlation of the data exists where correlation is expected.

8.10.5.5 Review all the QA/QC data taken in compliance with the specific data quality objectives.

9. Quality Assurance

9.1 Summary

The section provides guidance to the operator in determining how well the FT-IR sensor is operating. While this section is labeled "quality assurance", it is by no means adequate to serve as a quality assurance project plan or program plan. Project and program plans are meant to address the specific data quality objectives of a monitoring program, and the final use of the FT-IR data and cannot be adequately covered in this document. Some of the procedures are limited in scope because a satisfactory procedure has not been developed at this time.

9.2 The Determination of Method Noise or Method Noise Equivalent Absorption

9.2.1 Purpose. The purpose of this section is to allow the operator to determine the method noise. This determination should form part of the routine quality assurance checks made of the instrument. It should be made at least once a day for extended programs and every time the instrument is moved or otherwise changed. This procedure is used to judge whether the instrument is operating properly but not as a gauge of the quality of the data.

9.2.2 Assumptions

9.2.2.1 This procedure assumes that spectra have been acquired with the same operating parameters (number of co-added scans, resolution, etc.) as the field spectra. The one exception is that the spectra used to determine the method noise should be taken so that no time elapses between them.

9.2.2.2 It is also assumed that software exists that will allow this determination to be made automatically by computer.

9.2.3 Additional Sections Referenced. No other sections are referenced.

9.2.4 Methodology. Instrumental noise is generally considered to be the random fluctuations in the recorded signal. That is not exactly true for the FT-IR system when the data are acquired along a long, open path. Evidently, the time required to allow small but measurable changes in the gaseous atmospheric constituents is short compared to the normal acquisition time of the spectra. Because of that, when two spectra are used to create an absorbance spectrum there is a variability in the result that is not electronic noise alone. This is defined here as the method noise. It is important because it cannot easily be done away with and will contribute to the error of the measurement.

The determination of method noise uses the statistical quantity called the RMS deviation. The mathematical routine normally used for this calculation performs a linear least-squares fit (linear regression) using the data points over a specified wave number region and calculates the RMS deviation from that line. The RMS deviation is defined as the square root of the sum of the differences squared divided by the quantity N-2. The number N is the total number of data points. The differences are calculated by taking the difference between the actual data point and the line; they are then squared and added.

The actual range of wave numbers that can be used changes with resolution, but the number of data points does not. The number of data points used should be 80 points. Thus for a 1-cm^{-1} resolution, the range of wave numbers is 40, because the instrument acquires a data point every half resolution unit. Since this measurement is considered to be the determination of an instrument parameter, the wave

number region or regions should be chosen to minimize the effect of water vapor. The water vapor concentrations along the path are known to change rapidly, and that will perhaps cause most of the variability in the signal.

The two single beam spectra that are used to measure the noise should be taken without any time lapse between them. These two spectra are then used to create an absorbance spectrum. Which of the two that is used as the so-called background is irrelevant. Three wave number regions are then used for this determination. For this procedure, the regions are based on a 1-cm^{-1} resolution and are 968–1008, 2480–2520, and 4380–4420 cm^{-1}, respectively. Other regions may be used, but the operator should try to cover the range of wave numbers that are being measured. The 80 data points used in the measurement should also be adhered to. This data should then be recorded and plotted on a quality control chart for comparison purposes.

9.2.5 Procedure

9.2.5.1 Record two spectra with the same operational parameters that will be used for the acquisition of the field spectra. Do not allow any time to elapse between these spectra.

9.2.5.2 Create an absorbance spectrum by using either of the two spectra taken in Section 9.2.5.1 as a background.

9.2.5.3 Analyze this absorbance spectrum for the RMS deviation in the three wave number regions 968–1008 cm^{-1}, 2480–2520 cm^{-1}, and 4380–4420 cm^{-1}.

9.2.5.4 Record this data in a notebook and plot it on a quality control chart.

9.3 The Measurement of the Return Beam Intensity

9.3.1 Purpose. This section provides guidance to the measurement of the return beam intensity in the case of the monostatic system or the intensity of the IR source at the FT-IR in the case of the bistatic system. This procedure needs to be done only once as long as the detector or the infrared source does not change.

9.3.2 Assumptions. In order that these measurements be realistic, the stray light component or the black body radiation should be subtracted from the spectra. This means those measurement results should be available to the operator or should be made in conjunction with this measurement.

9.3.3 Additional Sections Referenced. Refer to Section 9.4, Measurement of Stray Light, and Section 9.5, The Measurement of Black Body Radiation, if applicable.

9.3.4 Methodology. The return beam intensity determines the operational signal-to-noise ratio of the FT-IR system. This intensity is a variable and depends on the path length chosen, the water vapor in the atmosphere, and other atmospheric conditions. The primary atmospheric conditions that make the return beam intensity change are fog, rain, snow, and sleet. Of these, fog has by far the largest effect. Another cause for a change in the return beam intensity is pollen in the atmosphere. This happens in the spring in areas where there are a large number of pine trees. Finally, for the monostatic geometry, which uses a retroreflector, condensation on the mirror can make dramatic changes in the return beam intensity. There are also instrumental causes of changes in the return beam intensity but they are beyond the scope of this document.

For these reasons, it is prudent to include in a quality assurance program the measurement of the return beam intensity. If the return energy has been degraded by an unacceptable amount, the operator must change the length of the path. Whether the return is acceptable or not is dependent on the data quality objectives from the quality assurance program plan.

This procedure is separated into two parts. The first is a procedure for measuring the return beam intensity as a function of path length. The second is the measurement of return beam intensity as a function of time.

There are two reasons to measure the return beam intensity as a function of path length. The first is to determine when the energy becomes intense enough to saturate the detector. The second is to determine when the infrared energy becomes too small to measure. These measurements then determine experimentally the minimum and maximum usable path length. There are a number of reasons why the return beam intensity should be monitored as a function of time. The primary one is that the return beam intensity will change according to varying weather conditions. The operator must become familiar with the magnitude and the rapidity of these changes.

9.3.5 Procedure

9.3.5.1 Return Beam Intensity as a Function of Path Length.

9.3.5.1.1 Place the light source or the retroreflector at a short distance, say 25 meters, from the detector.

9.3.5.1.2 Align the system to maximize the return signal.

9.3.5.1.3 Record a spectrum and convert this spectrum to a single beam spectrum.

9.3.5.1.4 Record the intensity levels in the 987-cm^{-1} region and in the 2,500-cm^{-1} and the 4,400 cm^{-1} regions. The reason the wave numbers are not given specifically is that the operator should select a maximum in the baseline return intensity in these regions.

9.3.5.1.5 Examine the detector cutoff region at about 650 cm^{-1}. If a dip occurs in this region or the baseline is elevated above zero, then the detector is already saturated.

9.3.5.1.6 If there is no indication of saturation, move the light source or the retroreflector so that the distance separating it and the detector is smaller. Repeat Sections 9.3.5.1.1 through 9.3.5.1.5.

9.3.5.1.7 Continue this process by cutting the distance in half until the single beam spectrum exhibits saturation as described above in the 650-cm^{-1} region. Record this distance. This distance represents the minimum path length that can be used with this particular instrument without altering the instrument.

9.3.5.1.8 Next, move the light source or retroreflector to a distance of 100 m.

9.3.5.1.9 Realign the instrument to maximize the signal.

9.3.5.1.10 Record a spectrum and convert it to a single beam spectrum.

9.3.5.1.11 Record the intensity levels at the same wave numbers as used above.

9.3.5.1.12 Repeat Sections 9.3.5.1.8 through 9.3.5.1.11 by increasing the path length in 50-m increments until the intensity levels no longer change. For the monostatic geometry mode, this will occur when all the energy being recorded comes from the stray light in the instrument. For the bistatic mode, the return signal will diminish to zero in the 4000-cm^{-1} region and then will evolve into the black body radiation spectrum.

9.3.5.1.13 Plot a graph of the return intensity versus path length.

9.3.5.2 Measurement of the Return Beam Intensity as a Function of Time. At least once every day of operation the return beam intensity should be recorded at the wave number regions given above. More frequent measurements should be made when the atmospheric or other conditions listed in Section 9.3.4 occur. The atmospheric conditions should also be recorded. Water vapor plays an important role in the recorded beam intensity so that the partial pressure of water should also be calculated and recorded. A continuous plot of these data should be made showing the intensity as a function of time. The graph should include notations for the various atmospheric conditions listed above.

9.4 The Measurement of Stray Light

9.4.1 Purpose. The monostatic FT-IR systems are prone to having stray light in the instrument. To obtain the best possible accuracy, this stray light component must be subtracted from the field spectra before the analysis is performed. This section describes how to measure the stray light component and is applicable to only the monostatic geometries that modulate the beam with the interferometer before the infrared energy is transmitted along the path and that use a second beam splitter to direct the beam. There are other sources for stray light that arise from overfilled optical components. These are a problem for the manufacturer and are not addressed in this document.

9.4.2 Assumptions. The primary assumption for this procedure is that the FT-IR system being used is of the monostatic geometry. The system has been operating sufficiently long to be past any warm-up periods and it is using the same resolution as when it is acquiring the normal field spectra.

9.4.3 Additional Sections Referenced. No other sections are referenced.

9.4.4 Methodology. The easiest way to measure the stray light with a monostatic system that modulates the beam before the energy is transmitted along the path is to simply slew the system away from the retroreflector. Once this is done, the operator should acquire a spectrum using a large number of co-added scans. If the time required to acquire this spectrum cannot be at least 4 times the length of time to acquire the field spectra, he should then use the longest time possible. The issue here is one of electronic noise, and the electronic noise should diminish as the square root of the time needed to acquire the spectrum. Changes in the atmospheric constituents play no role in this measurement.

This spectrum should be saved as a single beam spectrum with an appropriate name, and it must be subtracted from the single beam field spectra before they are converted to absorbance spectra.

A second way to measure the stray light is to cover the receiving telescope with some opaque, non-reflecting material. Any material that is reflecting acts as a mirror and will give erroneous readings. Any material that is not opaque will allow some of the beam returning from the retroreflector to be transmitted to the detector. This method is not recommended.

This measurement must be done at the beginning of operation and every time the instrument is altered in any way. For those programs that are short-term field programs, the measurement should be made at the beginning of each field program.

9.4.5 Procedure.

9.4.5.1 Set up the instrument in exactly the same way as it will be used to acquire field spectra.

9.4.5.2 Slew the transmitting telescope off the retroreflector so that there is no beam return signal.

9.4.5.3 Acquire a spectrum.

9.5 The Measurement of Black Body Radiation

9.5.1 Purpose. FT-IR systems generally have a field of view larger than the solid angle that the light source or the retroreflector subtends at the far end of the path. The bistatic systems (or those that do not transmit the beam through the interferometer before it transmitted along the path), therefore, admit radiation to the detector from the surrounding background. These systems also respond to any radiation coming from the instrument itself (the instrument is also a radiator of energy). This radiation is

commonly referred to as the black body radiation and it must be subtracted from the single beam spectra before the analysis is performed. This procedure describes how to measure that radiation.

9.5.2 Assumptions. The instrument must be set up in the same manner and with the same background that will be in its field of view during the acquisition of the field spectra.

9.5.3 Additional Sections Referenced. No other sections are referenced.

9.5.4 Methodology. The FT-IR systems available today use some form of a heated element as a source of infrared energy. These elements generally have a temperature in the vicinity of 1500°K. The terrestrial surroundings in which the FT-IR operates generally have a temperature around 300°K. All things above absolute zero radiate energy according to their temperature and have a very well known energy distribution in wave number. The distribution of energy peaks at a wave number that is temperature dependent with the cooler body having a peak at lower wave numbers. Also, the energy distribution of a cooler body is lower in intensity at all wave numbers than the distribution of a hotter body. The question arises of what the ratio of intensities is of these two sources. This ratio at the peak of the 300 degree source is about 5. That is, the surroundings can represent about 20% of the energy of the source. Therefore, it must be subtracted from the spectra before the analysis is performed.

The simplest way to acquire a black body spectrum is to set up the instrument in exactly the same way it will be run to take the field spectra. A spectrum should then be acquired with the light source turned off. This spectrum should be saved with an appropriate name.

This spectrum does not appear to change dramatically when the instrument is pointed at terrestrial targets such as buildings or trees. Nor does it change dramatically with slight changes in the ambient temperature (±10°K). A 10% change in temperature will shift the peak by 10%, and that may become important. Remember, however, that a 10% change in temperature is about 30°C. The black body spectrum does, however, change dramatically if the sky is included in the instrument's field of view. In this case an emission spectrum appears from the atmosphere, and this is very difficult to handle. The black body spectrum can also change dramatically if hot sources other than the primary light source are allowed into the field of view of the instrument. The operator is advised to take precautions so that these conditions are avoided.

In order to minimize the noise introduced by the subtraction process, the number of scans used to acquire the spectrum should be large. An acquisition time of more than 15 min is probably excessive. It is prudent to run such a spectrum at least once every day during the study. These spectra should be investigated for changes, particularly when there are large swings in temperature. This is possible during the early fall, when the temperature can range from cold at night to quite warm in the daytime.

9.5.5 Procedure

9.5.5.1 Set up the FT-IR along the same path that will be used to acquire the field spectra.

9.5.5.2 Acquire a spectrum over a long acquisition time with the infrared source off.

9.5.5.3 Store the spectrum with an appropriate name.

9.6 The Determination of the Detection Limit

9.6.1 Purpose. The purpose of this routine is to provide the operator with a mechanism for determining the detection limits for the various gases. The definition of the detection limit is given here as the minimum concentration of the target gas that can be detected in the presence of all the usually encountered spectral interferences.

9.6.2 Assumptions. The instrument is operating with the same parameter settings as those used for collecting the field spectra. That is, the path length, resolution, number of co-added scans, and the apodization function are the same in both cases. If the instrument has an ancillary gas cell, this must be empty.

9.6.3 Additional Sections Referenced. No other sections are referenced.

9.6.4 Methodology. The detection limit of the FT-IR systems is a dynamic quantity that will change as the atmospheric conditions change. The variability of the target gas, water vapor, and all of the other interfering species concentrations contributes to the variability of this measurement. Some researchers have suggested that the I_0 spectrum used to create the absorption spectrum when measuring the detection limits be the same as that used for the field spectra. However, that cannot be done if a synthetic background is used since the field spectra are expected to contain some quantity of the target gas. If any other arbitrary background is used the measurement will certainly reflect the variability of the target gas, at least. To overcome most of the effects of this problem, the operator should use spectra whose acquisition times are no longer than about five minutes. If the field spectra are acquired at shorter times then the shorter time should be used. If the field spectra are acquired at longer times because the anticipated variability of the target gas is small, then it is appropriate to use the longer times.

The detection limit as determined in this procedure is the result of a calculation using a set of 15 individual absorption spectra. The 16 individual single beam spectra used for this determination are acquired in 5-min intervals and no time is allowed to elapse between them. The absorption spectra are then created by using the first and the second single beam spectra, the second and the third, and the third and the fourth, and so on until the 15 absorption spectra are obtained. These absorption spectra are analyzed in exactly the same way that all field spectra are to be analyzed and over the same wave number region. The analysis should result in a set of numbers that are very close to zero because most of the effects of the gas variability have been removed. The numerical results should be both positive and negative and for a very large set of data should average to zero. Three times the standard deviation of this calculated set of concentrations is defined to be the detection limit.

There is reason to believe that this procedure gives the most optimistic (lowest) value for the detection limit because it removes most of the effects of the interfering species. However, the other suggested procedures seem to introduce as much uncertainty, and this procedure may actually be used for further diagnostics of the post-analysis review of the data (see Section 8.10).

9.6.5 Procedure.

9.6.5.1 Acquire a set of 16 single beam spectra in exactly the same manner that will be used for the field spectra.

9.6.5.2 Use the first spectrum as a background to create an absorbance spectrum from the second spectrum.

9.6.5.3 Use the second spectrum as the background and create an absorbance spectrum from the third spectrum.

9.6.5.4 Continue this process until all 15 absorbance spectra have been created.

9.6.5.5 Analyze each of the spectra for the target gas concentration.

9.6.5.6 Calculate the standard deviation of the set of concentration values.

9.6.5.7 Multiply the result of Section 9.6.5.6 by 3 to obtain the detection limit.

9.7 The Determination of Precision

9.7.1 Purpose. Precision is a measure of the FT-IR system's ability to make repeatable measurements when challenged with the same sample. This section provides guidance to the operator on how to make that determination for some gases.

9.7.2 Assumptions. The FT-IR system has the capability for installing a gas cell in the beam so that the entire beam passes through it. This is something that the manufacturer has to build into the design of the system and is not under the control of the operator. While the measurements are being made, the instrument is operating in the same way that it is used to collect the field spectra.

9.7.3 Additional Sections Referenced. No other sections are referenced.

9.7.4 Methodology. The precision with which a measurement is made with the FT-IR instruments is, at the present time, very difficult to measure. The best method that has been suggested is one that uses a cell of some sort that is filled with a high concentration of gas and is then placed in the beam. However, this process is quite error-prone and it has not been shown to work well with a mixture of gases. A second difficulty is that it cannot be used for all the gases that can be potentially measured with the FT-IR. The primary reason is that the concentration of the gas in the cell has to be high in order to produce a measurable absorption. Many gases have a vapor pressure that is too low to achieve these concentrations. No procedure has been established for making these measurements of polar compounds. Additionally, not all the commercially available instruments have at the present time been designed to accept a cell in an appropriate position of the optical path.

However, for those instruments and for those gases that can be measured, the procedure is as follows. A cell whose length is short compared to the path length is filled with a high concentration of gas. The cell is placed in the infrared beam so that all of the energy passes through the cell. Then a set of spectra is acquired and these are converted to absorption spectra. These absorption spectra are analyzed for the target gas. The relative standard deviation of this set of measurements is given as the precision.

This procedure is also quite similar to the procedure for the measurement of accuracy. The measurement of precision, however, does not require an exact knowledge of the concentration of the gas, but rather the gas concentration must remain constant. Thus the gas concentrations used can be made up in the field at a lower cost to the monitoring program.

Determining the precision of the FT-IR monitoring system is complicated by the fact that the measurements are made over an open path in the atmosphere. It cannot be assumed that the concentration of the various atmospheric gases will be constant in time, and this fact will impact the precision measurements. This procedure calls for the precision measurements to be made by using the same path length that is generally used for acquiring field spectra. Therefore, the precision will vary in time and will be dependent on the variability of not only the target gas but also the variability of the interfering species. The precision measurement described is therefore a method precision and includes all of the parameters that must be considered in the field spectra analysis.

The cell can be filled in a number of ways, but the preferred way is to use a gas of the appropriate concentration from a prepared cylinder that has been purchased for this purpose. The proper mixture can be calculated as follows:

- The absorption coefficient of the gas can be calculated from the reference spectrum by using $\alpha = A/cl$, where A is the absorbance at the peak of the reference spectrum and cl is the

concentration-path length product, which is supplied with the reference spectrum for the reference gas.

- Next, the desired absorbance when the cell is filled is selected. This can be set at 0.05.

- Then c is calculated from $c = A/\alpha l$, where $A = 0.05$, α is the absorption coefficient calculated above, and l is the length of the cell in meters if the reference gas has a concentration-path length product in parts per million per meter.

- The concentration calculated above has units of parts per million if the concentration-path length product for the reference gas has units of parts per million per meter. This is the concentration to use when purchasing a cylinder of gas. The fill gas of the cylinder must not absorb in the infrared, and the gas preferred for this is nitrogen.

Before the target gas is introduced into the cell, the cell should be flushed with nitrogen until at least five volumes of the cell have passed through it. At the present time the preferred method for introducing the target gas is with a flowing system. The gas should remain flowing during the measurement.

9.7.5 Procedure.

9.7.5.1 Calculate the appropriate concentration for the target gas and obtain a cylinder of that concentration.

9.7.5.2 Set up the instrument as it will be used to acquire the field spectra.

9.7.5.3 Place the cell in the instrument and flush it with dry nitrogen so that at least five volumes of the cell have passed through it.

9.7.5.4 Flow the target gas through the cell, and after three volumes of the cell have passed through, acquire a set of 15 spectra.

9.7.5.5 Analyze these spectra for the target gas.

9.7.5.6 Express the relative standard deviation of this set of concentrations as the precision.

9.8 The Determination of Accuracy

9.8.1 Purpose. Accuracy is a measure of the ability of the FT-IR to measure a known concentration of gas. This procedure may allow the operator to determine the accuracy of the FT-IR measurements for some gases. This measurement is very difficult to make and no exact procedure has been accepted.

9.8.2 Assumptions. The FT-IR must have the capability for installing a gas cell that is short compared to the path length in the instrument so that the entire infrared beam passes through it. This must be included in the manufacturer's design of the instrument, and whether or not the cell can be placed in the beam is not under the control of the operator. The measurements for accuracy should be made with the instrument operating in the same way as it is when acquiring normal field spectra.

9.8.3 Additional Sections Referenced. No other sections are referenced.

9.8.4 Methodology. The general procedure to be used for the determination of accuracy is essentially identical to the procedure for the determination of precision. The difference is that for the measurement of accuracy the concentration of the gas in the cell must be known. Obtaining this knowledge poses some special problems, and preparation of the sample gas by the individual operators is not recommended at this time. Rather, whenever possible a cylinder of prepared gas should be purchased; for convenience, this prepared mixture is called the reference gas for the rest of this procedure. However, the vapor pressure of some gases is too low to allow the purchase of appropriate

concentrations. Even if a cylinder is purchased, there is some difficulty with knowing what the concentration in the cell is, particularly for the polar compounds.

If a cell is to be used for this measurement then the first step is to calculate the concentration that is required. It is anticipated that the accuracy of the measurement is dependent on the concentration that is being measured. Therefore, the operator must make some judgement of what that concentration is to be. To obtain the concentration in the cell, the operator must multiply the anticipated concentration by the ratio of the path length used for the monitoring program to the cell length. Thus if the path length to be used in the acquisition phase is 100 m and the cell length is 20 cm, then the operator must multiply the anticipated concentration by 500 to get the required concentration of the reference gas in the cell.

Once the proper mixture of gas has been obtained, the operator must introduce it into the cell. At the present time it is recommended that the gas should be flowed through the cell continually during the measurement. Before the measurement is attempted, the gas should be allowed to flow through the cell until at least five volumes of the cell have passed through it.

At the beginning of this measurement the cell should be flushed with dry nitrogen and then a spectrum should be acquired. The reference gas is then flowed through the cell and a second spectrum acquired while the gas is flowing. The cell should then be flushed with dry nitrogen again and a third spectrum recorded.

The average value of the target gas concentration found from the first and third spectra is subtracted from the value determined for the target gas from the second spectrum. This value is then used as the recorded value for the measurement. This procedure is repeated five times in a day, and the average value of these five measurements is used as the accuracy measurement. The percent accuracy is then defined as the average value found above divided by the known concentration of the cylinder gas value times 100. This value should be recorded and plotted on a control chart made for that purpose.

If a flowing system is used, the flow rate must be small so that there is no measurable pressure change in the cell. Flow rates of a few cubic centimeters per minute are acceptable and would require no measurement of the pressure. When the cell is purged to remove the target gas, the volume of purge gas used should be at least 5 times the volume of the cell.

The procedure described here has not been studied in depth, and little written material exists in the literature. Questions such as what the material of the lead lines are to be made of, whether the pressure must be measured in the cell, and whether the lines have to be heated have not been answered at this time. It is also not clear whether this procedure can be used with a mixture of gas or if only a single species must be used at a time. It seems possible that, in the future, a procedure using the water in the atmosphere can be used for this measurement. Absorbance due to water is in every important part of the spectrum that is used with FT-IR measurements, and it will be in every spectrum. Water can also be measured independently with techniques other than the FT-IR so that a verification step can be performed. However, the use of water has not been explored at all.

9.8.5 Procedure.

9.8.5.1 Calculate the required concentration of the reference gas and obtain a cylinder with that concentration.

9.8.5.2 Set up the FT-IR with the same operating conditions used to acquire the field spectra.

9.8.5.3 Install the cell in the beam if necessary and flush it with dry nitrogen.

9.8.5.4 Acquire a spectrum.

9.8.5.5 Flow the reference gas through the cell so that at least five volumes of the cell pass through it.

9.8.5.6 Acquire a second spectrum with the reference gas flowing.

9.8.5.7 Flush the cell with dry nitrogen again and acquire a third spectrum.

9.8.5.8 Analyze all three spectra for the target gas by using the same background as used for the field spectra.

9.8.5.9 Find the concentration of the reference gas from the result of analyzing the second spectrum minus the average value of the first and third spectra.

9.8.5.10 Repeat Sections 9.8.5.3 through 9.8.5.9 five times in any one day of operation.

9.8.5.11 Determine the percent accuracy as the average value of the five measurements divided by the known concentration of the reference cell times 100.

9.9 The Measurement of Resolution

9.9.1 Purpose. The purpose of this procedure is to provide the operator with a means for measuring the resolution of the FT-IR instrument.

9.9.2 Assumptions. The spectra used to make this determination have been acquired with the same instrumental parameters as those used for the field spectra. Particularly, the apodization function and the path length must be the same.

9.9.3 Additional Sections Referenced. No other sections are referenced.

9.9.4 Methodology. The resolution of the FT-IR is an important parameter in that it determines the specificity of the measurements. The instrument resolution does not exhibit dramatic changes from day to day and needs to be measured infrequently. However, whenever any change is made to the instrument optics, including the light source, the resolution must be remeasured. The resolution can also change when the path length changes if the instrument does not have an appropriate field stop to clearly define the field of view regardless of the optical path length. If that is the case, the resolution should be measured at whatever path lengths are used. The FT-IR resolution is also dependent on the apodization function that is used when single beam spectra are created from interferograms, and if more than one apodization function is used then the resolution should be measured for each. The operator needs to be aware of the instrument resolution for a number of reasons. The spectra from two instruments cannot be compared if the resolutions are not the same. The use of reference spectra at resolutions different from that of the instrument creates problems with accuracy. Subtracting one spectrum from another with different resolutions is also a problem. The manufacturers of these devices list the nominal resolution, but a listed resolution of, for example, 1 cm^{-1} should not be interpreted as an exact number.

To measure the resolution, an absorption spectrum must be used. An absorption line that is narrow in comparison to the instrument's line function must be used, and the spectral line used must be a single line. If changes in the instrument resolution occur, they should be noticeable in the high-wave-number region first.

Six primary atmospheric constituents are present in every spectrum. They are water vapor, methane, carbon dioxide, nitrous oxide, ozone, and carbon monoxide. Of these, only the absorption features of water vapor and carbon monoxide can be used to measure the instrument resolution. If the path length is great enough and the water vapor concentration is large enough, then the atmospheric constituent deuterated water can also be used.

In addition to these, absorption features from other gases in high concentrations in conjunction with a short cell can be used. The important feature of any line that is selected for resolution measurements is that it be a single line and be narrow compared to the instrument's nominal operating resolution. Thus methane cannot be used because the lines are not single lines. Whatever feature is chosen, it must not be impacted by any interfering species, as this has the same effect as having double lines. The absorption features of ammonia or hydrogen chloride can be used. HCl is actually a good choice because it absorbs in the high-wave-number region. However, it is not generally present in high enough quantities in the atmosphere to be measured in every spectrum.

There are a number of lines that can be used in the water vapor spectrum that can be used for this measurement. They are at the wave numbers 1014.2, 1149.46, 1187.02, and 2911.88. It should be noted that many of the water lines are already saturated as far as the instrument response is concerned at a vapor pressure of 3 torr. So any line used must be checked to make sure it is not saturated. For carbon monoxide there is at least one line at 2168.9 that can be used. These lines should easily be observed in spectra that have been taken with path lengths greater than 100 m (total).

The resolution for the FT-IR is defined as the full width at half maximum (FWHM) for either of the these lines. Thus to determine the instrument's resolution, an absorbance spectrum must be created with a synthetic background. The operator needs to have a large number of data points across the line in order to make this measurement, and it should be remembered that the system takes only two data points per nominal resolution element. The best way to create this absorption spectrum is to record an interferogram and then zero fill by at least a factor of 4 before computing the Fourier transform. If that is not possible, then the absorbance spectrum must be interpolated to increase the number of data points.

The absorbance at the peak must be measured, and any non-zero baseline value must be subtracted from that measurement. The result of this subtraction is the peak height. Then the entire width of the line at one-half the peak absorbance is measured in wave numbers. This is the required measure of the resolution of the instrument.

9.9.5 Procedure.

9.9.5.1 Obtain an interferogram with the FT-IR operating at the same path length as will be used for the acquisition of the field spectra.

9.9.5.2 Zero fill the interferogram by at least a factor of 4.

9.9.5.3 Perform the Fourier transform on the interferogram.

9.9.5.4 Create an absorbance spectrum using a synthetic background.

9.9.5.5 Isolate one of the lines and measure the peak height.

9.9.5.6 Subtract any non-zero baseline measurement.

9.9.5.7 Measure the full width of the line at one half the absorbance measured in Section 9.9.5.6. This is the resolution.

9.10 The Determination of Nonlinear Instrument Response

9.10.1 Purpose. The FT-IR instrument can respond nonlinearly to changes in the light intensity for several reasons. There are two instrumental conditions that must be guarded against, and these are discussed here. The first is that the electrical gain is set too high, and this can cause the analog-to-digital (A/D) converter to be saturated. The second is that the light source itself is too intense, and this causes the detector response to become nonlinear. This procedure is intended to give the operator a means for determining when either of these conditions exist.

9.10.2 Assumptions. The instrument is operating under the same conditions as it will be to acquire the field spectra.

9.10.3 Additional Sections Referenced. No other sections are referenced.

9.10.4 Methodology. A nonlinear response can be caused by excessive source intensity or amplifier gain. All of the FT-IR systems that are used for remote sensing use A/D converters to convert the analog detector signal to a digitized form. Most use either a 16 bit or an 18 bit converter, and that defines the range of voltages that can be monitored. If the source intensity and amplifier gain combination is too high, then the A/D converter can be saturated. This manifests itself as a sudden drop in the signal being recorded when the source or the retroreflector is moved closer to the detector. When this happens, the system gain must be lowered, if that possibility exists, or the path length must be changed.

The second type of nonlinear response is somewhat more difficult to determine. This occurs if too much light falls on the detector. The detector converts the incident light photons to an electrical signal. There is a limit for how many photons can be converted to electrons, and when this limit is exceeded the detector response becomes nonlinear.

There may also be a nonlinear response from the fact that HgCdTe detectors exhibit nonlinear behavior in their response to infrared energy. This circumstance is not covered here and should be corrected by the manufacturer.

In everyday operation, the easiest way to detect the second kind of nonlinearity is to examine the portion of the single beam spectrum at wave numbers below the detector cutoff. This is in the 650–680-cm^{-1} region for most HgCdTe detectors. If a dip below zero occurs in that region or if the signal is above zero at wave numbers below that region, the system's response may be nonlinear.

There are two ways to check the system's response. Both involve the use of screens to diminish the light intensity while the response is being viewed. If the screens have meshes that reduce the intensity by known amounts, the response should be diminished by that amount also. If the instrument responds differently, the system is nonlinear.

Wire screens can be purchased in a number of mesh sizes, and the mesh size determines how much light will get blocked. Plastic screens should not be used because they may exhibit selective absorption. Aluminum screening that is used for window screening is satisfactory but may not reduce the intensity enough. It is best to use screens of different mesh when using the procedure described below rather than two layers of screening with the same mesh.

The following procedure needs to be done only if the operator suspects that the system is operating in a nonlinear way.

9.10.5 Procedure.

9.10.5.1 Set the FT-IR system up as it will be used for acquisition of the field spectra.

9.10.5.2 Move the source or the retroreflector to twice the original distance.

9.10.5.3 Examine the signal. If a sudden increase in the signal strength occurs, then the A/D converter is saturated.

9.10.5.4 With the source on and the retroreflector at the distance used for the field spectra, acquire a single beam field spectrum and examine the intensity in the detector cutoff region. If a dip occurs, the detector may be saturated.

9.10.5.5 If the dip that is described in Section 9.10.5.4 occurs, insert a wire screen in the beam so that it covers the entire beam and record the signal level.

9.10.5.6 Insert a second screen in the beam and record the signal again. If the screens are the same, each should diminish the beam in the same ratio. If that does not happen, the system is nonlinear in response and the infrared energy must be decreased by some means such as increasing the path length, closing the iris in the instrument, etc.

9.11 The Determination of Water Vapor Concentration

9.11.1 Purpose. It is suggested that the water vapor content in the atmosphere be monitored independently of the FT-IR measurements. This is not an individual procedure like the preceding portions of this method in that it does not explain the siting criteria for making water vapor measurements. It is rather a discussion as to why the measurement is important.

9.11.2 Assumptions. There are no assumptions about the FT-IR system associated with this process.

9.11.3 Additional Sections Referenced. No other sections are referenced.

9.11.4 Methodology. Absorption due to water vapor is the predominant feature in the spectra acquired by the FT-IR remote sensor. It also seems to be one of the most difficult compounds to deal with in the analysis. There are measurable changes in the observed water vapor from spectrum to spectrum. Data from a local airport weather service is not satisfactory to understand the changes and their effects on the analysis. Large and abrupt changes in the water vapor content can be expected. When that occurs it is likely that the background spectrum and the water vapor reference spectrum will have to be remade. But the only way to know that these changes have occurred is to measure the water independently.

Some argument can be made that the water vapor concentration can be obtained by simply adding water to the list of analyzed gases. However, it is not simple to make that measurement. Many of the water vapor lines are very strongly absorbing when the vapor pressure is 3 or 4 torr. The atmospheric vapor pressure in most areas is at least 5 times higher than that. That makes line selection for analysis quite problematic.

Since the water vapor can easily be measured in a continuous fashion it seems prudent to make the measurement independently of the FT-IR. One post-analysis check of the data is to look for a correlation between the concentrations of the target gas and water vapor. To accomplish that, the operator must determine what the water vapor concentration is. The following discussion describes a way of doing that.

The water vapor concentration can be obtained by measuring the relative humidity and the ambient temperature. These values, along with the Smithsonian psychrometric tables, are then used to calculate the water vapor concentration. The psychrometric tables can be found in the *Handbook of Chemistry and Physics* (14), which is published yearly.

There are solid-state devices available today that allow reliable measurements of the relative humidity and the ambient temperature. These devices give results to within a few percent of relative humidity and a few tenths of a degree for the temperature. The operator will need a way to record the output from these devices. This can be accomplished with a data logger that allows for multichannel, multiday recording.

The sensors can be placed anywhere along the path but must be shielded from the sun. A complete description of how to configure the placement of these devices is well outside the scope of this document.

For a complete discussion of these measurements, the operator should consult the following document: *Quality Assurance Handbook for Air Pollution Measurements, Volume IV—Meteorological Measurements* (15). Once the water vapor concentration is known, it should be plotted as a function of time and then compared with the target gas concentration as discussed in the procedure for post-analysis data checking (see Section 8.10). The operator should pay particular attention to the periods where abrupt changes in the water vapor occur.

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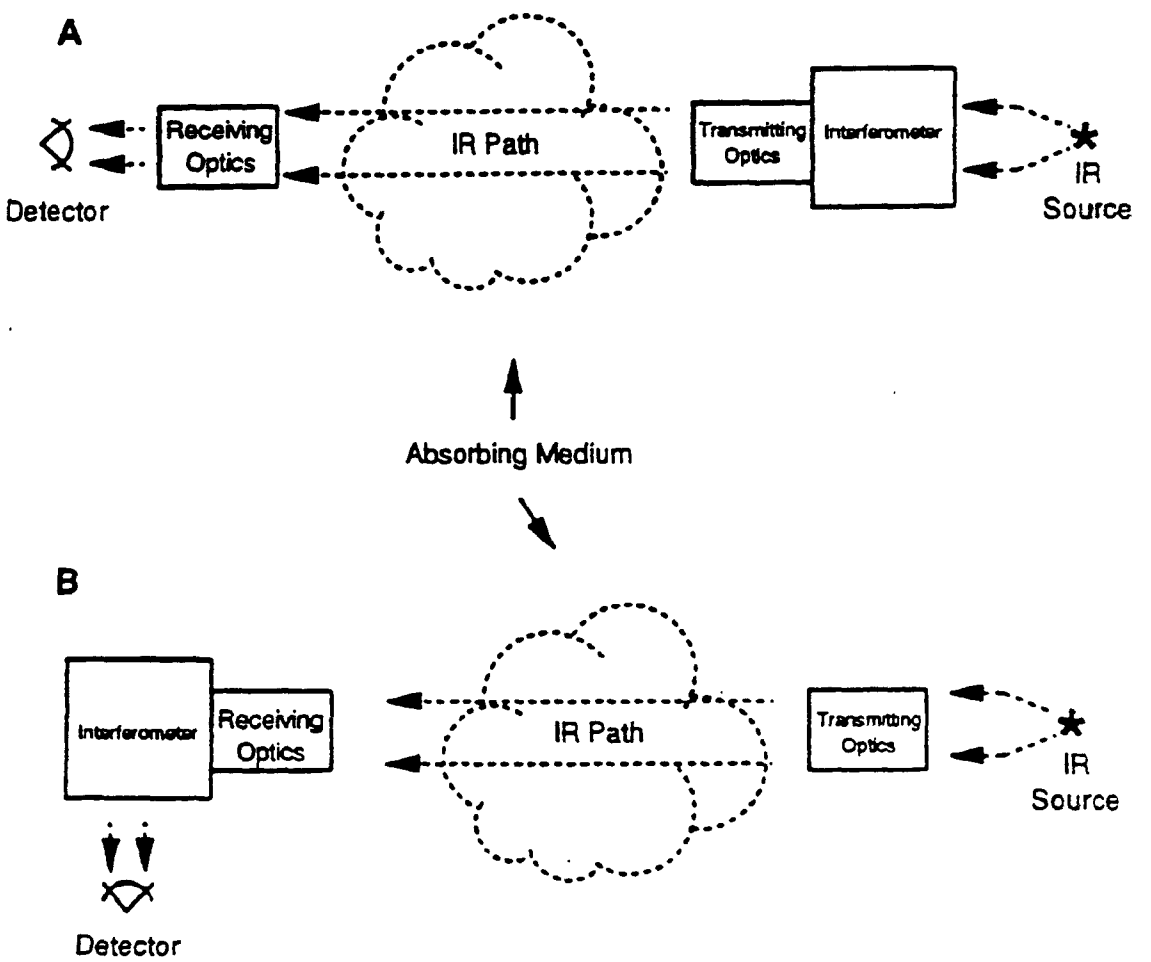


Figure 1. The bistatic configuration of an FT-IR system.

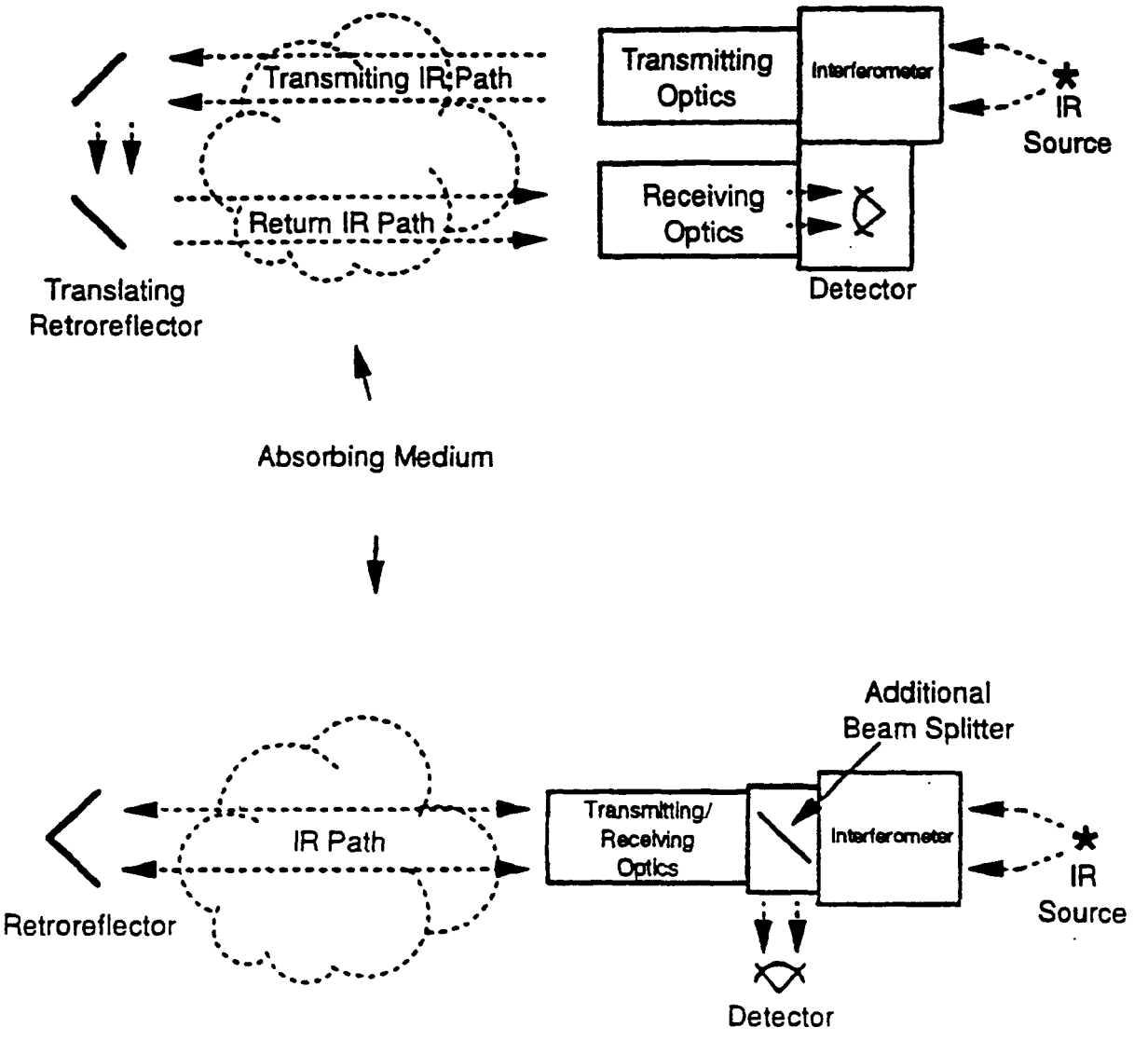


Figure 2. The monostatic configuration of an FT-IR system.

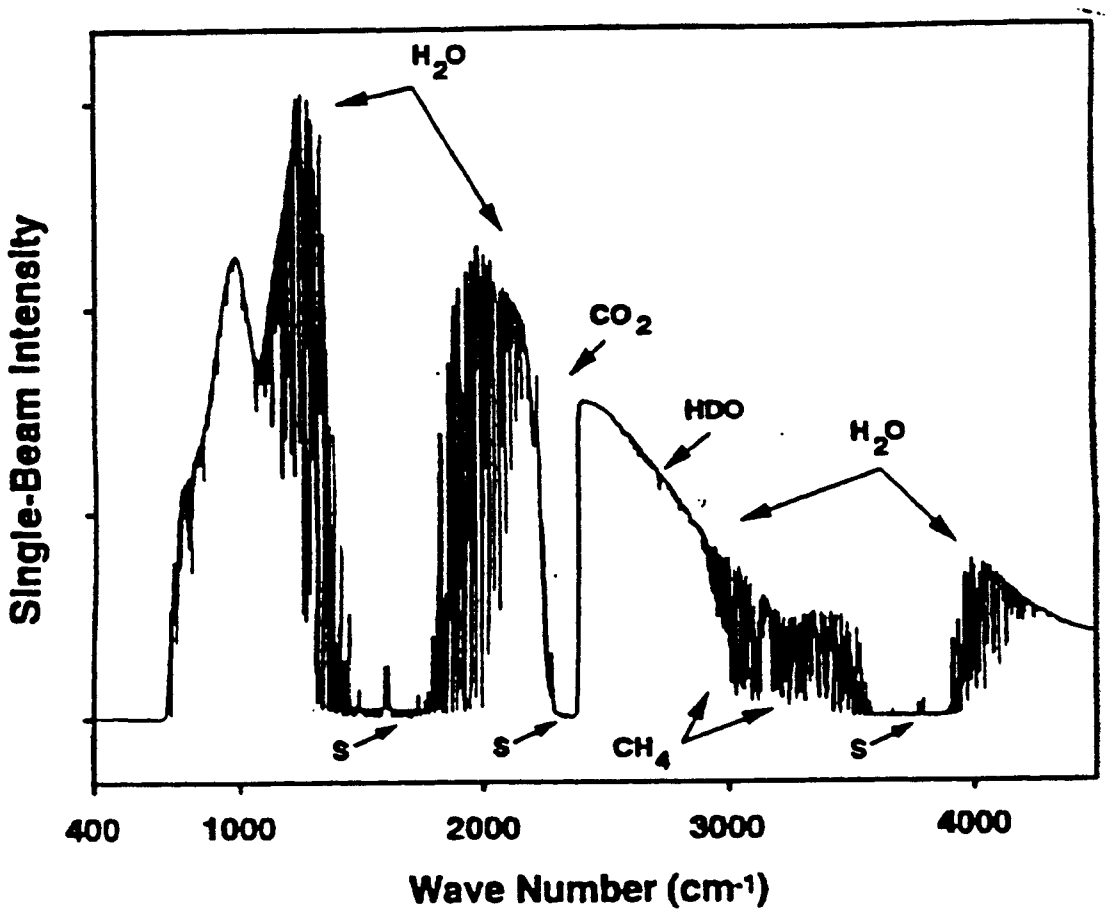


Figure 3. Single-beam spectrum acquired by using a monostatic system and a 414-m path. *[Note: S indicates stray light.]*

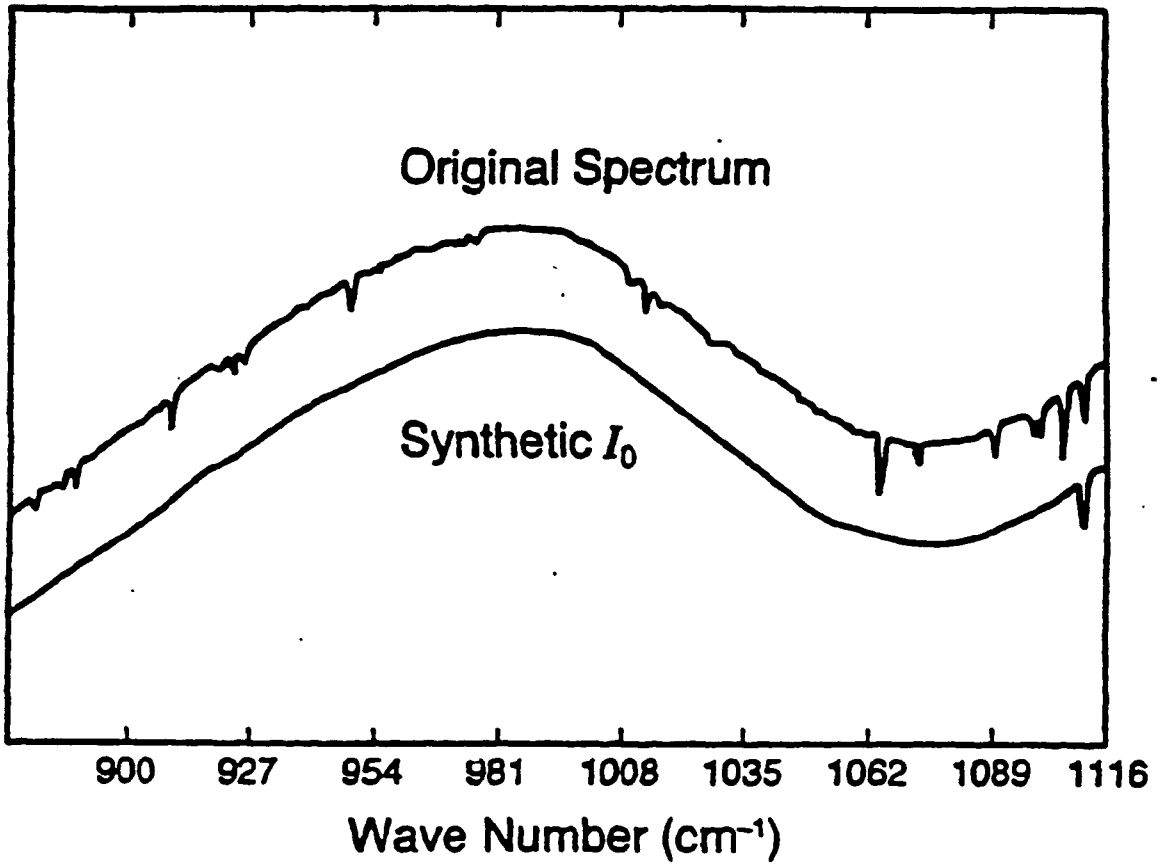


Figure 4. Synthetic I_0 spectrum for an FT-IR absorbance.
[Note: The peak at 1110 cm^{-1} has intentionally been left in as a fiducial point.]

National Specialty Workshop
Technical Tools for Air Toxics Assessment

- State and Local Participatory Programs
  - National Volatile Organic Monitoring Contract
    - Speciated NMOC
    - Urban Air Toxics
    - Carbonyls
    - Photochemical Assessment Compounds

- *Dave-Paul Dayton*
  Eastern Research Group
  Morrisville NC

National Volatile Organic Monitoring Contract

- What the Program Includes
- Compounds
- Relationship to Toxics
- Options and Costs
- How Can I get Access

National Volatile Organic Monitoring Contract

- Program Supports Three Distinct Components
  - Urban Air Toxics Measurments
  - Speciated NMOC (and Nonspeciated NMOC)
  - Photochemical Assessment Monitoring for Volatile Organics

National Volatile Organic Monitoring Contract

- Each Program Component Provides
  - Sampling and Analysis Support
  - Sampling Equipment (UATMP/SNMOC/Carbonyls)
  - Site Installation and Training
  - Site Support
  - Central Laboratory Analysis
  - Quarterly and Annual Reports
  - AIRS-AQMS data entry

National Volatile Organic Monitoring Contract

- **Central Laboratory Analysis Includes:**
  - Compendium Method TO-14 for Air Toxics (thru 96 program)
  - Compendium Method TO-15 for Air Toxics (starting 97 program)
    - Polar Fuel Additives
  - Compendium Method TO-11 for Carbonyls
  - Compendium Method TO-12 for NMOC
  - Speciated Nonmethane Organic Compounds
  - Photochemical Assessment Monitoring Compounds

National Volatile Organic Monitoring Contract

- **Urban Air Toxics**
  - 49 compounds from TO-14
  - 13 carbonyl compounds
  - 9 additional "polar" compounds from TO-15
    - includes 4 fuel additive compounds

National Volatile Organic Monitoring Contract

- **Speciated NMOC**
  - 80 Hydrocarbon species including
    - Saturated Hydrocarbons
    - Unsaturated Hydrocarbons
    - Single ring aromatics
    - Includes 12 UATMP target compounds

National Volatile Organic Monitoring Contract

- **Photochemical Assessment Monitoring**
  - QA/QC Support
    - Retention Time Standards
    - Site Setup Ongoing Support for automated GC monitoring
  - 57 Hydrocarbon species from PAMS Technical Assistance Document
    - Includes 11 UATMP Target Compounds
  - 13 of the Compendium Method TO-11 carbonyl compounds

National Volatile Organic Monitoring Contract

- Program Costs
  - State Accessable through 105 Grant Funds
  - Independent Access through Non-Federal Funds
  - Base Sites Include:
    - UATMP
    - SNMOC
    - PAMS
  - Site Options are available for each base
    - Toxics
    - Carbonyls
    - SNMOC

National Volatile Organic Monitoring Contract

- Program Access and Contacts

  - Neil Berg - EPA Delivery Order Manager
  - Kathy Weant - EPA Project Officer

  - Dave-Paul Dayton - ERG Program Manager
  - Tim Hanley - ERG Site Coordinator

Table 1

NMOC, UATMP, and PAMS Networks Base Program and Associated Costs (1997)*

Line Item		Cost ($)	Shipping ($)	Total ($)
1.0	NMOC Base Site Support • (Frequency, 4 months, 5 days per week, 1 sample per day equals 92 samples) • Canister Cleaning and Shipping • Instrument Certification and Installation • Travel • NMOC Analysis • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	15,869	3,840	19,709
2.0	Speciated Base NMOC Site Support • (Frequency, 4 months, 5 days per week, 1 sample per day equals 92 samples) • Canister Cleaning and Shipping • Instrument Certification and Installation • Travel • Speciated Analysis • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	30,058	3,840	33,898
3.0	Toxics Option to NMOC Base Site* • (10 Samples) • Sampler Certification • Toxics or Polar Organic Compound Analysis • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	5,614	NA	5,614

*Cannot be selected as stand-alone program.

Table 1

(Continued)

Line Item		Cost ($)	Shipping ($)	Total ($)
4.0	Carbonyl Option to NMOC Base Site* • (10 samples) • Carbonyl Analysis for 16 Target Compounds • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	1,663	NA	1,663
5.0	Speciated NMOC Option to NMOC Base Site* • (10 samples) • Speciated Hydrocarbon Analysis • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	2,872	NA	2,872
6.0	Toxics Base Site Support • (1 year, 1 sample per 12 days, includes 10% duplicates equals 34 samples) • Canister Cleaning and Shipping • Instrument Certification and Installation • Travel • Toxics or Polar Organic Compound Analysis by GC/MSD-FID • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	28,254	1,564	29,818

*Cannot be selected as stand-alone program.

Table 1

(Continued)

Line Item		Cost ($)	Shipping ($)	Total ($)
7.0	Carbonyl Option to Toxics Base Site* • (1 year, 1 sample per 12 days, includes 10% duplicates equals 34 samples) • Instrument Certification and Installation • Carbonyl Analysis for 16 Compounds • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	3,798	NA	3,798
8.0	Technical Site Support • Any of a combination of the following PAMS site support activities - On-Site Instrument Setup, - QA/QC Support, Standards, & Round Robin Support, - On-site Technical Assistance and Consultation	24,650	NA	24,650
9.0	PAMS Site - Frequency A • (Eight, 3-hr every 3rd day and one 24-hr sample every 6th day during the monitoring period of June, July, and August equals 284 samples, includes 10% duplicates) • Canister Cleaning and Shipping (canisters provided by State or local agency) • Instrument Certification and Installation (instrument provided by State or local agency) • VOC Analysis • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	70,014	11,960	81,974

*Cannot be selected as stand-alone program.

Table 1

(Continued)

Line Item		Cost ($)	Shipping ($)	Total ($)
10.0	PAMS Site - Frequency B • (Eight, 3-hr every day during the monitoring period of June, July, and August and one 24-hr sample every 6th day year round equals 818 samples, includes 10% duplicates) • Canister Cleaning and Shipping (canisters provided by State or local agency) • Instrument Certification and Installation (instrument provided by State or local agency) • VOC Analysis • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	146,814	36,662	183,476
11.0	PAMS Site - Frequency C • (Eight, 3-hr samples on 5 peak ozone days plus each previous day, eight 3-hr samples every 6th day and one 24-hr sample every 6th day during the monitoring period of June, July, and August equals 236 samples, including 10% duplicates) • Canister Cleaning and Shipping (canisters provided by State or local agency) • Instrument Certification and Installation (instrument provided by State or local agency) • VOC Analysis • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	37,181	10,028	47,209

*Cannot be selected as stand-alone program.

Table 1

(Continued)

Line Item		Cost ($)	Shipping ($)	Total ($)
12.0	PAMS Site - Frequency D • (Eight, 3-hr samples every 3rd day during the monitoring period of June, July, and August equals 266 samples, including 10% duplicates) • DNPH Cartridges • Carbonyl Analysis for 16 Compounds • QA/QC Program • Data Validation, Reduction, Reporting, and AIRS Input	21,109	552[b]	21,661
13.0	PAMS Site - Frequency E • (Eight, 3-hr samples, every day during the monitoring period of June, July, and August equals 810 samples, includes 10% duplicates) • DNPH Cartridges • Carbonyl Analysis for 16 Compounds • QA/QC Program • Data Validation, Reduction, Reporting, and AIRS Input	61,608	1,500[c]	63,108
14.0	PAMS Site - Frequency F • (Eight, 3-hr samples on 5 peak ozone days plus each previous day, eight 3-hr samples every 6th days, and one 24-hr samples every 6th day during the monitoring period of June, July, and August equals 236 samples, includes 10% duplicates) • DNPH Cartridges • Carbonyl Analysis for 16 Compounds • QA/QC Program • Data Validation, Reduction, Reporting, and AIRS Input	18,054	250[d]	18,304

[b]Cannot be selected as stand-alone program.

Table 1

(Continued)

Line Item		Cost ($)	Shipping ($)	Total ($)
15.0	PAMS Supplemental Auto GC Canister Support Frequency • (One 24-hr sample every 6th day equals 60 samples) • Canister Cleaning and Shipping (canisters provided by State or local agency) • VOC Analysis • QA/QC Program and Standards • Data Validation, Reduction, Reporting, and AIRS Input	19,373	2,944	22,317

[a]Select base and optional programs desired and return the information to Neil Berg at U.S. EPA Office of Air Quality Planning and Standards, MD-14,
Research Triangle Park, North Carolina 27709.
[b]If selected in combination with Line Item No. 9.0, shipping for this item is not applicable.
[c]If selected in combination with Line Item No. 10.0, shipping for this item is not applicable.
[d]If selected in combination with Line Item No. 11.0, shipping for this item is not applicable.

[e]Cannot be selected as stand-alone program.

NATIONAL SPECIALTY WORKSHOP ON TECHNICAL TOOLS FOR AIR TOXICS ASSESSMENT

State and Local Participatory Program:
Particulate Compounds Including PM_{10}, $PM_{2.5}$,
and Filter Analysis for Toxic Species

EPA Contract 68D30029
Work Assignment 3-118

Neil Berg
Work Assignment Manager
Monitoring and Quality Assurance Group
Emissions, Monitoring, and Analysis Division
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

Stan Sleva
TRC Environmental Corporation
6340 Quadrangle Drive, Suite 200
Chapel Hill, NC 27514

Tuesday Afternoon Session
June 17, 1997

1.0 INTRODUCTION

The U.S. Environmental Protection Agency (EPA) is encouraging State and local air pollution control agencies to conduct short-term, multi-site ambient air pollutant monitoring studies using the technique known as saturation monitoring. Saturation monitors are non-reference or non-equivalent sampling methods for measuring particulate matter, carbon monoxide and NOx. The samplers are small, portable, and relatively easy to set up and operate. Because they are relatively inexpensive, it is customary to "saturate" a geographical area with the samplers to assess the air quality in areas where high concentrations of pollutants are possible. Such information is helpful to air pollution control agencies in evaluating their ambient air monitoring networks for consistency with the 40 CFR Part 58 air quality surveillance regulations, which require an annual network review and approval by EPA. EPA initiated the Saturation Monitor Repository (SMR) in 1993. The SMR includes a pool of saturation samplers and related equipment which agencies use when it becomes necessary for them to upgrade or borrow saturation sampling equipment. The SMR provides limited services to quality assure the samplers and assist in field studies upon request.

Occasionally, State and local agencies will find that the concentrations of particulate matter measured at locations in their ambient air monitoring networks exceed the PM-10 national ambient air quality standard (NAAQS). In order to understand the nature of the particulate matter responsible for the exceedance, EPA has provided filter analysis assistance to the agencies operating their particulate matter network.

Under work assignment 3-118, TRC Environmental Corporation (TRC) is providing

technical assistance to EPA in operating and maintaining the SMR, conducting special field studies using the saturation samplers, and analyzing particulate matter filters.

2.0 MINI VOL PORTABLE AIR SAMPLER

The Airmetrics portable minivol air sampler can be used to collect ambient air samples for TSP, PM10, and PM2.5 and CO and NOx. The sampler is compact, lightweight, battery-operated, and constructed from durable PVC. It can be operated from either AC or DC power supplies. An internal programmable timer can make up to six sampling runs within a 24 hour period, while an elapsed time totalizer records total pump operation time. The sampler also continuously monitors the battery voltage and air flow rate, automatically shutting off sampling if limits are exceeded. Figure 2-1 shows the sampler and hanging apparatus. Figure 2-2 shows the preseparator and filter holder. Figure 2-3 shows the battery/sampler connection points and Figure 2-4 shows the integrated gas sampling arrangement.

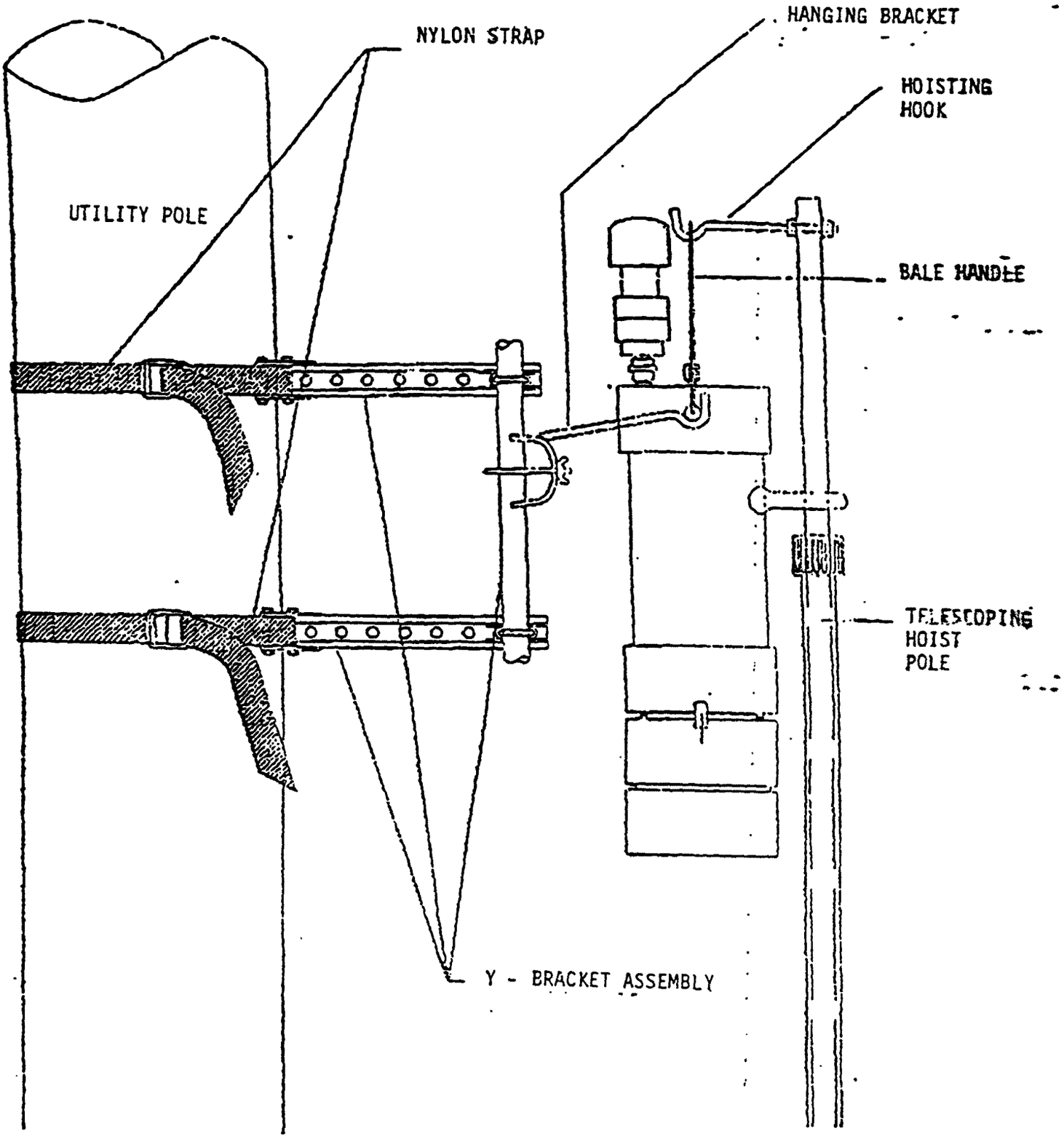


Figure 2-1 Sampler and Hanging Apparatus

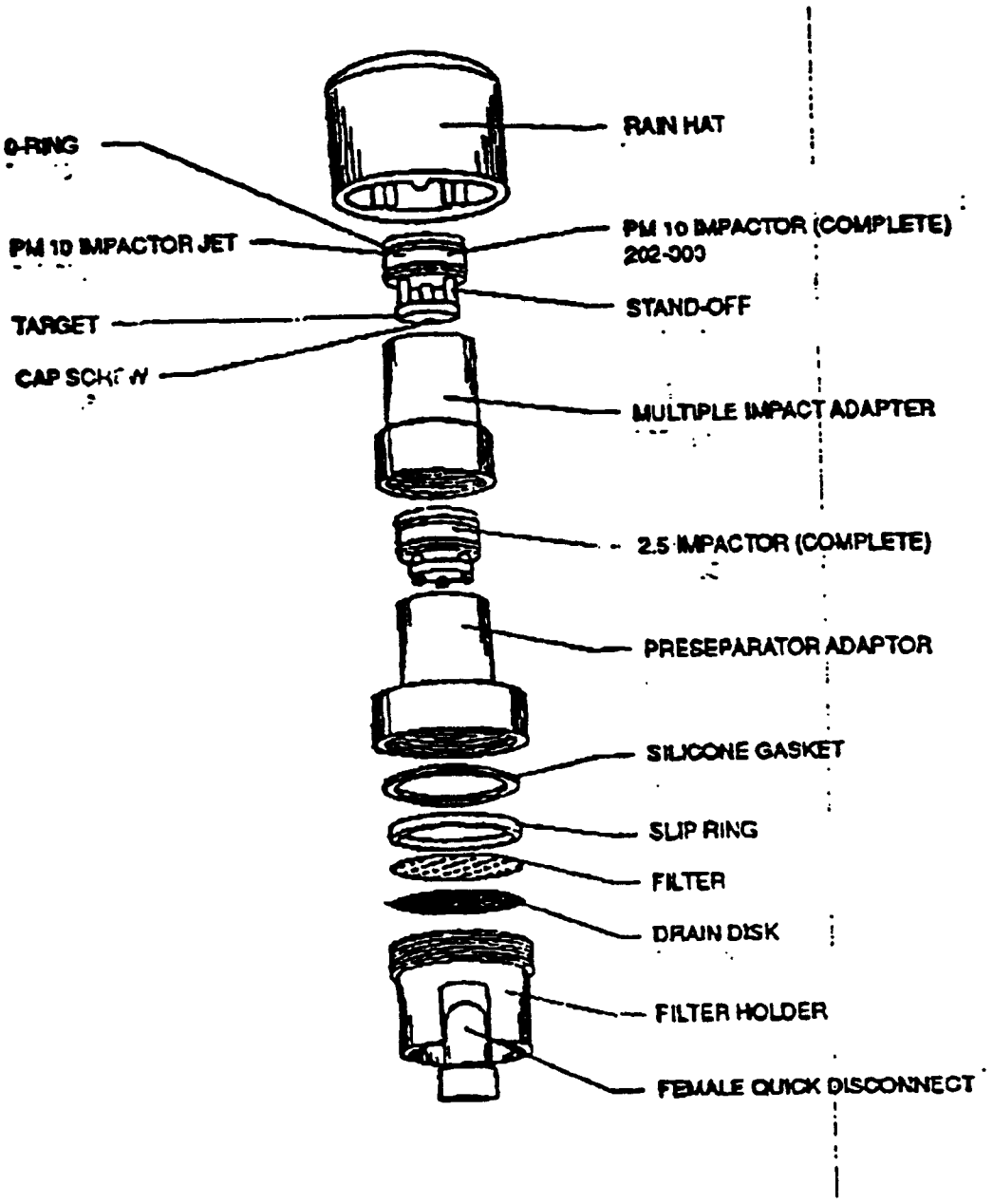


Figure 2-2 Preseparator and Filter Holder Assembly

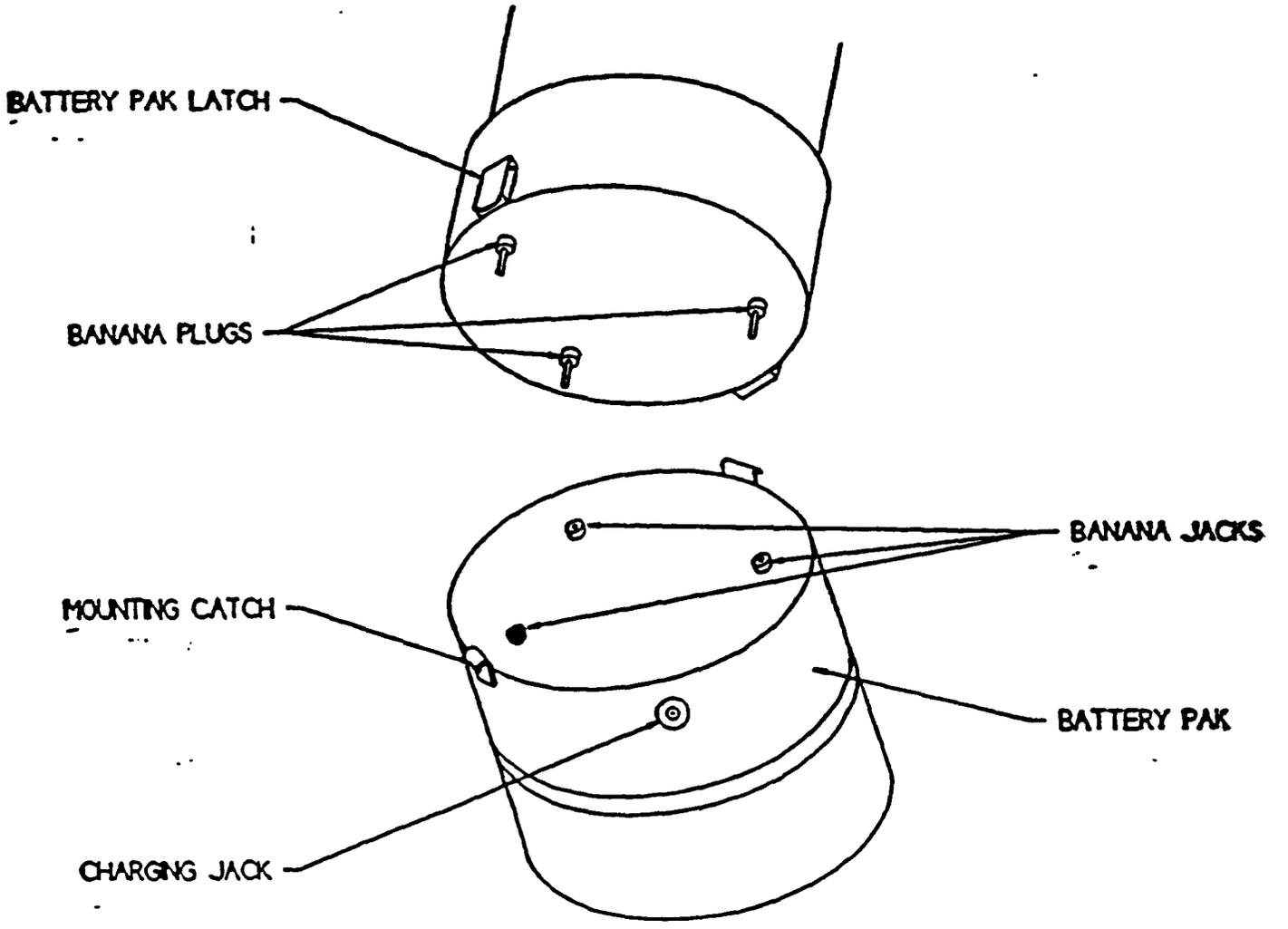


Figure 2-3 Battery/Sampler Connection Points.

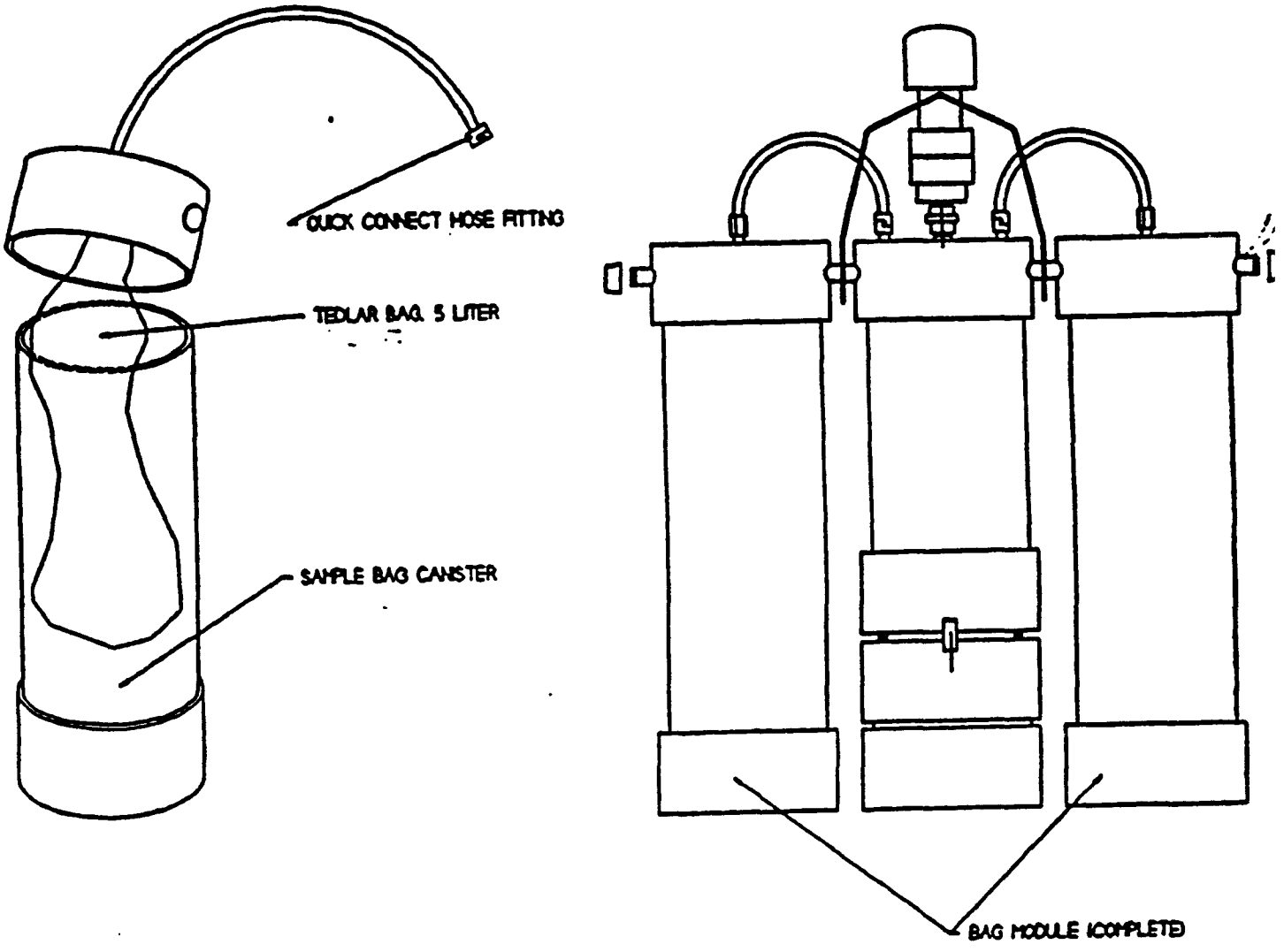


Figure 2-4 Integrated Gas Sampling Arrangement

3.0 STATUS OF THE SATURATION MONITORING REPOSITORY

Table 1 shows the status of the SMR as of May 31, 1997:

TABLE 1. STATUS OF SATURATION MONITORING REPOSITORY

Location	*No. of Monitors*	*Status*
In-House	35	Available
Cincinnati	2 (PM-2.5)	Due June 1997
City of Indianapolis - ERM	8 (PM*)	Due January 1998
EPA - RTI Special Study	6 (PM-2.5)	Due August 1997
Missouri - Jefferson City	6 (PM-2.5)	Due December 1997
New Jersey - Holland Tunnel	2 (1 PM, 1 CO)	Due October 1997
NC DEHNR - Asheville	2 (PM-2.5)	Due May 1998
NC DEHNR - Washington	1 (PM)	Due September 1997
Region 3 - Philadelphia	4 (PM-2.5)	Due December 1997
Region 7 - Kansas City	5 (PM-2.5)	Due October 1997
Region 8 - Tribes	5 (PM-2.5)	Due July 1997
USDA Agricultural Research Service	20 (PM*)	Due June 1997
Washington State University	15 (PM*)	Due January 1999
WI DNR - Milwaukee	4 (PM-2.5)	Due October 1997
TOTAL	115	

* Includes PM-2.5 inlets

4.0 COMPLETED STUDIES

The following studies were completed during the last six months:

Study #1: PM-10/2.5 Saturation Study in Washington N.C.
Agency: NCDEHNR - Washington Regional Office
Request: 11 PM-10 and 2.5 samplers
Purpose: To determine PM-10 and 2.5 levels at selected sites

Time Period:	1996 through January 1997
Pre- and Post-Filter Weighing:	No

Study #2:	Region VIII/ORD Reference Sampler Study
Agency:	Region VIII
Request:	3 PM-2.5 samplers
Purpose:	To compare with proposed FRM
Time Period:	November 1996 through January 1997
Pre- and Post-Filter Weighing:	No

Study #3:	Ventura County California
Agency:	Ventura County Air Pollution Control District
Request:	10 PM-2.5 samplers
Purpose:	To determine PM 2.5 levels at selected sites
Time Period:	Summer 1996 through March 1997
Pre- and Post-Filter Weighing:	No

5.0 ONGOING STUDIES

The following studies were ongoing as of May 31, 1997:

Study #1:	PM-2.5 Special Study
Agency:	Cincinnati
Request:	2 PM-2.5 samplers
Purpose:	To determine PM concentrations around burning landfill (~1 month), followed by periodic sampling at selected sites
Time Period:	July 1996 through June 1997
Pre- and Post-Filter Weighing:	No

Study #2:	Holland Tunnel PM/CO Study, New Jersey
Agency:	Municipal Environmental Commission
Request:	1 CO, 1 PM-2.5 sampler
Purpose:	To determine PM and CO outflow from the Holland Tunnel.
Time Period:	February 1996 through September 1997
Pre- and Post-Filter Weighing:	No

Study #3:	PM-2.5 Saturation Study in Asheville, North Carolina
Agency:	NC DEHNR
Request:	2 PM-2.5 samplers
Purpose:	To determine the impact of suspended PM sources near residences located at valley exit
Time Period:	May 1996 through May 1998
Pre- and Post-Filter Weighing:	No

Study #4:	Saturation Sampler Study in Washington, North Carolina
Agency:	NC DEHNR
Request:	1 PM sampler
Purpose:	To determine sampler/battery operation
Time Period:	March 1997 through September 1997
Pre- and Post-Filter Weighing:	No

Study #5:	PM-2.5 Study
Agency:	EPA Region VII
Request:	5 PM-2.5 samplers
Purpose:	To determine PM levels in urbanized area
Time Period:	March 1996 through September 1997
Pre- and Post-Filter Weighing:	No

Study #6:	PM-10 Study in Big Springs, Texas
Agency:	USDA Agricultural Research Center
Request:	20 PM samplers (8 with PM-10 inlets, 6 with PM-2.5 inlets, 6 with no size selection on the inlet)
Purpose:	To determine the relationship between PM-10 readings and soil erosion by wind.
Time Period:	February 1994 through June 1997
Pre- and Post-Filter Weighing:	No

Study #7:	PM-10 Study
Agency:	Washington State University
Request:	15 PM samplers
Purpose:	To determine PM emissions from windblown dust at three different elevations at a site near Spokane, Washington.
Time Period:	February 1994 through December 1998
Pre- and Post-Filter Weighing:	No

Study #8:	PM Saturation Study in Jefferson City
Agency:	Missouri Department of Natural Resources
Request:	6 PM-2.5 samplers
Purpose:	To determine PM levels at selected sites in Missouri
Time Period:	November 1996 through November 1997
Pre- and Post-Filter Weighing:	No

Study #9:	PM-2.5 Saturation Study - Northern Cheyenne, Confederated Salish and Kootenai Tribes
Agency:	EPA Region VIII
Request:	5 PM-2.5 samplers
Purpose:	To better characterize the PM emissions in Montana's tribal nonattainment areas to allow EPA to better target control strategies.
Time Period:	November 1996 through June 1997
Pre- and Post-Filter Weighing:	No

Study #10:	PM-2.5 Monitoring Study
Agency:	WI DNR - Milwaukee
Request:	4 PM-2.5 samplers
Purpose:	To determine PM levels at selected urban area sites
Time Period:	November 1996 through September 1997
Pre- and Post-Filter Weighing:	No

Study #11:	PM-2.5 Monitoring Study
Agency:	City of Indianapolis - ERM
Request:	8 PM-2.5 samplers
Purpose:	To determine PM levels at selected urban area sites
Time Period:	November 1996 through September 1997
Pre- and Post-Filter Weighing:	No

Study #2:	PM Monitoring Study
Agency:	EPA Monitoring and Quality Assurance Group
Request:	6 PM-2.5 samplers with different PM2.5 inlet configurations
Purpose:	To compare with proposed FRM
Time Period:	April 1997 through August 1997
Pre- and Post-Filter Weighing:	Yes

6.0 PLANNED STUDIES

The following saturation studies are planned for the upcoming period:

Study #1:	PM 2.5 and PM 10 Monitoring Study

Agency:	EPA Region II
Request:	10 PM-2.5 samplers and 3 PM 10 samplers
Purpose:	Determine PM2.5 levels in Queens, NY
Time Period:	To be determined
Pre- and Post-Filter Weighing:	Yes

Study #2:	PM 2.5 Monitoring Study
Agency:	Puerto Rico Air Quality
Request:	15 PM-2.5 samplers
Purpose:	Determine PM2.5 levels selected areas of Puerto Rico
Time Period:	To be determined
Pre- and Post-Filter Weighing:	No

7.0 FILTER ANALYSIS COST ESTIMATES

Analysis	Cost $/Sample
Gravimetric Analysis (Pre and post sampling weighing)	8-11
Elemental Analysis (34 elements) (X-ray Fluorescence)	40
Total Carbon, Organic Carbon, Elemental Carbon (Thermal/Optical Reflectance)	35
Total Carbon, Organic Carbon, Elemental Carbon, Carbonate Carbon (Thermal/Optical Reflectance)	70
Sulfate, Nitrate, and Chloride (Ion Chromatographic Analysis, IC)	30
Ammonium or Nitrite Ion (Automated colorimetric analysis, AC)	30
Single Elements, Sodium or Potassium (Atomic Absorption Spectroscopy, AA)	30

F.E.M.A. BURN STUDY -- TRYON ROAD SITE

LEGEND

(A): Downwind site for Episode 1, Upwind site for Episodes 2,3,4,5 (Fixed Location)

(B): Source Site for Episode 1,2,3,4,5 (Fixed Location)

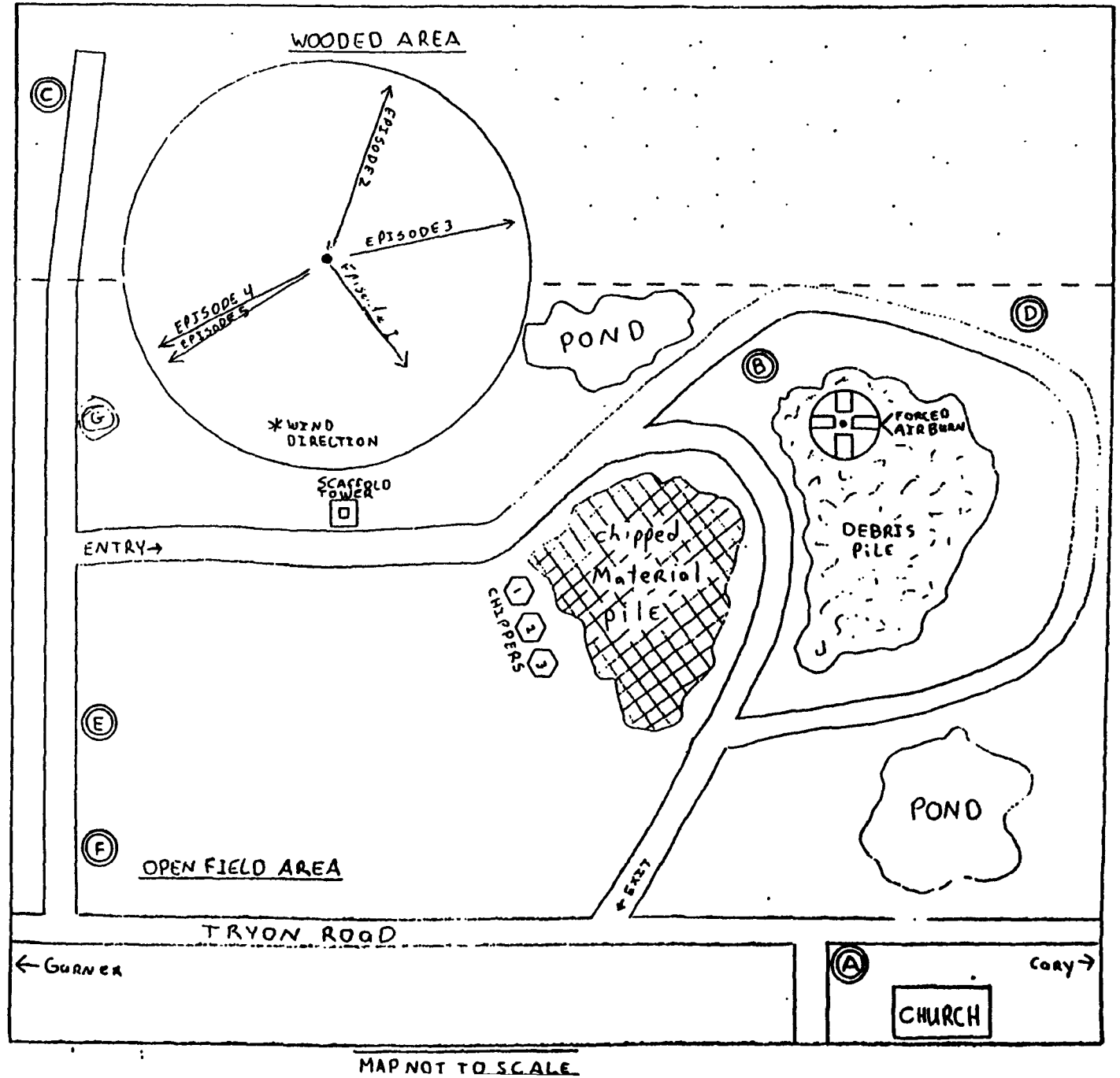
(C): Upwind site for Episode 1, Downwind site for Episodes 2,3,4,5 (Fixed Location)

(D): Rover site for Episode 3 (location based on visual observation of wind direction)

(E): Rover site for Episode 4 (location based on visual observation of wind direction)

(F): Rover Site for Episode 5 (location based on visual observation of wind direction)

(G): Entrance of site [illegible] (Fixed Location)



MAP NOT TO SCALE

In: Proceedings of the EPA/A&WMA Symposium, "Measurement of Toxic and Related Air Pollutants," April 29 - May 1, 1997, Research Triangle Park, NC

CMB8: New Software for Chemical Mass Balance Receptor Modeling

Charles W. Lewis
National Exposure Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park NC 27711

ABSTRACT

The Chemical Mass Balance (CMB) method for receptor modeling of ambient air pollutants has been in use for over two decades. Over the past year the U.S. Environmental Protection Agency's Office of Research and Development and Office of Air Quality Planning and Standards have jointly sponsored the development of a new generation of CMB software, CMB8. Developmental work has been performed by the Desert Research Institute, Reno, NV. Changes embodied in CMB8 include (1) switch from a DOS-based to a Windows-based environment, (2) increased attention to volatile organic compounds (VOC) applications, (3) correction of some flaws in the previous version (CMB7), (4) more options for input and output data formats, (5) addition of a more accurate least squares computational algorithm, (6) a new treatment of source collinearity, (7) multiple defaults for sources and fitting species, and (8) choice of fitting criteria. Details of the changes and the procedure for obtaining CMB8 are given.

INTRODUCTION

The Chemical Mass Balance (CMB) method for receptor modeling of ambient air pollutants has been in use for over two decades. The CMB model can be written as

$$C_i = \sum_{j=1}^{p} a_{ij} S_j, \quad i = 1, n \tag{1}$$

where C_i is the ambient concentration of specie i, a_{ij} is the fractional concentration of specie i in the emissions from source j, S_j is the total mass concentration contributed by source j, p is the number of sources, and n is the number of species, with $n > p$. The C_i and a_{ij} are known and the S_j are found by a least squares solution of the overdetermined system of equations (1). While the system is simple in appearance its solution is not, because of the need to take account of uncertainties in both the C_i's and the a_{ij}'s.

The U.S. Environmental Protection Agency (EPA) has tacitly approved CMB as a regulatory planning tool through the Agency's approval of numerous State Implementation Plans (SIPs) which have had a CMB component. Since about 1990 EPA has supported and freely distributed the current version of the CMB software (CMB7). Over the past year EPA's Office of Research and Development and Office of Air Quality Planning and Standards have jointly sponsored the development of a new generation of CMB software, CMB8, and associated documentation and guidance. The work is being performed by the Desert Research Institute, Reno, NV. During the development period the evolving versions of CMB8 have been available to an informal network of over 20 interested individuals for testing.

In the following an overview of CMB8 is presented. The procedure for obtaining a copy of the software and documentation is also given.

CMB8 FEATURES

Windows Environment

CMB8 is designed for use with Microsoft Windows®. Both 16-bit and 32-bit versions are available for Windows 3.x and Windows 95, respectively. CMB8 is not available as a DOS application. The switch to a Windows environment offers a number of advantages. Species and profile selections can be done more quickly under mouse control, and the user can choose to immediately view the current selections in display windows (or have them continuously present) during a session. In general, use of a mouse has encouraged a richer choice of options and gives more immediate access to them.

Species and Source Selection Defaults

In CMB8 the user can specify any one of up to ten sets of fitting species that can be chosen at random by mouse-clicking on a software button. A set can be created or modified at any time during a session. Similarly, up to ten sets of source profiles can be defined and accessed. It is anticipated that this feature will provide a vast improvement in the efficiency of searching through many source and fitting species combinations in order to find the best fit -- a very time-intensive aspect of using CMB7.

Input File Options

Necessary inputs for a CMB calculation include an ambient data file, which lists all the measured chemical information for a series of ambient samples, and a source profile data file, which lists the chemical composition of a collection of candidate source profiles. CMB7 required these files to be blank-delimited ASCII text files (supplementary software was available to externally convert spreadsheet- and database-type files to the required CMB7 format). In CMB8 the direct input of ambient and source data files may be done in a variety of formats: blank-delimited ASCII(*.*TXT*), blank-delimited ASCII with columns and rows interchanged (*.*CAR*), comma-separated value (*.*CSV*), xBASE (*.*DBF*), and Lotus 123 spreadsheet (*.*WKS* and *.*WK1*).

Output File Options

The calculated results from a CMB8 session are available in two output files whose default names are *CMBOUTRP.TXT* and *CMBOUTDB.TXT*. The "report" file *CMBOUTRP* is an electronic copy of the output results that are displayed and printable during the session. File *CMBOUTRP.TXT* is the analogue of *CMBOUT.DT1* in CMB7. Similarly, the "database" file *CMBOUTDB.TXT* is the analogue of the CMB7 file *CMBOUT.DT2*.

A new feature of these files in CMB8 is that not only their names (both prefix and suffix) but also their directories may be changed by the user during a session, allowing for better grouping and identification of results generated during a lengthy session. The last choices in a session become the defaults for the next session. In the case of the file *CMBOUTDB*, the only allowed suffixes are *.TXT*, *.CSV*, *.DBF* and *.WKS*. Each can be selected with a software button, which causes the file to have the corresponding format type.

Collinearity Treatment

Collinearity in a CMB context refers to a situation in which the compositions of two or more source profiles are so similar that it is difficult to infer the separate impact of each. Collinearity is a form of mathematical *ill conditioning*, and its presence is associated with additional serious problems beyond the one just noted. The basis

than either χ^2 or r^2 alone.

OBTAINING CMB8

Until CMB8 is finalized, and is formally accepted and supported by EPA, the current version of the CMB8 software and documentation is available from the developer, DRI, via anonymous ftp. The address is:

eaf.sage.dri.edu:/cmb80/model/16bit/win3MMDD.exe

where MMDD stand for month and day to identify the development version (the directory may contain a few earlier versions in addition to the latest one). The file *win3MMDD.exe* is a PKZIP self-extracting file, so the user should use a binary mode of file transfer. In addition to the *CMB8.EXE* program the file also contains sample input files and a tutorial/users manual. A Windows 95 version may be obtained by changing the last part of the address to *32bit/wn32MMDD.exe*.

CONCLUSIONS

Features of the new version of CMB software (CMB8) have been described. It is anticipated that CMB8 will significantly increase the convenience, efficiency and accuracy of performing receptor modeling by the CMB method.

ACKNOWLEDGEMENTS

The DRI CMB8 development team consists of John Watson, Norman Robinson and Judy Chow. We are indebted to those individuals who made substantial contributions to improving the CMB8 software through their suggestions and testing efforts during the development period. They include Teri Conner, Tom Coulter, William Ellenson, Eric Fujita, Douglas Lowenthal, Elizabeth Vega, and Robert Willis. Richard Scheffe was instrumental in coordinating the joint support of EPA's Office of Research and Development and Office of Air Quality Planning and Standards to serve both the research and regulatory interests of the Agency.

DISCLAIMER

The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under Purchase Order No. 5D1607NAEX to the Desert Research Institute. It has been subjected to Agency review and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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NEW DATA ANALYSIS TOOLS for Ambient Air Quality Data

Presentation for National Speciality Workshop on Technical Tools for Air Toxics Assessment

June 17, 1997

James Hemby

Air Quality Trends & Analysis Group
OAQPS

OVERVIEW

- Demonstrate two recently developed software tools
  - PAMSDAS
  - VOCDAT
- Other miscellaneous tools
- Ambient air quality data characterization project

Air Quality Trends & Analysis Group
OAQPS

PAMSDAS: Description

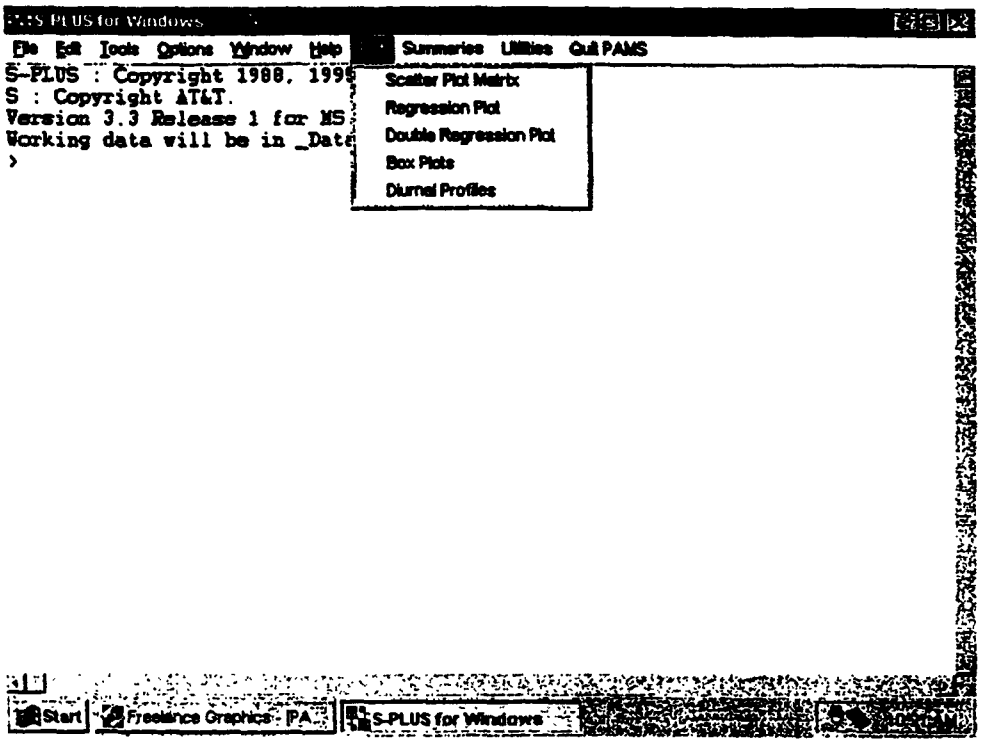
- PAMS Data Analysis System
- Software module that facilitates exploratory PAMS analysis
- Design
  - Menu driven; easy to learn & use
  - No programming experience needed
- Once complete (October '97), the module will be posted on the web and distributed to Regions/States

Air Quality Trends & Analysis Group
OAQPS

PAMSDAS (continued)

- System Requirements
  - PC based (Pentium)
  - Minimum 16 MB RAM
- Operating Environment
  - S-PLUS front-end menu-driven system
  - Windows NT/Windows 95/Windows 3.x
- Capabilities (demonstrated on next several slides)

Air Quality Trends & Analysis Group
OAQPS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S : Copyright AT&T.
Version 3.3 Release 1 for MS
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Regression Plot
Double Regression Plot
Box Plots
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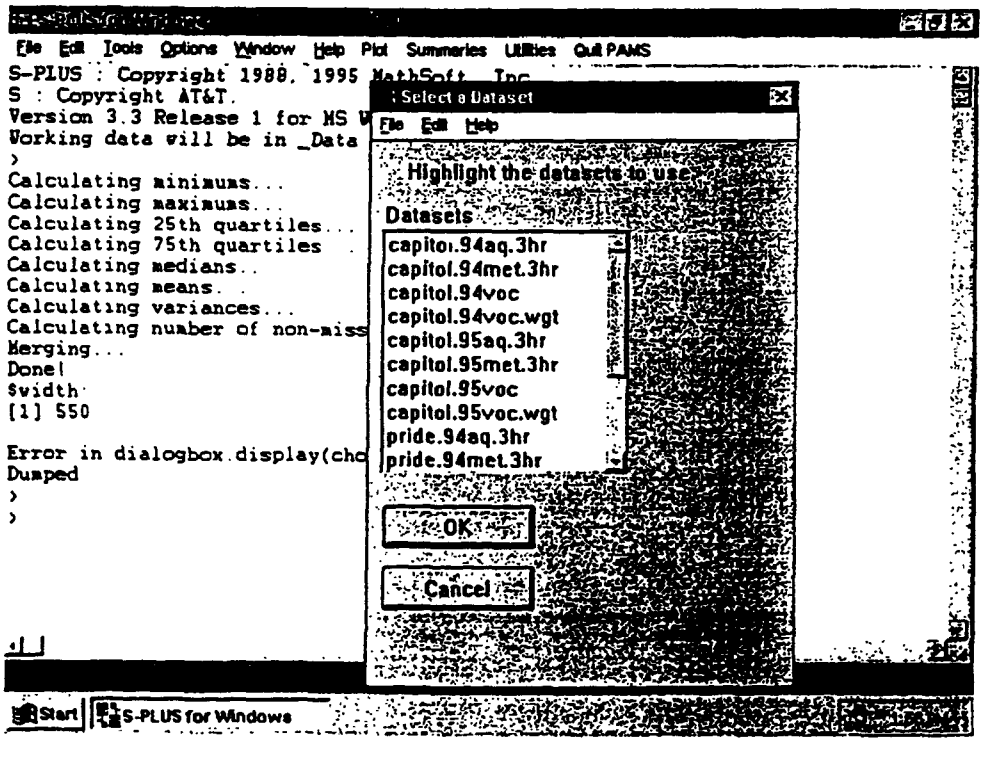
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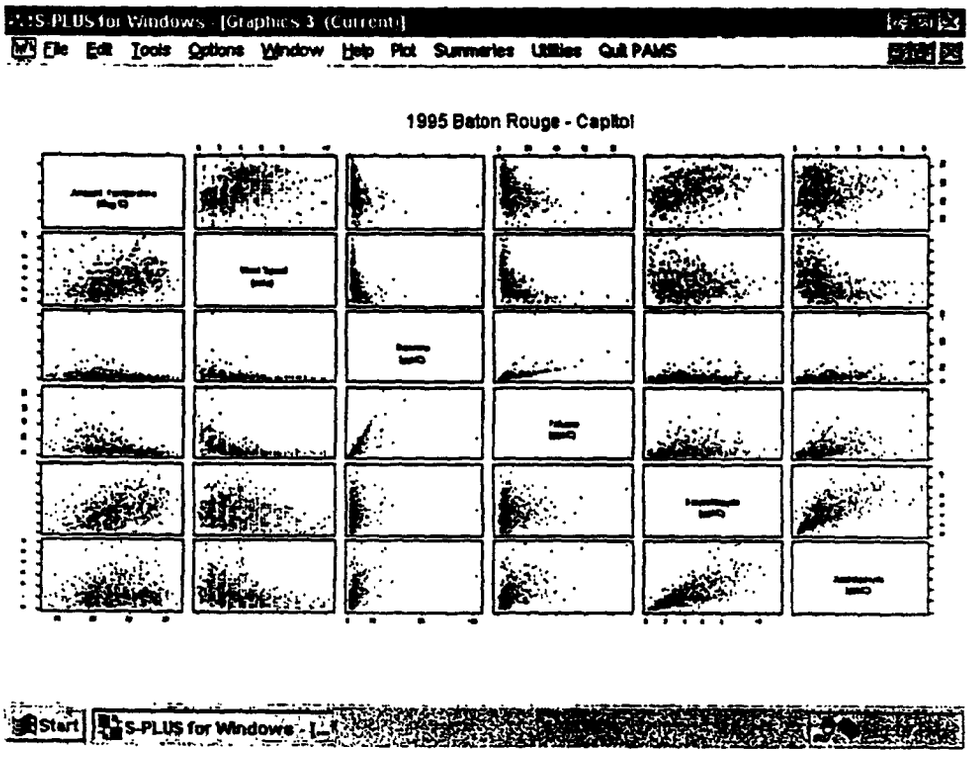
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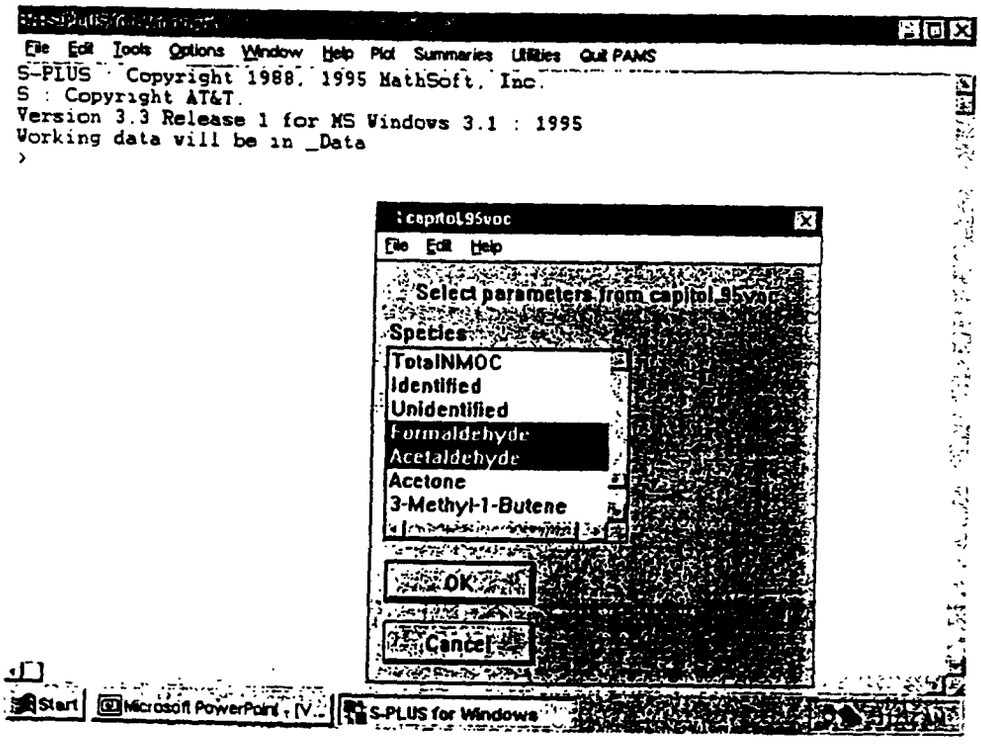
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Acetaldehyde
Acetone
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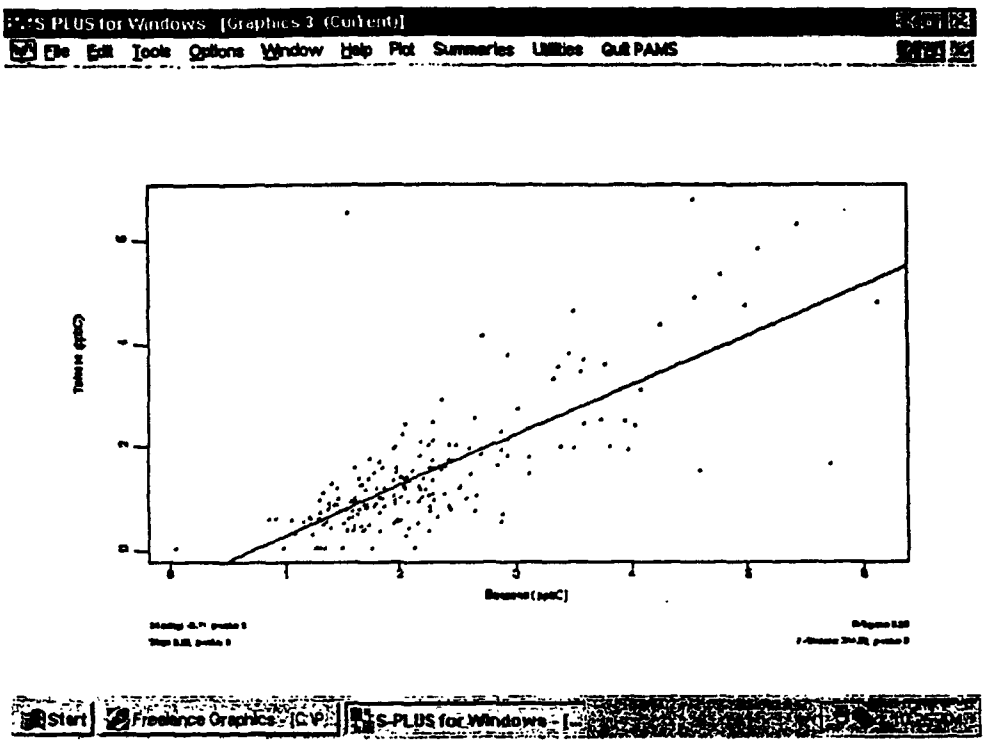
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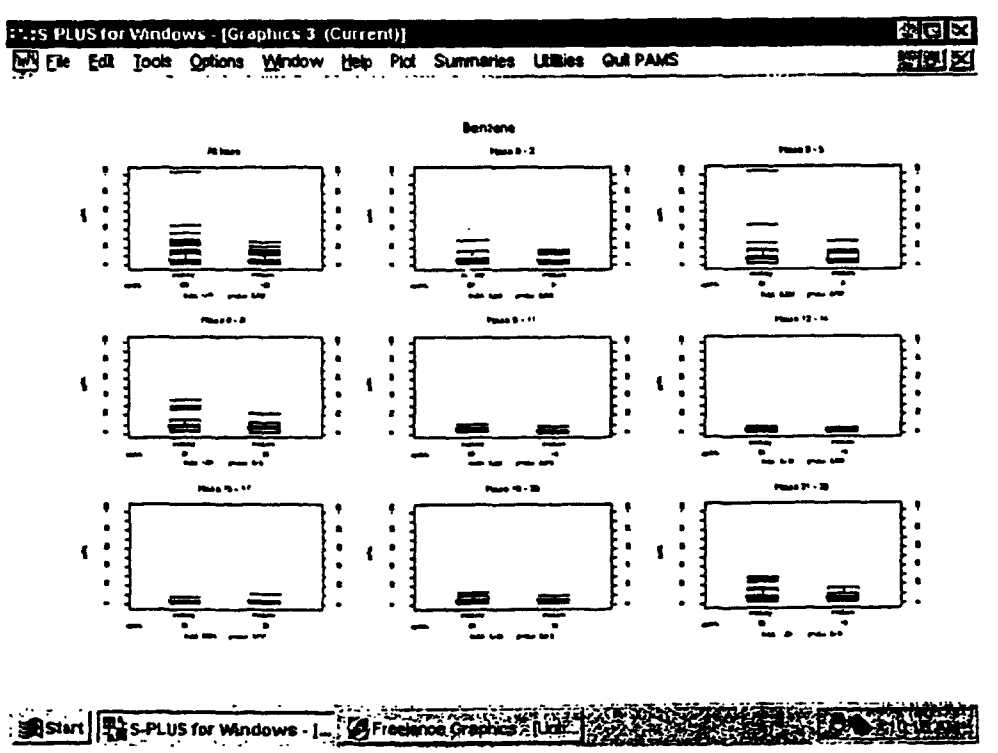
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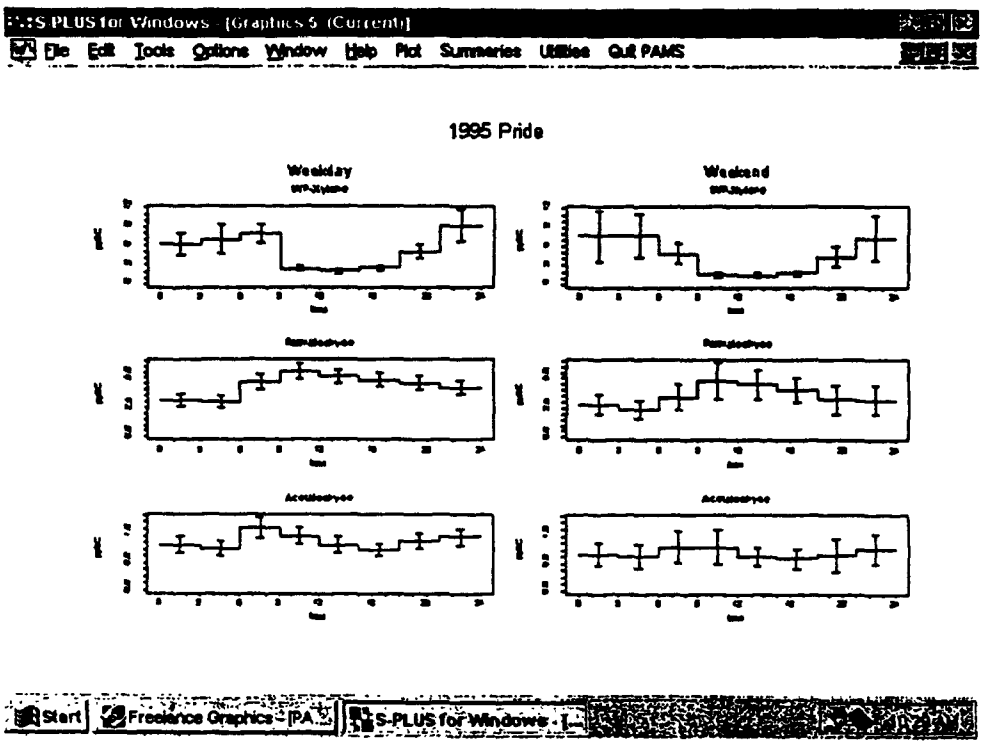
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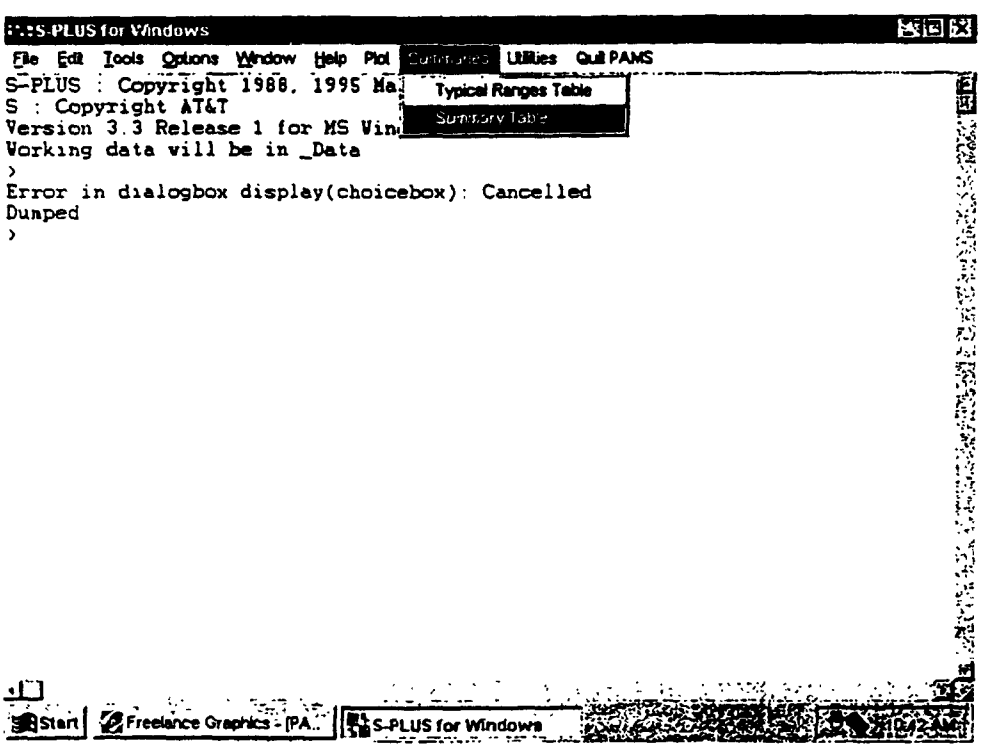
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capitol.95voc

	VOC	Min	1st Qu.	Median	3rd Qu.	Maximum	Mean	S.D.
5	Acetaldehyde	0.05	0.74	1.14	1.76	5.90	1.36	0.94
6	Acetone	0.04	1.49	2.36	3.45	14.31	2.57	1.44
7	Acetylene	0.05	1.51	2.74	4.86	23.17	3.76	3.47
8	Alpha-Pinene	NA	NA	NA	NA	NA	NA	NA
9	3-Methyl-1-Butene	NA	NA	NA	NA	NA	NA	NA
10	2-Methyl-2-Butene	NA	NA	NA	NA	NA	NA	NA
11	1-Butene	0.05	0.65	1.09	2.10	36.60	1.88	2.52
12	Benzene	1.23	2.93	4.29	6.95	103.23	5.90	6.20
13	Beta-Pinene	NA	NA	NA	NA	NA	NA	NA
14	2,2-DiMethylbutane	0.05	0.40	0.68	1.26	8.79	0.99	1.04
15	2,3-DiMethylButane	0.05	0.63	1.14	2.34	15.24	1.81	1.85
16	1,2,3-TriMethylBenzene	0.05	0.14	0.26	0.50	5.90	0.43	0.56
17	1,2,4-TriMethylBenzene	0.05	0.45	0.84	1.60	25.91	1.57	2.29
18	1,3,5-TriMethylBenzene	0.05	0.05	0.47	1.06	19.51	0.80	1.26
19	Cis-2-Butene	0.05	0.15	0.33	0.69	17.06	0.64	1.16
20	Cis-2-Hexene	NA	NA	NA	NA	NA	NA	NA
21	Cis-2-Pentene	0.05	0.44	0.78	1.31	12.29	1.14	1.22
22	CycloPentane	0.05	0.47	0.72	1.16	11.09	0.94	0.80
23	CycloPentene	NA	NA	NA	NA	NA	NA	NA
24	CycloHexane	0.05	0.37	0.71	1.46	8.70	1.22	1.43
26	EthylBenzene	0.05	0.66	1.03	1.97	10.59	1.65	1.77
27	Ethane	0.05	8.16	15.51	20.40	256.93	24.90	30.53
28	Ethylene	0.05	2.48	5.01	10.43	60.06	8.73	9.06

Start | S-PLUS for Windows | Page37c.424 - Notepad

VOCDat: QC Software for VOCs

VOCDat Ver. 1.1
Volatile Organic Compound Data
Display, Quality Control, and Analysis

Developed as part of:

NARSTO-Northeast

For technical support contact:

Sonoma Technology, Inc.
5510 Skylane Blvd., Suite 101
Santa Rosa, CA 95403
(707)527-9372

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VOCDat: Description

- Windows-based, menu-driven program providing a graphical platform to display VOC data and to perform QC tasks.
- Allows QC code changes on-screen, keeps log of changes.
- Import/Export AIRS format files (including null codes).
- Prepares summary of species groups.
- Options to apply reactivity factors or create wt% NMHC.

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OAQPS

VOCDat: Planned Enhancements

- Modify AIRS output to include 0 concentrations for PAMS target species that are missing.
- Create sum of target species and output to AIRS.
- Allow user customization of target species list.
- Create module(s) to run statistical checks and comparisons to enhance QC/QA activities.
- Finalize program in October/November - plans to make available via EPA Internet site

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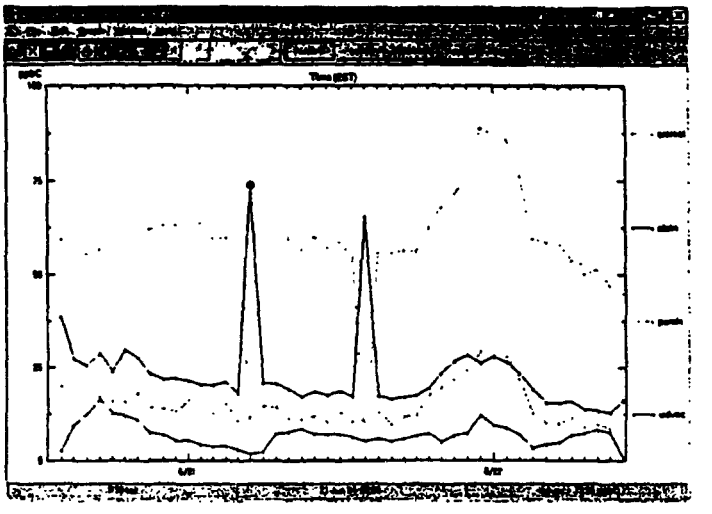
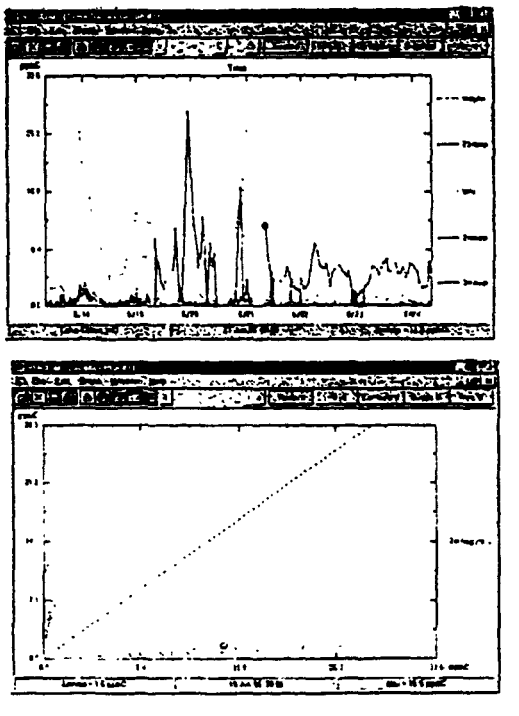
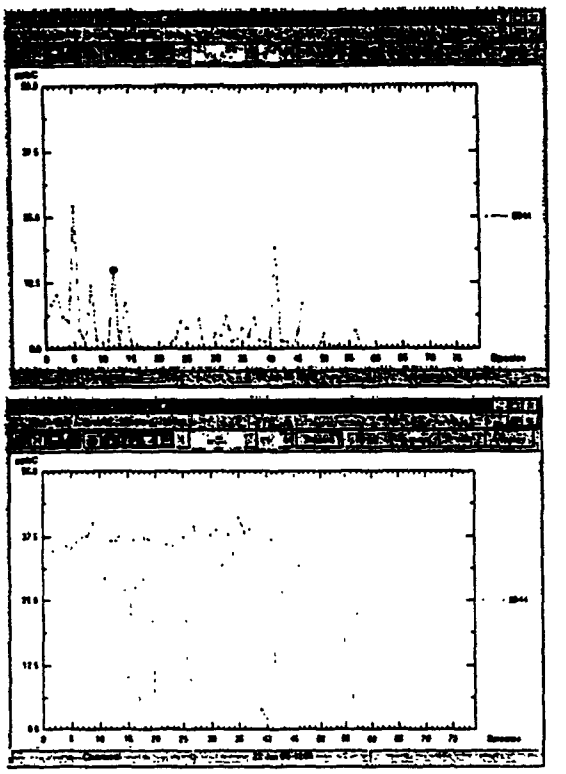


Time series plot of several species groups at Stafford, CT in 1994. Example of misidentification of a paraffin for an unidentified peak. (Level 0, preliminary data, CT DEP)



Example of finding species misidentification in a data set using a time series plot (top) and scatter plot (bottom). Data were collected at the Lake Clifton, MD PAMS site during June 1995 (Level 0, AIRS)



Fingerprint plots of 1995 samples at Chamizal (El Paso), TX. Examples of typical (top) and calibration (bottom) fingerprints. (Level 1, AIRS data)

OTHER ANALYSIS TOOLS

- VOYAGER
- EnvironmentalStats for SPLUS
- Output Format Software

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AMBIENT AIR QUALITY CHARACTERIZATION PROJECT

- Goal: Assess air toxics issue using ambient air quality data
- Two aspects:
  - Collect and analyze ambient data
  - Develop and apply indicators
- Products:
  - Annual data catalogue
  - Annual trend/indicator assessment

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OAQPS

National Air Toxics Emissions Inventory

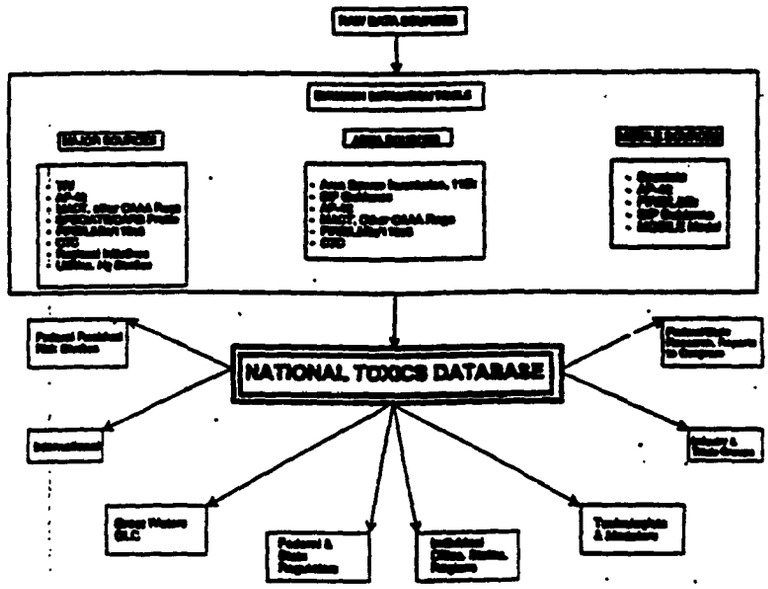
June 18, 1997

Air Toxics Modeling & Exposure Workshop

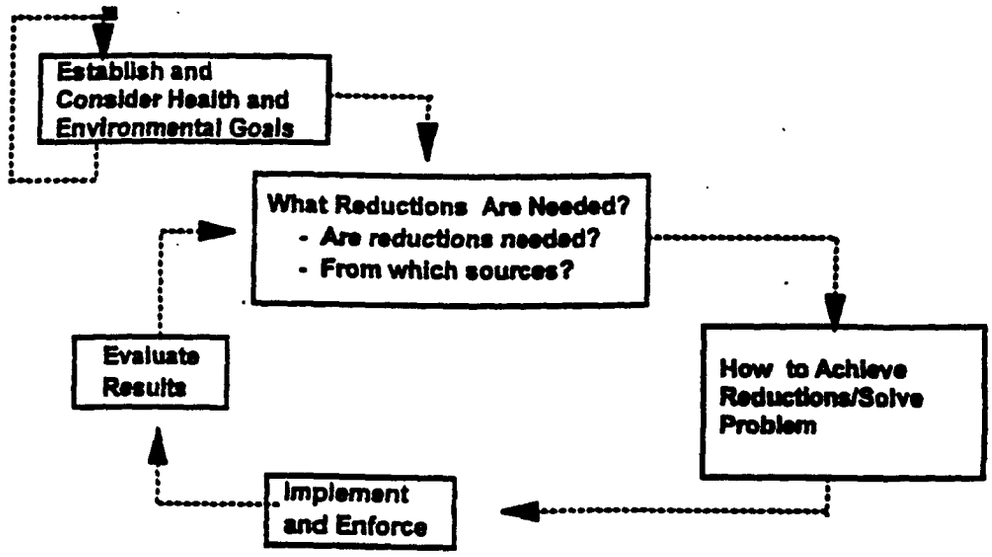
CAA Requirements for NTI

- Section 112(d), MACT
  - Source category & HAP listing/delisting
  - MACT Tracking
- Section 112(k), Urban Area Source Program
- Section 112(c)(6)
- Section 112(f), Residual Risk Program
- Section 112(m), Great Waters Program
- Section 112(n), Special Studies, e.g., Hg

NTI Database Estimation Tools and Stakeholders



AIR TOXICS MANAGEMENT MODEL



112(c)(6) HAPs

- Alkylated lead
- Hexachlorobenzene
- Mercury
- PCBs
- POM
- 2,3,7,8-TCDD
- 2,3,7,8-TCDF

112c6 Category Listing

- Open Burning of Scrap Tires

- Gasoline Distribution Stage I Aviation

- Wood Treatment/Wood Preservatives

Potential 112(k) HAPs

- Acetaldehyde
- Acrolein
- Acrylamide
- Acrylonitrile
- Arsenic compounds
- Benzene
- Beryllium compounds
- Bis(2-ethylhexyl)phthalate
- 1,3-Butadiene
- Cadmium compounds
- Carbon tetrachloride
- Chloroform
- Chromium compounds
- Coke oven emissions
- 1,4-Dichlorobenzene
- 1,2-Dichloropropane
- 1,3-Dichloropropene
- Dioxins/furans
- Ethyl acrylate
- Ethylene dibromide
- Ethylene dichloride
- Ethylene oxide
- Formaldehyde
- Hydrazine
- Lead compounds
- Manganesecompounds
- Mercury compounds
- Methyl chloride
- Methylene chloride
- Methylene diphenyl diisocyanate
- Nickel compounds
- POM
- Quinoline
- Styrene
- 1,1,2,2-Tetrachloroethane
- Tetrachloroethylene
- 1,1,2-Trichloroethane
- Trichloroethylene
- Vinyl chloride
- Vinylidene chloride

Risk Identification Process - List of 37 HAPs of Interest

- Acetaldehyde
- Acrolein
- Acrylamide
- Acrylonitrile
- Antimony compounds
- Arsenic compounds
- Benzene
- Beryllium compounds
- bis(2-chloroethyl) ether
- 1,3-Butadiene
- Cadmium compounds
- Chloroform
- Chromium compounds
- Coke oven emissions
- Ethylene dibromide
- Ethylene dichloride
- Ethylene oxide
- Formaldehyde
- Glycol ethers
- Hydrazine
- Lead compounds
- Managanese compounds
- Mercury compounds
- Methylene chloride
- Methylene diphenyl diisocyanate
- Nickel compounds
- Phosgene
- POM
- Styrene
- 2,3,7,8-TCDD
- 2,3,7,8-TCDF
- Tetrachloroethylene
- Toluene
- 2,-4-Toluene diisocyanate
- Trichloroethylene
- Vinyl chloride
- Xylenes (include o,m, and p)

NTI Data Sources:

- Inventory Approach

  Source-specific data where available
  - State/local HAP inventories
  - MACT data
  - Industry data
  - TRI data

  Estimates using efs and source activity data

Types of NTI Data

- Annual emission estimates in ton/yr
- Physical location of emissions
- Data sources
- Miscellaneous fields related to data processing
  - Data entry dates
  - Allocation codes
- Auxillary information used to estimate emissions
  - Activity data
  - Population
  - Number of facilities
  - Employment data

NTI System Construction

- FIPs state and county codes
- SCCs
- CAS numbers/Pollutant names
- SIC codes
- Allocation codes to define source categories as area, point or mobile
- Primary and secondary references
- US Census population data to define inventory areas as either urban or rural
- VOC or PM codes to identify VOC and PM HAPs
- Date of inventory

NTI System Design

- Database uses SAS

- Hardware requirements: Pentium 200 MHz or Unix system

- Data Storage Space

Auxiliary Data -	120 Megabytes
Local Inventory Data -	50 Megabytes
Dictionary Data -	15 Megabytes
Inventory Data -	200 Megabytes
Data Processing Space -	1-2 Gigabytes
System Memory	64 Gigabytes

NTI Pollutant and Source Category Coverage

- 188 HAPs
- 780 unique point, area, and mobile (on-road & off-road) source categories
- 3141 counties in 50 states

Example Data Outputs

Planned Improvements to NTI

- MACT data
- Facility specific data for major sources
- Update NTI with 112(k) and 112(c)(6) data
- State/Local HAP inventories
- Title V data
- Gap-filling in source/pollutant data
- Better correlation between monitoring and emission inventory data (Qualitative)

STAPPA/ALAPCO Survey

- Source Characteristic
- Toxic Chemical Characteristics
- Risk Assessment
- Ambient Data
- Data Accessibility

Dear State and Local Air Toxics Regulators:

EPA is beginning to work on the implementation of the residual risk requirements mandated by Section 112(f) of the Clean Air Act. In order to understand the residual risks that a source or source category may present after implementing MACT, it is necessary to know what toxic air pollutants they emit. The best sources of the type of information EPA needs for this effort are the state and local regulatory agencies who work most closely with the facilities.

The following is a short survey developed by STAPPA, ALAPCO and EPA. It attempts to gather information about which state and local air agencies collect air toxics emission data and what types of data they have. IT DOES NOT ACTUALLY REQUEST THAT YOU SUBMIT THE DATA! It is merely an attempt to determine what information may be available. The questionnaire also asks that you provide the name of a person to contact if we need follow-up information -- someone familiar with your agency's air toxics efforts as a whole and who can direct us to specific technical staff people, if needed.

Please send your responses to Mary Sullivan Douglas of STAPPA/ALAPCO at m4clnair@sso.org by June 2, 1997. Thank you for your participation!

If you have questions about this survey in general, please direct them to Carol Piening, Washington State Department of Ecology, Air Quality Program. email: cpie461@ecy.wa.gov phone: (360) 407-6858 fax: (360) 407-6802

If you have questions about the ambient air quality portion of the survey, please direct them to James Hemby, EPA, OAQPS email: hemby.james@epamail.epa.gov (919)541-5459 (voice) (919) 541-1903 (fax)

***AIR TOXICS DATA SURVEY - May, 1997 ***

DEFINITIONS:
For the purposes of this survey, please consider the following definitions:

TOXIC CHEMICAL - any chemical on the list of hazardous air pollutants found in Section 112(b) of the Clean Air Act.

SOURCE or SOURCE CATEGORY - a source category listed by EPA for development of MACT standards pursuant to Section 112(c) of the Clean Air Act. Categories of AREA sources include chrome electroplaters, dry cleaners, commercial sterilization facilities, halogenated solvent cleaners, and secondary lead smelting. MOBILE sources includes both on-road and off-road vehicles.

BENCHMARK - the guidelines or standards currently in use by your state or local agency.

PART 1 - SOURCE CHARACTERISTICS:

In general, for what kinds of sources do you collect source characteristic information? (X all that apply)

Point _
Area __
Mobile ___
Some specific-source categories ___

In general, how often are data for a particular source reported?
ie. annually_____

Does your agency collect emission point information? Yes ___ No ___

Does your agency collect emission unit information? (X all that apply)

Stack height: Yes __ No __
Inside diameter: Yes __ No __
Exit temperature: Yes __ No __
Exit velocity: Yes __ No __
Distance(s) to property line: Yes __ No __
Geographical location: Yes __ No __ (e.g. latitude and longitude for GIS applications)
Emission rates: Yes __ No __
Maximum hourly emission rate: Yes __ No __

Are facility data coded by (X all that apply)

SCC __
AMS __
SIC __
Plant or facility ID: name __, address __, ID __, FIPS county codes __

In general, how accurate and complete are the data collected?

1 (poor) __ 2 __ 3__ 4 __ 5 (good) __

PART 2 - TOXIC CHEMICAL CHARACTERISTICS

Does your agency collect information for toxic chemical emissions by CAS number?
Yes __ No __ On a case-by-case basis.

In what units are the toxic chemical emissions information? (X all that apply)

Lb/hour ___
Lb/year ___
Kg/hour ___
Kg/yr ___
Other _____

PART 3 - RISK ASSESSMENT INFORMATION

Has your agency performed or evaluated any risk assessments on source categories?
__Yes - approximate number:_____ No __

Has your agency performed or evaluated any risk assessments on individual sources within those source categories?
__Yes - approximate number:____ No __

What type of benchmarks are used by your agency for cancer endpoint evaluations? (X all that apply)

Cancer: EPA unit risk values __
State/local unit risk values __
Both __
Cancer unit risk value not used __
Derived from occupational guidelines __

If your cancer benchmarks are derived from occupational guidelines, what factors do you apply to them? _____

What type of benchmarks are used by your agency for non-cancer endpoint evaluations? (X all that apply)

Non-cancer: EPA reference concentration/reference dose ___
State-derived (NOAEL/LOAEL approach) ___
Derived from occupational guidelines ___

If your non-cancer benchmarks are derived from occupational guidelines, what factors do you apply to them? _____

What averaging period is used for your benchmarks? (X all that apply)
Annual ___
24 hour ___
8 hour ___
1 hour __
Other ___

PART 4: AMBIENT DATA

Has your agency collected any ambient data on air toxics?
Yes_____ No_____

Are these monitoring efforts best characterized as
Special studies directed at particular sources _____
Characterizations of representative ambient conditions _____
Both _____

What option(s) below best describes the duration of the monitoring effort
One year ____ (please indicate year _____)
Multi-years _____ (please indicate years _____)
Ongoing _____ (please indicate initial year _____)
Other _____

Does your agency have plans to conduct any ambient toxics monitoring in the future?
Yes _____ No_____

If yes, please provide a brief description (objectives, duration, etc.). Ongoing, as part of ozone precursor study.

PART 5: DATA ACCESSIBILITY
Is the data available in a computerized file format? (i.e. ASCII, spreadsheet, database files?)

Source Characteristic data Yes ___ some ___ No ___

Chemical Characteristic data Yes ___ some ___ No ___

Risk Assessment information Yes ___ some ___ No ___

Ambient data Yes ___ some ___ No ___

Are/were ambient data submitted to the Aerometric Information Retrieval = System (AIRS) database?
Yes ___ No ___

Are the data accessible via the Internet?
Yes ___ No ___

Is the data organized in a central location, or dispersed among several people in your agency?
Centralized ___ Dispersed ___

PART 6: ONE CONTACT PERSON

If there are follow-up questions about your air toxics program and the data you have collected, who would be the appropriate primary contact?

Name and title:
Agency or organization:
Mailing address:
Phone:
Fax:
E-mail:

YOU ARE FINISHED WITH THIS SURVEY! Please send your responses, electronically if possible, to Mary Sullivan Douglas of STAPPA/ALAPCO.
email: m4clnair@sso.org
phone: (202) 624-7864
fax: (202) 624-7863

THANK YOU for your time and assistance. This information will be compiled and made available to state and local air pollution control agencies, EPA regional offices, and EPA headquarters. As we get a better idea of what information we need, and who has more information available, we will likely ask the contact person for additional help.

Status of STAPPA/ALAPCO Survey - June 16

Alabama	
Alaska	
Arizona	rec'd
Arkansas	
California	
Bay Area	rec'd
Ventura	rec'd
Monterey	rec'd
Colorado	rec'd
Connecticut	rec'd
Delaware	rec'd
Florida	
Georgia	
Hawaii	
Idaho	
Illinois	rec'd
Indiana	
Iowa	
Kansas	
Wyandote	rec'd
Kentucky	rec'd
Louisiana	rec'd
Maine	rec'd
Maryland	
Massachusetts	
Michigan	rec'd
Minnesota	rec'd
Mississippi	
Missouri	
Montana	
Nebraska	
Nevada	
New Hampshire	
New Jersey	
New Mexico	
New York	rec'd
North Carolina	rec'd
North Dakota	rec'd
Ohio	
Oklahoma	rec'd
Oregon	
Pennsylvania	rec'd
Rhode Island	

South Carolina	rec'd
South Dakota	rec'd
Tennessee	
Texas	
Utah	
Vermont	rec'd
Virginia	rec'd
Washington	rec'd
Puget Sound	rec'd
West Virginia	
Wisconsin	rec'd
Wyoming	
DC	

TABLE 1. PROPOSED EMISSION INVENTORY RULEMAKING PROVISIONS.

Provision	Statewide Point Source Inventory			
	Significant Sources[1,2]	Major Sources[2]	Emission Statements	3-Year Inventory
CAA citation	§ 110(a)(2)(F)	§ 110(a)(2)(F), § 112	§ 182(a)(3)(B)	§ 172(c)(3), § 182(a)(3)(A), and § 187(a)(5)
Frequency of reporting	Annual	Every three years	Annual	Every three years
Estimating period	Annual	Annual	Annual and Daily[5]	Annual and Daily[6]
Areas to which provision applies	Entire U.S.	Entire U.S.	Ozone NA areas and attainment areas in ozone transport regions	Ozone, CO, and PM-10 NA areas
Pollutants and source size thresholds	Pollutant / tpy[3] SO_2 2,500 NO_x 2,500 VOC 250 PM-10 250 CO 2,500	Pollutant / tpy SO_2 ≥ 100 NO_x ≥ 100 VOC ≥ 100 PM-10 ≥ 100 CO ≥ 1,000 Pb ≥ 10 [4]HAPs ≥ 10 Major source thresholds vary in nonattainment areas depending on classification.	Pollutant / tpy Ozone NA areas: VOC ≥ 25 NO_x ≥ 100 Attainment areas in ozone transport region: VOC ≥ 50 NO_x ≥ 100	Pollutant / tpy Ozone NA areas: VOC ≥ 10 NO_x ≥ 100 CO ≥ 100 CO NA areas: CO ≥ 100 PM-10 NA areas: PM-10 ≥ 70 Inventory includes: • Point sources ≥ specified tpy. • Area sources < specified tpy. • On-road mobile sources. • Nonroad mobile sources. • Biogenic sources.

Great Lakes Commission

Great Lakes Regional Air Toxics Emissions Inventory

Overview

Air regulatory agencies in the eight Great Lakes states agree that a collaborative effort is vital to successfully implement a compatible regional database of airborne toxic pollutant emissions. They have been working cooperatively toward this goal since 1987. Once a quality controlled/quality assured data inventory has been established, the states and the U.S. Environmental Protection Agency can begin to work separately and in concert to define and regulate sources; evaluate control technology; establish guidelines for siting new facilities; and reduce airborne deposition of persistent toxic chemicals to the Great Lakes.

Purpose

This inventory will assist in the successful implementation of key provisions of the Great Lakes Toxic Substances Control Agreement, signed by the Great Lakes governors in 1986. In addition, this work is consistent with the state activities for the implementation of the Urban Area Source Program required under sections 112(c) and 112(k) under the Clean Air Act Amendments of 1990 and the assessment of atmospheric deposition to the Great Lakes under the efforts of U.S. EPA's Great Waters Program.

- Section 112 of the Clean Air Act
- Great Lakes Governors' Toxic Substances Control Agreement of 1986

Background/History

An Overview of Inventory Development

The Great Lakes states, working together through the Great Lakes Commission, are creating this regional database with funds from the Great Lakes Protection Fund and U.S. EPA. Specifically, the program's goal is to establish a baseline using 1993 data on point and area source emissions of 49 toxic air pollutants that have been identified as significant contributors to the contamination of the Great Lakes.

Steering Committee for the Great Lakes Regional Air Toxics Inventory Project

The steering committee guides development of the regional inventory and associated products, including RAPIDS and the *Air Toxics Emissions Protocol*. Emission inventory specialists from the Great Lakes states, U.S. EPA and the province of Ontario work together closely.

49 Toxic Pollutants

The Great Lakes Regional Air Toxics Emissions Inventory targets 49 compounds that have been identified as significant contributors to the contamination of the Great Lakes. These compounds, and the programs or agencies that have targeted them, are listed.

AirToxics E-mail Archive

The Great Lakes Regional Air Toxics Emissions Inventory Project successfully demonstrates the cost-effective and time-efficient use of the Internet as an aid to solving regional environmental problems. Project members use an e-mail list server to discuss project developments, drastically reducing the need to travel to meetings and hold expensive conference calls. An archive of the e-mail messages provides a history of this interaction.

Products

Air Toxics Emissions Inventory Protocol for the Great Lakes States

The protocol provides instructions necessary for the Great Lakes states to develop a regional inventory that is complete, accurate and consistent from state to state. The protocol was tested during the Southwest Lake Michigan Pilot Study. It is being used to guide the efforts of all eight Great Lakes states in 1995-96 as they prepare the first full statewide toxic air emissions point and area source inventories and populate the regional repository. Further additions and refinements may be expected after the first full eight-state inventory.

Regional Air Pollutant Inventory Development System (RAPIDS) client/server software

RAPIDS, the Regional Air Pollutant Inventory Development System, is the first-ever multi-state pollutant emissions inventory software. Designed and implemented for the Great Lakes Commission and the eight Great Lakes States, RAPIDS was tested by the lead states of Illinois, Indiana and Wisconsin in their joint development of the Southwest Lake Michigan Urban Areas Air Toxics Emission Inventory. At least 49 toxic pollutants were targeted, in addition to several other important nontoxic compounds.

Southwest Lake Michigan Pilot Study

Illinois, Indiana and Wisconsin, working together through the Great Lakes Commission, have completed the first multistate inventory of emissions of toxic air contaminants that are identified as being potentially harmful to the Great Lakes ecosystem or human health. Specifically, these states created an inventory of small point and area sources of toxic air emissions from the combined 12-county urban areas of Chicago, Gary and Milwaukee.

Scope Study for Expanding the Great Lakes Toxic Emission Regional Inventory to include Estimated Emissions from Mobile Sources

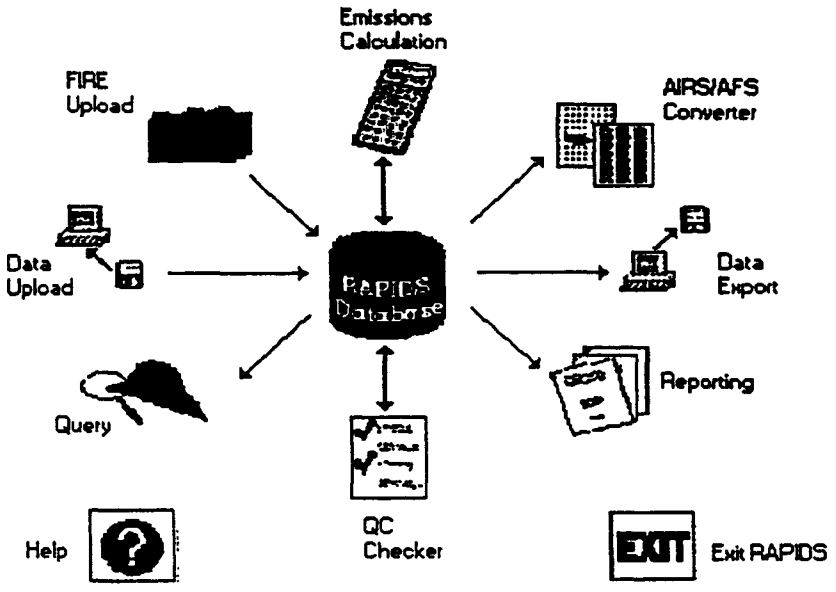
This study explores expanding the Great Lakes Toxic Emission Regional Inventory to include estimated emissions from mobile sources.

Comments or questions about the regional inventory? Contact Project Manager Carol Ratza, cratza@glc.org.

Great Lakes Commission

Overview of the RAPIDS System

RAPIDS is a client/server system consisting of an ORACLE back-end database (version 7.0), designed using ORACLE CASE tools, and a suite of front-end applications developed using various software tools (e.g., primarily PowerBuilder and SAS). The RAPIDS system includes the following components:



- RAPIDS Database
- FIRE Upload client/application
- Data Import and Data Export client applications
- Query
- QC Checker client/application
- Report Generator
- Data Converter client/application
- Emission Estimator client/application

The RAPIDS Database

The RAPIDS database includes the following components:

- An ORACLE back-end database consisting of various ORACLE data tables of emissions data and estimates located on a separate (i.e., separate from the front-end client applications) file server at each participating state;

- A set of Data Entry client/applications developed in PowerBuilder that consists of various forms/screens to enter various types of emissions data, and emission estimates derived external to RAPIDS;

- A set of ORACLE data tables of emissions data and estimates located at the Great Lakes National Program Office (GLNPO) containing emissions data and estimates obtained from each of the participating states (i.e., a regional database of emissions data and estimates). RAPIDS includes a client/application that uploads (GLNPO Upload) each state's set of ORACLE tables to the regional repository located at GLNPO.

RAPIDS Data Model

The RAPIDS data model is the cornerstone of the RAPIDS system and includes entities that are shared by most mission critical applications. As more applications are added to the RAPIDS system, the core data model will be extended to support them.

FIRE Upload

A FIRE Upload client/application (this application is under development) that will upload the emission factors contained in FIRE into a reference table used to calculate emissions. The Factor Information Retrieval System or FIRE is an emission factor database repository developed by U.S. EPA. The emission factors contained in FIRE have been incorporated into RAPIDS and used within the system to compute emission estimates for certain source categories.)

Data Import and Data Export

Data Import and Data Export client applications facilitate the import of emissions data and estimates maintained by the states external to RAPIDS into the back-end database, and the export of data from the back-end database into ASCII files (i.e., import file format).

Query

The QUERY application provides the user with access to InfoMaker (the InfoMaker software is not provided with RAPIDS), a powerful, easy-to-use ad-hoc reporting tool that lets users query the RAPIDS database and create custom reports of

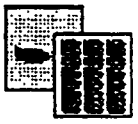
data. This ad-hoc query and reporting tool supplements the pre-defined reports created by the Reporting client/application.

QC Checker

A QC Checker client/application that perform various statistical checks on the emissions data and estimates contained in the ORACLE back-end database. A sample QC Checker screen shows the various options available to the user for performing these statistical checks. Additional statistical checks are expected to be added to the QC Checker application over time.

Report Generator

A Report Generator consisting of various client/applications that generate summary reports of the emissions data and estimates contained in the ORACLE back-end database. A sample Tier 1, 2, 3 Reporting screen shows the various reporting options available to the user for this particular report.



Data Converter

A Data Converter client/application converts the emissions data and estimates into U.S. EPA's AIRS Facility Subsystem (AFS) transaction records. A sample AIRS Converter screen shows the various options available to the user for creating AFS transaction record from RAPIDS.

Emission Estimator

An Emission Estimator client/application allows the user to compute emission estimates using a variety of emission estimation techniques [e.g., product of activity data and an approved emission factor, speciation of either particulate matter (PM) or VOC emission estimates or user-defined algorithms] that match pre-established

SCC/compound-specific methodologies listed in the *Air Toxics Protocol.* (The protocol is a comprehensive document that describes the methodologies the participating states will use to compile the regional inventory, including the procedures to resolve differences of opinion). A sample emission estimation screen shows the various options available to the user for estimating emissions.

RAPIDS software was designed with several features:

- An easy-to-use Windows format built with state-of-the-art database management tools.
- A menu-oriented design with an interface that maintains a consistent "look and feel" throughout the various system modules.
- Data storage and management for point source and area source emissions estimates. Although a fugitive emissions data model is not presently a RAPIDS feature, the system is designed to accommodate this component at a later date.
- Specific emissions estimates for states, facilities, devices, processes or streams can be incorporated.
- Source-specific emission factors can be stored and used to calculate emission estimates.
- Batch and interactive emission estimation capabilities, using emission factors, activity data, mass balance and speciation.
- Batch input and on-line updates.
- Various QA/QC checks and routines on the emissions data and estimates are performed, including range checks, outlier checks, acceptable value checks, missing value flags and other techniques, to identify suspicious or unacceptable data.
- Point and area source data and estimates stored in RAPIDS are converted into the U.S. EPA's Aerometric Information Retrieval System (AIRS) transaction format.
- Emissions summary report generation.

Comments or questions about RAPIDS? Contact Project Manager Carol Ratza, cratza@glc.org.

● Return to the RAPIDS Home Page

Table 1: List of Target Compounds for the Regional Toxic Air Emissions Inventory

		Toxic List			
		Great Lakes Waters	Great Lakes Commission	CAA 112(c)(6)	
1	Arsenic	Yes	Yes		7440-38-2
2	Atrazine	Yes			1912-24-9
3	Benz(a)anthracene (1,2-Benz(a)anthracene Benzo(a)anthracene)		Yes		56-55-3
4	Benzo(a)pyrene	Yes	Yes		50-32-8
5	Cadmium	Yes	Yes		7440-43-9
6	Carbon tetrachloride	Yes	Yes		56-23-5
7	Chlordane	Yes			57-74-9
8	Chromium	Yes	Yes		7440-47-3
9	Chrome VI		Yes		18540-29-9
10	Chrysene (Benz(a)phenanthrene)		Yes		218-01-9
11	Cobalt	Yes			7440-48-4
12	Coke oven emissions	Yes			8007-45-2
13	Copper	Yes			7440-50-8
14	1,2-Dichloroethane		Yes		107-06-2
15	Diethlyhexyl phthalate (Bis(2-ethylhexyl) Phthalate)		Yes		117-81-7
16	Di-n-butyl phthalate		Yes		84-74-2
17	Di-n-octyl phthalate		Yes		117-84-0
18	Dioxins	Yes			
19	Ethylbenzene	Yes			100-41-4
20	Fluoranthene (1,2-Benzacenapthene Benzo(jk)fluorene)		Yes		206-44-0
21	Heptachlor	Yes			76-44-8
22	Hexachlorobenzene	Yes	Yes	Yes	118-74-1
23	Hexachlorobutadiene		Yes		87-68-3
24	Hexachloroethane		Yes		67-72-1
25	Lead	Yes	Yes		7439-92-1
26	Alkylated lead compounds		Yes	Yes	7439-92-1
27	Manganese & compounds	Yes			
28	Mercury	Yes	Yes	Yes	7439-97-6
29	Methoxychlor Dimethoxy-DDT	Yes			72-43-5
30	Methylene Chloride Methane Dichloride Freon 30	Yes			75-09-2
31	Naphthalene		Yes		91-20-3

		Toxic List			
		Great Waters[1]	Great Lakes Commission[2]	CAA 112(c)(6)[3]	
32	Nickel and compounds Ni carbonyl Ni cyanide NI subsulfide	Yes			 13463-39-3 557-19-7 12035-72-2
33	Parathion	Yes			56-38-2
34	Pentachloronitrobenzene (PCNB) (Quintobenzene)	Yes			82-68-8
35	Pentachlorophenol (PCP)	Yes			87-86-5
36	Phenol (Carbolic Acid)	Yes			108-95-2
37	Total polychlorinated biphenyls (PCBs)	Yes	Yes	Yes	1336-36-3
38	Total polychlorinated dibenzodioxins (PCDDs)	Yes	Yes		
39	Total polychlorinated dibenzofurans (PCDFs)		Yes		
40	Total polycyclic aromatic hydrocarbons (PAHs)	Yes	Yes		
41	Polycyclic organic matter (POM)	Yes		Yes	
42	2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD)		Yes	Yes	1746-01-6
43	2,3,7,8-tetrachlorodibenzofuran (TCDF)	Yes	Yes	Yes	51207-31-9
44	Tetrachloroethene (Tetrachloroethylene 1,1,2,2-Tetrachloroethylene Perchloroethylene PERC)		Yes		127-18-4
45	Trichloroethene (Trichloroethylene)		Yes		79-01-6
46	1,1,1-trichloroethane		Yes		71-55-6
47	2,4,5-trichlorophenol		Yes		95-95-4
48	2,4,6-trichlorophenol		Yes		88-06-2
49	Trifluralin (2,6-Dinitro-n,n-dipropyl-4-(trifluoro-methyl) benzenamine)	Yes			1582-09-8

1. Compounds listed (among others) on U.S. EPA Great Waters Program's list of targeted toxic chemicals.
2. Compounds originally targeted by the Great Lakes Commission. The full GLC list now includes all 49 compounds listed above.
3. Compounds identified (among others) in the U.S. Clean Air Act, as amended in 1990 (Section 112 (c)(6)).

Emission Estimation: Techniques and Tools

Guidance and Assistance Tools from the Emission Factor and Inventory Group, OAQPS, U.S. EPA

Presented by:

Anne Pope, U.S. EPA
Mary Anne Barckhoff, Lockheed Martin

Emission Estimation Methods

- ✓ Continuous Emissions Monitoring
- ✓ Source Tests
- ✓ Material Balances
- ✓ Emission Factors

Material Balances

- ✓ **Air Emissions = Input - Solid wastes - Products - By-products**
- ✓ **Can be used when source test data and emission factors are not available**
- ✓ **Best used for screening purposes where reasonable assumptions can be made about the fate of compound**
- ✓ **DO NOT USE for processes where material is reacted to form products or otherwise significantly chemically changed**

Providing Preferred and Alternative Methods

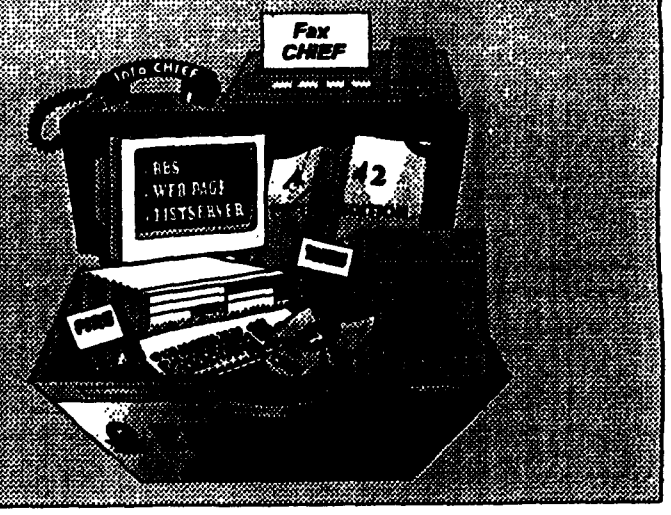
- ✓ A preferred method should result in the best estimate, and can be accomplished by a typical agency.
- ✓ Alternative methods may be less demanding to accomplish, but may provide a less dependable estimate or less detail.
- ✓ A well-done alternative method may be preferable to a badly done preferred method.

Emission Factor

An Emission Factor is a ratio that relates quantity of pollutant emitted to the activity level of a specific source.

(Example: kg PM/Mg coal burned)

EPA's Emission Estimation Tools



AP-42

Volume I -- Point and area sources

Volume II -- Mobile sources

Contains criteria and HAP emissions information on:

- ✓ Types of sources emitting criteria air pollutants
- ✓ General process descriptions
- ✓ Identification of potential release points
- ✓ Emission factors for controlled and uncontrolled processes

Available from GPO, EPI, CHIEF BBS, Web Page, Fax CHIEF and on Air CHIEF CD

LOCATING AND ESTIMATING SERIES

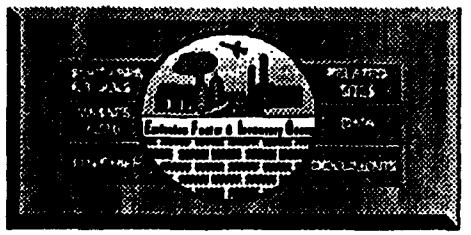
"L & E'S"

Pollutant or source category specific reports that contain detailed emission information on:

- ✓ **Types of sources emitting hazardous air pollutants**
- ✓ **General process descriptions**
- ✓ **Identification of potential release points**
- ✓ **Emission factors for controlled and uncontrolled processes**
- ✓ **Reviewed by S/L agencies, industry, consultants, and EPA**

EFIG WEB SITE

http://www.epa.gov/oar/oaqps/efig/



Emission Factor and Inventory Group
Office of Air Quality Planning and Standards,
US EPA

Fax CHIEF

- ✓ **What is it?**
  - **AP-42 is loaded on our fax machine to be retrieved from your fax machine**
- ✓ **How do I use it?**
  - **Call (from a fax machine) (919) 541-5626 or 0548. A recording will coach you through the process.**
- ✓ **Suggestion!!!**
  - **Choose document 000001 (the code list for the Document Index) as your first request.**
- ✓ **For help. . .**
  - **Call Info CHIEF (919) 541-5285**

EFIG Listserver

- ✓ Receive CHIEF Newsletter (no longer available in print format) via email
- ✓ Receive timely EFIG news updates via email
- ✓ How to Subscribe:
  - **Email a message to: listserver@unixmail.rtpnc.epa.gov**
  - **type "Subscribe CHIEF *Firstname Lastname*"**

AIR CHIEF CD-ROM

- ✓ Contains EPA reports and databases in one easy-to-use CD-ROM including:
  - **FIRE**
  - **L&E's**
  - **AP-42**
  - **SCC List**
  - **SIC List**
  - **AP-42 Background Documents**
- ✓ **Install copies**
  - **FIRE**
  - **TANKS**
- ✓ **NEW (version 5.0)!**
  - **EIIP Documents**
  - **Adobe Acrobat Reader**

Air CHIEF CD-ROM
Version 5.0

Version 5.0 will be available Fall 1997

- ✓ NEW! Adobe Acrobat format
- ✓ Verity search engine
- ✓ Links between EIIP and AP-42 documents
- ✓ System Requirements
  - **Requires IBM-compatible PC**
  - **486 or better**
  - **Microsoft Windows**
  - **CD-ROM reader**

Call Info CHIEF for more information,
(919) 541-5285

National Emission Trends Viewer CD-ROM

- ✓ Microsoft Access program
- ✓ Includes emission inventory data for 1985-1995
- ✓ Emission reports available by:
  - **Pollutant source-type grouping (chemical manufacturing)**
  - **National, state, county or non-attainment area**
  - **Year**
- ✓ Summary reports export to dbf, txt, and wkl file types.

TANKS version 3.0

- ✓ **Calculational software to estimate emissions from organic liquid storage tanks**
- ✓ **Based on revised equations in Chapter 7 of AP-42**
- ✓ **Calculates emissions for:**
  - **Horizontal and Vertical Fixed Roof Tanks**
  - **External and Internal Floating Roof Tanks**
  - **Underground Storage Tanks**
- ✓ **Calculates total VOC and individual HAP emissions**
- ✓ **Calculates monthly and annual emissions**

FIRE version 5.0b

- ✓ Searchable database containing EPA's recommended emission factors
  - Criteria pollutants
  - Toxic pollutants
- ✓ Complete Source Classification Code (SCC) Listing
- ✓ Standard Industrial Codes (SIC)
- ✓ Available for download from EFIG web page (www.epa.gov/oar/oaqps/efig/)

Info CHIEF Help Desk
(919) 541-5285

Staffed under contract by

LOCKHEED MARTIN

- ✓ Locate Emissions and Inventory Material
- ✓ Help with using databases and CD-ROM
- ✓ Help with CHIEF BBS and Internet problems
- ✓ On-site training

Presentation Notes
Mike Fishburn
Panel #3: Air Toxic Emissions Inventory

When Are Emissions Inventory Tools Adequate?

Perceived Deficiencies, Problems and Some Solutions:

Training and Materials

Reading List

Satellite Training/Video Tapes/PC-Based Training

Accessibility of Data and Available Tools

There were a number of tools and sources mentioned in the comments (AP-42, FIRE, L&E documents, TTN BBS (CHIEF, CAA, EMTIC, etc), SPECIATE), but there was also a need expressed for improvement in tools in a variety of areas.

New SPECIATE Database

Guidance

List of Chemicals?

List of Categories?

Level Setting

Help with Methodology and Format(s):

What type of inventory information and format is most useful to the modelers and the people that do exposure and health risk assessment?

Is a holistic inventory (every possible source category) necessary or only an inventory of selected categories?

What about hot spots?

Consistency

There is a need for a concise list of toxic area source categories to be studied that would be consistent across states and locals (or a list of chemicals to be inventoried and related source categories).

There's a perceived need for EPA to assist in establishing consistent across-the-board "levels of significance" in regard to HAPs reporting, i.e., how quantity (1 lb. per year, 10 lbs. per year, 10 tons per year, etc.) of a particular HAP should be reported because levels at or above that should be of concern.

Consistency (cont.)

There may be a need to develop a consensus-type process, similar to the Emissions Inventory Improvement Program's (EIIP), to compile existing inventory methodologies and/or develop new methodologies. This would help assure that different states and locals used the same steps or procedures in developing toxic emissions estimates.

Where should inventories be sent (i.e., what database)? What format(s) should be used?

Specific or Special Guidance Issues

Improved speciation for on-road and off-road

Guidance in how to use the new MOBTOX module

Relating Emissions Levels of HAPs to Exposure and Health Risk Assessment

There is a need for some way to meaningfully relate health risk assessment and impacts to emissions levels so that emissions data become more meaningful as a consequence (a weighting scheme, screening model?) In this way those category/chemical combinations that are more significant could be put into priority bins that would allow everyone involved to better focus their efforts.

Atmospheric Transformation/Secondarily-formed Pollutants

Provide some means of dealing with secondarily formed pollutants without running a regional oxidant model. Current tools are not very amenable to doing a good analysis

for things like formaldehyde.

TRI/EI Overlap

Concerns were expressed about the seeming overlap in responsibilities between Emissions Inventory and the Toxic Release Inventory (TRI). There needs to be a clarification of the areas of responsibility.

Responsibility for Establishing New Toxic Emissions Inventory Requirements

Federal Role

Role of the State and Local Agencies

The Legalistic Approach--Because It's Required

Industry Accountability

Health Risk

Conclusion

If the priorities/needs of Emissions Inventory personnel in regard to toxic emissions inventories could be reduced to no more than a handful of major points they would be:

- Update current tools and make them easily accessible (i.e.TTN-BBS and CD-ROM), and provide assistance in developing emission inventories to state and locals by developing a reading list and conducting training.

  A particular emphasis should be placed on updating SPECIATE if it is inappropriate for use with point source toxic emssions inventories. Continue to provide updated HAP emission factors in FIRE and AP-42.

Conclusion (cont.)

- Create a uniform method for database development, develop an air toxic list of pollutants that are important, develop a significance level for each pollutant to minimize database size and maximize its use, and recommend a particular method for developing emissions so that there is a consistency within the state as well as between states (i.e. use AP-42 for point sources, etc.)

- Develop a requirement (regulation) that sources above certain significance levels must report emissions and create standards or some sort of ambient levels as a goal for specific toxic pollutants. This could also require that industry be held accountable for

its toxics emissions as well as criteria pollutants. And, if everyone uses these same parameters for inclusion in an inventory, then this would be one step towards providing consistency in both data collection and comparison.

Conclusion (cont.)

- Do whatever is regulatorily necessary to provide support to existing state air toxics programs.

- Ensure inventories are compatible with the models likely to utilize the emissions inventories.

Panel 3: Toxic Air Emissions Inventory
Additional Comments

Who should have the responsibility for establishing any new toxic emissions inventory requirements? Is there a need?

Federal Role?

"Should the federal government be the primary party responsible for promulgating programs and regulations aimed at emissions reductions of hazardous air pollutants?"

Role of the States and Locals

"How many states and locals are actually doing anything with toxic emissions inventories on a regular basis and what level of involvement do they want? For instance, is there the political will on the part of states to develop their own regulations if that was necessary to "fill the holes" in any federal rules that might be promulgated (Urban Area Source Program Team)?

"Who will bear the expense of any additional inventory requirements?"

Legalistic Approach--Because It's Required

"There is currently no federal requirement for area, non-road and on-road mobile source inventories toxic emissions inventories. What's on the horizon legally? What will be the outcome of the work on implementing sections of CAAA 112 that is being done through EPA's Urban Area Source Program?" What form should the any new guidance take?

"A recommendation is that EPA concentrate on a umbrella-type structure or framework (e.g., scientific research shows that a certain number of chemicals from certain categories cause health problems at X levels and a standard is to be established not to exceed X level) while leaving states and locals the flexibility to develop and implement the regulations and programs required to achieve reductions. The initial presumption should be that the states and locals should be and will want to be involved in developing the regulations and programs appropriate to their areas. That level of flexibility, built into the program, will assure that any new toxic emissions programs and regulations are more targeted and address local area-specific problems."

"Another point of view on the issue of EPA standard-setting is that it may not be workable to rely on the EPA to set the standards because it may take too long and may

not be workable. The history of the Maximum Achievable Control Technology (MACT) standards was cited to support this view of EPA in the standard-setting role. In this view states would assume more of the standard-setting role rather than waiting for EPA to take action."

"There is a legal requirement that all point sources establish their permitting category (Title V or non-Title V). To do this, a fairly thorough accounting of HAPs must occur to establish whether facilities are over or under the 10/25 ton thresholds for Title V permitting"

"Some States have air toxics programs that require an accounting and evaluation of many of the HAPs listed in the federal program.

"The experience of developing the 1990 Base Year Inventory and the 1993 Periodic Inventory have made it clear that while area source and nonroad mobile sources are becoming increasing larger percentages of the overall anthropogenic emissions inventory the quality of data available about activity levels is relatively poor. While some states may require that area sources report if they exceed fairly low threshold amounts there may be an equal or larger number of states that may be estimating emissions based on surrogates such as population or employment because of the paucity of actual information about activity levels. Since the area source and nonroad mobile source categories may either not lend themselves to survey work or survey work would be too resource intensive and expensive, there may be an issue of how to get reliable data to estimate toxic emissions. It may be counterproductive to raise people's level of concern based on emissions estimates allocated to a county-wide area when it may be that only the gas station at 12th and Vine is the source of the problem in its proximity to a daycare center.

There may be very little enthusiasm on the part of the federal government to mandate that such information be provided and collected. And, given the political climate and proximity to small business association lobbies, it seems highly unlikely that states will be requesting additional authorities to collect such information.

Unless there is a clear federal mandate or requirement placed on states or locals to develop toxic emissions inventories and/or the grant funding to develop inventories some panelists are of the opinion that states and locals that already have toxic emissions inventory programs in place will be likely to continue, some additional states and locals will comply with a voluntary program, but still others will not develop the inventories and may legitimately make their case that their agencies are resource constrained and are already having difficulty in meeting federal requirements."

Industry Accountability

"Industry has been held accountable for its emissions of the criteria pollutants since the onset of the Clean Air Act. Why shouldn't there be a comprehensive accounting of what toxics are being emitted into the air?"

Health Risk

"Is there a significant threat? The lesson of the new NAAQS: A frequently heard comment made in response to the proposed revisions in the NAAQS is that EPA has failed to make its case that there is a significant health risk sufficient to outweigh the costs entailed in achieving even greater emissions reductions than are currently mandated. If regulations are promulgated that mandate SIP-like targets for reductions in HAPs, then it seems critical to the successful implementation of those regulations that EPA make a strong, scientifically-based case that there is, in fact, a significant health risk from the exposure to various HAPs. It might be, given the availability of the evidence, that the risk from HAPs should be prioritized or that tiers, bins, or other groupings be established that would convey the level of associated risk. Anything else might result in inefficiencies, i.e., trying to inventory and control everything."

"Washington State has developed Ambient Source Impact Levels (ASILs) which are protective screening concentrations for TAPs to identify situations requiring further risk assessment. These numbers are based on EPA's IRIS database or occupational safety standards (threshold limit values (TLVs) if IRIS data not available. Sources undergoing New Source Review (new sources and modified sources) must undergo screening using ASILs."

"Once an accounting of HAP emissions has occurred, shouldn't there be some decision-making guidelines concerning the pursuit of evaluating ground level impact? For example, EPA could put the HAPs into "bins" that determine what emission rates of specific HAPs are significant enough to pursue a risk assessment strategy. These bins could also be used to determine what emission levels are significant enough to even include in the accountability portion of an inventory. Do we need to report emissions less than 1 lb (for example) for many of the HAPs? There needs to be some consideration of credibility in regards to the extent that regulatory agencies pursue emissions data. There also needs to be some guidelines for regulatory agencies in this matter in order to eliminate man-hours wasted in data entry and the hard copy forms needed to provide this information to the data entry personnel."

AIR TOXICS MODELING

-- OVERVIEW --

- Prior Emphasis on Criteria Pollutants
- Greater Focus on Air Toxics
- Past "Identity Crisis" for Air Toxics
- Hopeful Future

  -- Emphasis in CAA Title III on Risk
  -- Lessons learned from criteria pollutants

AIR TOXICS MODELING

-- DISCUSSION ISSUES --

- **Models for Air Toxics Assessments**

  -- Similarities to criteria pollutants
  -- Dense gas
  -- Chemistry
  -- Deposition
  -- Evaluation

- **Input Data** - Emissions/AirQuality/Meteorological

- **Screening Models**

- **Models** -- EPA vs Others

- **Averaging Times**

- **Sources of Meteorological Data**

- **Chemical Transformation**

- **Variable Emission Rates**

DIRECTIONS OF AQMG PROGRAM

- National Assessment to Demonstrate Risk Reduction

  -- Urban applications & evaluation
  -- Comparisons with national/regional assessments

- Assessments for Individual Source Categories

- Outreach

  -- Workshops
  -- Model Clearinghouse
  -- SCRAM Website

- Assistance to States on Risk Assessments

Lecture Notes For The National Speciality Workshop of Technical Tools for Air Toxics Assessment, Held June 17-19, 1997 in Research Triangle Park, NC

Dispersion Modeling Of Pollutant Impacts

by
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ABSTRACT

Since 1973 the U.S. Environmental Protection Agency (EPA) has provided a selection of numerical air quality dispersion modeling methods. Where once these models were distributed using computer magnetic tape, the distribution now is made via the Support Center for Regulatory Modeling which is available either through an electronic bulletin board service (telephone modem access, (919)541-5742), or through an Internet web page, http://www.epa.gov/scram001/. The goal of this presentation is to provide a basic understanding of the kinds of air dispersion models available and the purposes for which these dispersion models are best used.

For pollutants that can reasonably be treated as inert, Lagrangian models are made available, as such models provide direct tracking of individual impacts from each of the sources simulated. For chemically active pollutants, where the pollutant of interest is primarily the result of reactions during transport (as opposed to being emitted directly into the atmosphere), Eulerian grid models are made available for best treatment of the often complex chemistry.

The spread (or dispersion) of particles or gases within a smoke plume as it is transported downwind is often approximated as having a Gaussian distribution in the vertical and horizontal. This approximation regarding dispersion has been adapted into many Lagrangian air dispersion models, each of which has been tailored to treat a different set of situations, such as: dispersion from building complexes, near roads and intersections, near coastal areas, etc. Following a brief overview of Eulerian and Lagrangian modeling, a discussion is presented of the strengths and limitations of the Gaussian plume dispersion assumption.

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[1] On assignment to the Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency

BACKGROUND

The passage of the Clean Air Act in 1963 and its amendments (U.S. Congress, 1963), in particular the amendments of 1970 and 1977, formalized the need for routine access to air quality simulation models. This act and its amendments established the concept of air quality goals to protect public health and welfare. These goals were expressed in the form of National Ambient Air Quality Standards (NAAQS), which were specific maximum permitted air concentration levels. Limiting existing and future emissions such that these national standards were attained became the responsibility of the states. The states were charged with developing detailed plans and procedures that when enforced would assure attainment of the NAAQS. Air quality simulation models became the means by which demonstrations could be made that a source's emissions would not endanger attainment of the NAAQS.

Figure 1 provides a schematic representation of some of the concepts envisioned in the Clean Air Act. At the bottom of the cycle depicted, the basic decisions are whether human health and welfare are sufficiently protected. If not, then knowing the costs associated with alternative plans for reducing the health and welfare impacts, provides useful information for deciding next steps. The goal of effective costs/benefit analyses is to address at least the major consequences and relationships of alternative air pollution prevention strategies. Removing pollutants from stack gases before they are released to the atmosphere, creates a need and associated cost for the disposal of the pollutants removed. And the disposal of these pollutants must be properly addressed, otherwise the air pollution problem has only been transferred to another medium, such as the soil, which may in fact have a more severe and costly environmental impact.

If it is determined that adjustments are needed to attain the NAAQS, the next logical step (moving counter-clockwise), is to develop an emission inventory. Developing an inventory is usually an iterative process. An initial accounting for major known sources is developed. This initial inventory is used as input to an air quality simulation model. The modeled concentration values are compared to available measured concentration values. Then a series of analyses are considered to address whether the differences seen are 1) within acceptable bounds given known levels of natural variability, 2) resulting from deficiencies in the application of the air quality model, or 3) deficiencies in emission inventory. This iterative process may involve use of at first rather simplistic air quality simulation models, to provide first order checks of the emission inventory. Then progressively more refined air quality simulation models can be used as needed to further refine both the emission inventory and the air quality simulation to the level needed for the determination of health and welfare impacts.

Reducing ambient air impacts from specific sources can be accomplished by various means, as: changing to different fuels, adding control equipment to trap

material before it is released to the atmosphere, upgrading industries to use more modern (less polluting) equipment or practices. Each option alters the emissions and each option carries with it an associated cost.

ACCESS TO MODELING TOOLS

To provide access to available dispersion models, a User's Network for Applied Modeling of Air Pollution (UNAMAP) was developed in 1972 (Turner et al., 1989). Six air quality simulation models were made available to four mainframe computers that were accessible to the public. However, the system proved too awkward to manage, and in 1973 it was replaced by making available a computer tape of the FORTRAN source codes for the six models. Copies of the computer tape were distributed to the public by the National Technical Information Service (NTIS). Over the succeeding years new versions of the computer tape were provided to include additional air simulation models and updates to existing codes. In 1988, version 6 of UNAMAP provided codes for 24 different simulation models, and 19 associated processors and utility programs. The utility programs served various needs from reformatting meteorological data from standard archive formats, to processors that provided listings and analyses of generated results.

By the late 1980's, many of the simulation models made available through UNAMAP had attained the status of being routinely accepted for various regulatory assessment activities (Environmental Protection Agency, 1986). The updating of these models had to be carefully managed and coordinated within the Environmental Protection Agency and with the public. These demands and the advent of electronic Bulletin Board Systems (BBS) prompted a renovation in the manner in which simulation modeling products were provided. The Support Center for Regulatory Models (SCRAM) BBS started operation in May, 1989. Initially SCRAM consisted of 18 models and utility programs, with a total of about 50 files available for download. At that time, access to the SCRAM BBS was through 4 phone modem lines. Download activity was around 30 files per week during the first few months and has grown to an average of about 2100 files per week today.

Today, 40 modem lines are available at any given moment via a Technology Transfer Network (TTN). And the TTN now consists of over 15 separate BBS systems, providing a vast variety of information and services related to air pollution control. Over time the purpose of SCRAM was adapted and expanded to meet new user needs. In addition to the software for various air simulation models, SCRAM now also provides modeling guidance documents. Today, there are 46 models and utility programs made available via SCRAM, with over 3500 files available for download. On April 23, 1996, SCRAM became accessible via Internet. The web page address is: http://www.epa.gov/scram001/

AIR DISPERSION MODELING

Air quality simulation models can be characterized broadly by the manner in which the fate and transport of pollutants within the air are simulated. Models which employ algorithms of the physical processes that are stated relative to the dispersing material during transport downwind can be referred to as Lagrangian dispersion models. Lagrangian models are typically not used if the pollutant of concern is primarily formed through chemical and physical processes during transport, such as ozone. The chemical rates of production of secondarily formed pollutants are controlled by the combined effects of the emissions from all sources. For numerical efficiency, the simulation of atmospheric chemistry is typically stated relative to a volume of air fixed in space, through which the air moves. Such models can be referred to as Eulerian grid models. As discussed below, selecting an air simulation model for use for a particular situation involves not only an awareness of the pollutants being modeled, but also includes among other factors, the emission control options being considered and the chemical and physical process being simulated. Since this is a general discussion to emphasize principles, specific references have purposely not been provided. A useful general reference that discusses all and more than will be introduced here, and itself provides an excellent cross reference to other references, is Randerson (1984).

Eulerian Models

Shown in Figure 2 is a first-order implementation of a grid model. In this implementation, the entire modeling domain is one box. The emissions within this volume from area, point and line sources are assumed to be instantaneously well-mixed throughout the volume. The chemical reactions resulting from the interaction of the emitted species with each other and with incoming solar radiation are then simulated to produce volume average concentrations as a function of time. One-volume grid models are often used as aids in seeing if more comprehensive model simulations are worthwhile. A discussion and illustration of a popular single-cell grid model often used for screening analyses is provided on the Internet; the URL address is http://www.shodor.org/ekma/. A more complete characterization of the processes is obtained by dividing the modeling domain into horizontal grid cells, stacked in the vertical. This allows elevated point source emissions to be injected into the simulation into cells aloft and near-surface emissions to be injected in the grid cells next to the surface, to provide a more realistic characterization of the processes, (Environmental Protection Agency, 1990). Within these multi-grid models, the emissions are well-mixed within each cell they are emitted. Dispersion between grid cells occurs over time, and is typically a function of the time-dependent three-dimensional meteorological conditions within the modeling domain.

The impact of secondarily formed pollutants, typically involves small amounts of primary emissions from a multitude of widely dispersed sources, such as automobiles

or home heating. The formation through chemical and physical processes of pollutants during transport downwind takes time. The development of emission control strategies for secondarily formed pollutants rarely involves adjustments unique to particular individual sources. Hence, Eulerian grid models are very useful for assessing the effects of secondarily formed pollutants.

Lagrangian models

Shown in Figure 3 is a popular implementation of a Lagrangian model, namely the Gaussian plume model (Turner, 1970). Based on field tests of tracer gas dispersion, it has been determined that the crosswind concentration profile along the surface, downwind from a point source release, appears to generally have a bell-shaped profile (Gaussian). Even the vertical profile can be often approximated as having a Gaussian profile. Empirical data provide a basis for estimating the growth in the vertical and lateral dimensions of the dispersing plume as it moves downwind. Adjustments can be made to account for the fact that the vertical and lateral growth of the dispersing material will be faster over large trees and bushes versus over large lakes or bodies of water. Algorithms have been developed to account for the fact that most industrial source emissions are hotter than the surrounding ambient air, and tend to rise. As shown in Figure 3, the physical stack height, h, is less than the effective height of the plume, H, due to buoyant plume rise effects. Through the years, other adaptations have been developed from accounting for possible capture of the emissions upon release within the wake of nearby buildings, to accounting for alteration in the downwind course of the plume and rate of dispersion due to a hill being in the path of the plume. The plume model is limited to downwind distances for which the dispersive state of the atmosphere can be assumed to be steady-state. This limits the plume model to distances of order 30 km. However, the same Lagrangian concepts can be adapted to a puff model, where the emission is simulated as a series of overlapping puffs, which then allows nonsteady-state conditions (in time or space) to be appropriately simulated.

The major impacts from primary emissions are usually near the release, typically involving transport downwind of less than 15 km. Developing effective plans to mitigate impacts from primary emissions often involves unique limitations being placed on individual sources. One of the strengths of Lagrangian models is that they can be fashioned to address very local (source-specific) factors that greatly affect the local (near-field) dispersion and related concentration values. Since Lagrangian models track independently the contributions from each source, they are very useful for assessing the effects of primary emissions of pollutants.

NATURAL VARIABILITY VERSUS MODEL ACCURACY

Natural Variability

The differences seen in comparisons of model predictions and observations of atmospheric air concentrations may largely reflect an inherent uncertainty caused by the stochastic nature of turbulence within the atmosphere. This component of variance is inherent in that it is the component of the variance that can not be reduced significantly by improving the physics of the air quality models. At best air dispersion models provide an unbiased estimate of the average concentration expected over all realizations of an ensemble. An estimate of an ensemble can be developed from a set of experiments having fixed external conditions (Lumley and Panofsky, 1964). To accomplish this, the available concentration values are sorted into classes characterizing ensembles. For each of the ensembles thus formed, the difference between the ensemble average and any one observed realization (experimental observation) is then ascribed to natural variability, whose variance, σ_n^2, can be expressed as (Venkatram, 1988):

$$\sigma_n^2 = \langle (C^\circ - \langle C^\circ \rangle)^2 \rangle \qquad (1)$$

where C° is the observed concentration seen within a realization; the angle brackets refer to an average over all available realizations within a given ensemble, so that $\langle C^\circ \rangle$ is the estimated ensemble average. In (1) the ensemble refers to the infinite population of all possible realizations meeting the chosen characteristics of the ensemble. In practice, we will only have a small sample from this ensemble. Measurement uncertainty in C° in most tracer experiments is much less than $\langle C^\circ \rangle$, hence its inclusion in the above σ_n is deemed negligible. Available estimates suggest σ_n may be large, of order $\langle C^\circ \rangle$ (Hanna, 1993).

An illustration of concentration variability is presented in Figure 4. Project Prairie Grass (Barad, 1958, and Haugen, 1959) is a classic tracer dispersion experiment, where sulfur-dioxide (SO_2) was released from a small tube placed 46 cm above the ground. Seventy 20-minute releases were conducted during July and August, 1956, in a wheat field near O'Neil, Nebraska. The wild hay was trimmed to a uniform height of 5 to 6 cm in height. Sampling arcs were positioned on semicircles centered on the release, at downwind distances of 50, 100, 200, 400 and 800 m. The samplers were positioned 1.5 m above the ground, and provided 10-minute concentration values.

For the purpose of illustrating concentration variability, small ensembles of six experiments along the 400-m arc have been grouped together in Figure 4 using the inverse of the Monin-Obukhov length, L, a stability parameter (as 1/L approaches zero, the surface layer of the atmosphere approaches neutral stability conditions).

Concentration values from near-surface point sources are inversely proportional to the transport wind speed, U, and directly proportional to the emission rate, Q. To group the results of the six experiments together, the concentration values have been normalized by multiplying the concentration values by U/Q, where U was defined as the value observed at 8 m above the ground. The solid line shown for each group is a Gaussian fit to the results for each six experiment group. As mentioned earlier in this discussion, the lateral dispersion is seen to be well approximated by a Gaussian shape. The scatter of the normalized concentration values about this Gaussian fit can be statistically analyzed, to provide an estimate of the concentration variability not characterized by the Gaussian fit. From analyses of this and another tracer study (involving tracer injected into the emissions of a 186 m stack of an operating power plant), the stochastic fluctuations (natural variability), the distribution of $C^{o}/\langle C^{o}\rangle$ for centerline concentration values was found to have a somewhat log-normal distribution with a standard geometric deviation of order 1.5 to 2 (Irwin and Lee, 1996).

Model Accuracy

To set the context for the discussion to follow, it is important to realize that most of the model evaluation results currently available in the literature are for applied dispersion models that use ensemble average characterizations of the vertical and lateral dispersion, the chemical transformations, and the physical removal processes. Thus these applied dispersion models only provide a description of the average fate and dispersion of pollutants to be associated with each possible ensemble of conditions. Natural variability can and will result in large deviations to be seen in comparisons of individual observations (which are individual realizations from an ensemble of realizations) with modeling results (which are characterizing the ensemble average result).

Figure 5a shows a comparison of observed and simulated SO_2 concentration values in the vicinity of the Clifty Creek power plant which is located in a rural area near Madison, Indiana in the United States. There were 6 air quality monitors near this power plant, ranging in distance from 3 to 15 km from the power plant. This power plant has six coal-fired boilers each capable of producing 217 megawatts of power. For each pair of boilers there is one 208-m stack. The average hourly SO_2 emission rate for 1975 and 1976 was 8.67 kg/s. For each year (1975 and 1976) the maximum observed and simulated SO_2 concentration value for each receptor is shown for several averaging times, ranging from the 1-hour maximum to the annual average. Data files from Environmental Protection Agency (1982) for the CRSTER dispersion model (Environmental Protection Agency, 1977) were used to construct the data shown in Figure 5a. Through the years, CRSTER has been replaced by other Gaussian plume dispersion models, but the comparisons shown in Figure 5a are typical of those summarized in Hanna (1993) for characterization of SO_2 emissions from isolated power plants located in rural areas of the United States.

The trend to increasingly underestimate the maximum concentration as averaging time increases can be summarized using the average fractional bias (FB = 2(e-o)/(e+o), where e is the simulated value and o is the observed value). The average FB for each averaging time is: 24% (1-hr), 5% (3-hr), -6% (12-hr), -9% (24-hr), -43% (720-hr), and -77% (annual average). The standard deviation of FB (a measure of relative scatter) is relatively independent of averaging time, ranging from 34 to 47%. If we summarize these results by stability, it can be shown that there is a bias to overestimate concentrations during unstable conditions and to underestimate concentrations during stable conditions. The bias seen in the model performance may in part be traceable to the use of the Pasquill-Gifford dispersion parameters (Turner, 1970), in which the lateral dispersion has an implied averaging time of 3-minutes (hence the simulated lateral dispersion is too narrow for characterization of 1-hour average dispersion), and the vertical dispersion is typical for ground-level releases (which has various deficiencies for characterizing dispersion from tall stack emissions). Studies during the late 1980's of tall stack dispersion in convectively unstable conditions have shown that standard Gaussian plume models can not properly simulate the effects on dispersion of the highly organized convective eddies. As a consequence, standard Gaussian plume models tend to underestimate maximum surface concentration values from tall stack emissions during convectively unstable conditions.

Figure 5b shows the comparison of observed and simulated SO_2 concentration values for 1976 in the vicinity of St. Louis, Missouri in the United States. Seven of these monitors were within 13 km of downtown St. Louis, five were within 13 to 36 km, and the remaining site was about 50 km north of the downtown area. The SO_2 emission inventory included 208 point sources and 1989 area sources. Although the area sources only accounted for about 3.5% of the 29.76 kg/s of total SO_2 emissions, they are simulated to account for as much as 14 to 67% of the annual average concentration values for the 13 downtown monitors (Irwin and Brown, 1985). The comparison results shown in Figure 5b are listed in Turner and Irwin (1983), and are for RAM, a Gaussian plume dispersion model that is tailored for urban applications. The average FB for each averaging time is: 0% (1-hr), -18% (3-hr), -35% (24-hr), and -2% (annual average). The standard deviation of the FB varies as averaging time varies, as: 59% (1-hr), 46% (3-hr), 60% (24-hr), and 33% (annual average). The results shown in Figure 5b are typical of those summarized in Hanna (1993) for characterization of SO_2 emissions in urban areas of the United States. The dispersion parameters in RAM are based on tracer studies of dispersion conducted in an urban area. The tracer releases were conducted from ground-level releases and releases from the roof of a three-story building. The averaging time of these tracer experiments (and hence the urban dispersion curves in RAM) is approximately 1-hr.

CONCLUSIONS

Within the United States emphasis has been placed on the development, evaluation and application of air quality simulation models that allow development of air quality management plans to achieve defined national air quality goals. These plans involve development of emission control strategies sometimes for individual sources ('primary' impacts associated with pollutants emitted directly into the atmosphere) and sometimes for classes of sources ('secondary' impacts associated with pollutants formed during transport). Part of the decision of which model to select is dictated by insuring that the appropriate physical processes are addressed by the model. But, another part of the decision in model selection is the recognition that every model is a compromise, in that not all processes are included or else the computational demands would be excessive. Hence, model selection often involves expert judgment based on actual experience in the use and application of the various models available.

Typically Eulerian grid models can not treat individual source impacts, unless these impacts are several grid cells from the source. This limitation arises from the fact that current grid models uniformly mix the emissions within the grid cell, and thus do not properly address the initial growth and dispersion of the pollutants. Since grid models are most often addressing impacts from pollutants that are formed from other primary emissions, the lack of treatment of initial dispersion affects is typically assumed to be tolerable. Studies are showing that better characterization of the chemical reactions may require more direct and complete treatment of the initial dispersion effects. Hence, in the future we might expect the more advance chemical models to be 'plume-in-grid' models, where initial 'sub-grid' dispersion will be treated by a plume model. Grid model estimates of maximum ozone (a secondarily formed pollutant) are typically within 20 to 30% of those observed. Since the chemistry is strongly forced to track the presence of sunlight and the precursor emissions are often strongly correlated with surface temperatures, the model estimates show good correlation in time. The spatial correlation is dependent on the sophistication brought to bear on the analysis and characterization of the time and space varying three-dimensional wind field. Typically one of the more problematic inputs for grid models is the spacial and temporal characterization of the precursor emissions, which are most often deduced from assumptions of land use, activities patterns, traffic flows, etc., rather than on direct measurements of emissions.

Typically Lagrangian plume and puff models can at best only treat chemical processes that can be approximated as simple linear transformations in time. But Lagrangian plume and puff models can track individual source impacts, allowing for development of source specific air pollution control strategies. Since the uncertainties in the characterization of the direction of transport are of the order of the actual plume width, large differences are seen when concentrations are paired in time and space. But when comparisons are made of observed and simulated frequency distributions for

fixed receptors, current applied plume and puff models typically provide estimates of maximum concentration values within a factor of two or three of those observed. These differences are an order of magnitude larger than those seen for estimates of secondary pollutants, but are understandable when one considers the lack of any strong constraints in the dispersive processes that would insure correlation in time. Regardless of whether the model is Eulerian or Lagrangian, modeling the transport and dispersion of inert pollutants is an order of magnitude more difficult than simulation of secondarily formed pollutants whose reaction rates are strongly correlated by the availability of sunlight.

Recent investigations of the differences seen in comparisons of modeling results with observations for inert tracers suggest that much of the differences seen may be a result of natural variability. Future development of dispersion models and the methods used to characterize performance of these models will likely increasingly devote more attention to the characterization of the stochastic effects associated with atmospheric natural variability.

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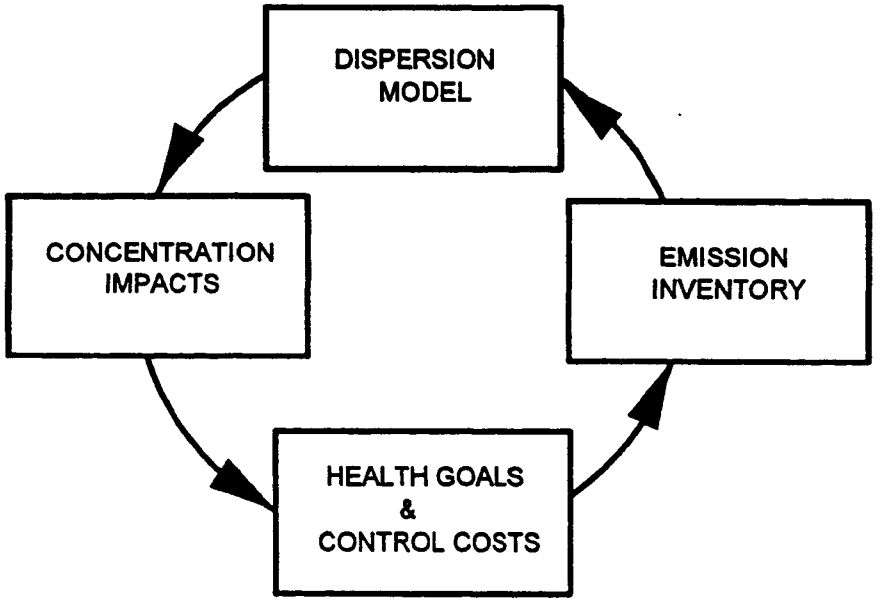


Figure 1. Illustration of the cycle of steps that often occur during an assessment of the consequences of emissions of pollutants.

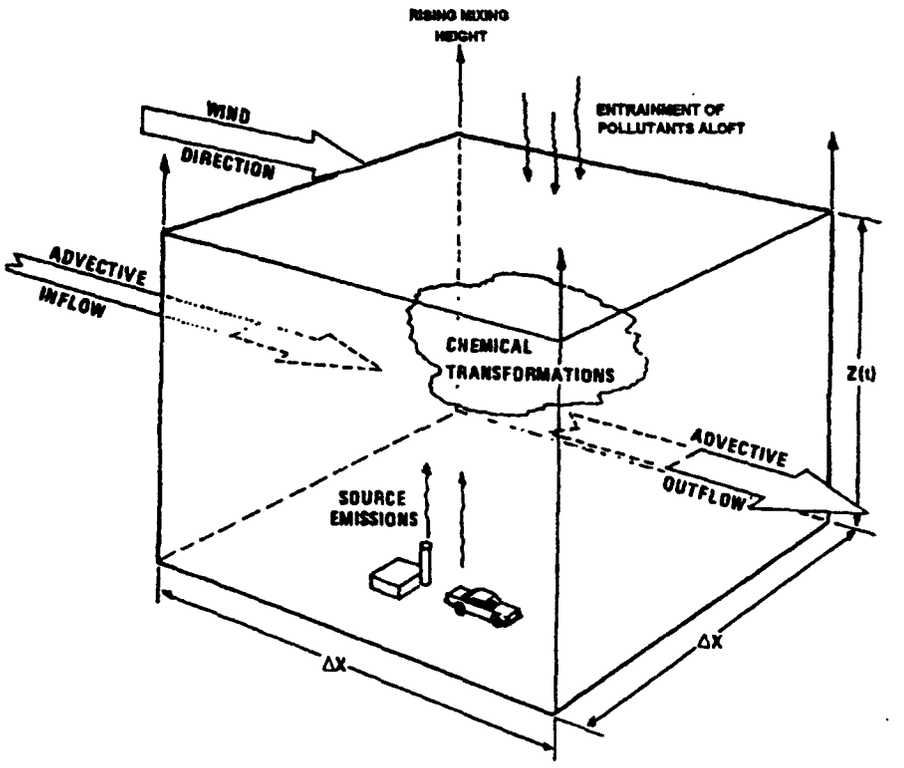


Figure 2. Schematic illustration of a photochemical box modeling domain (Schere and Demerjian, 1984).

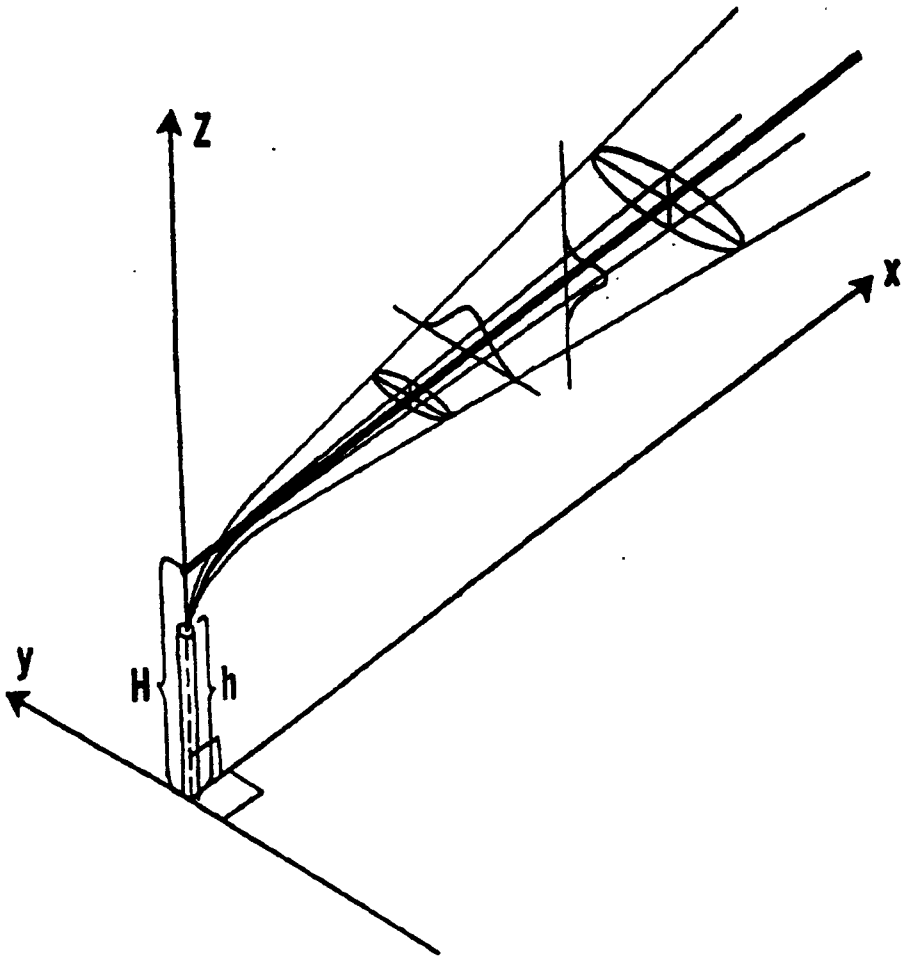


Figure 3. Schematic illustration of a Gaussian plume model (Turner, 1970).

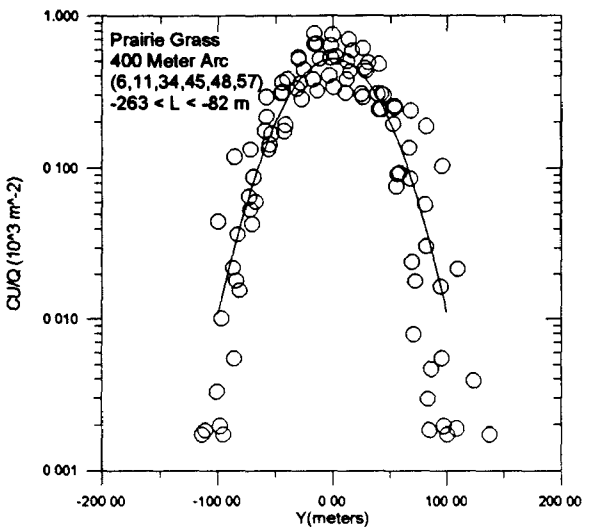


Figure 4a. Near-neutral unstable ensemble normalized concentration values. Experiment numbers are shown within the figure.

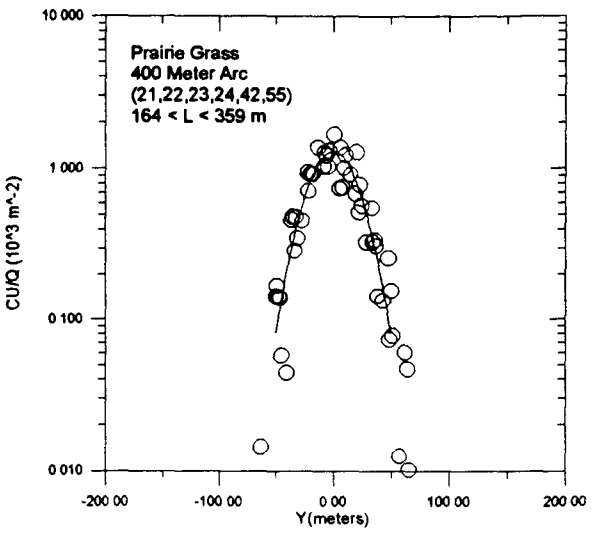
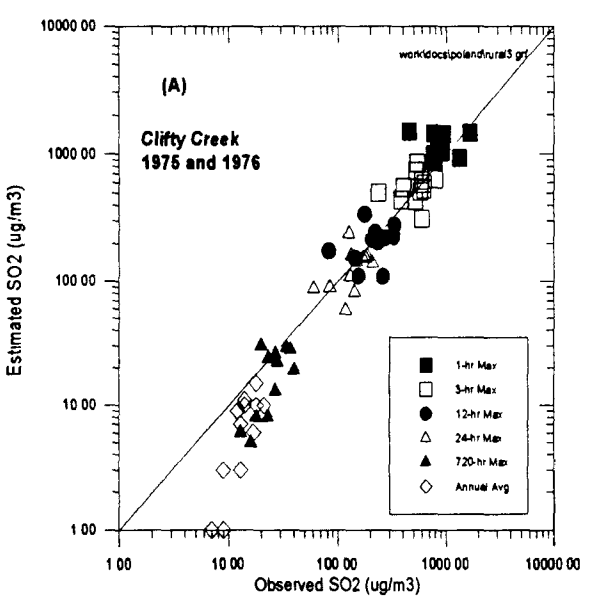


Figure 4b. Near-neutral stable ensemble normalized concentration values. Experiment numbers are shown within the figure.



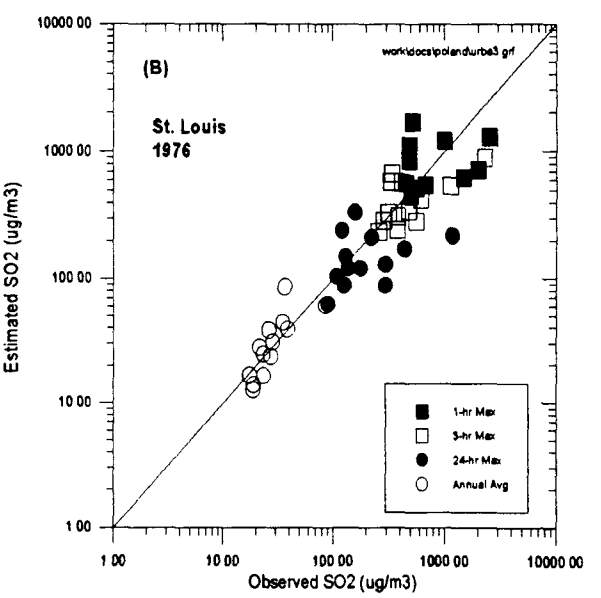


Figure 5. Comparison of observed and simulated SO2 concentrations for (A) an isolated power plant in a rural area, and (B) for an urban area in central United States.

Meteorological Data and Electronic Data Transfer

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June 18, 1997

Meteorological Data

- Required for refined modeling
- Data needed (2 types):
  - surface data
  - mixing height data
- Preprocessor needed (either):
  - PCRAMMET - NWS data
  - MPRM - on-site data

Meteorological Data

- PCRAMMET processing
  - surface data - 3 formats
    - SCRAM - EPA (1984-1992)
    - SAMSON - NCDC (1961-1990)
    - TD-1440 (CD-144) - NCDC (all years)
  - mixing height data - 1 format
    - SCRAM - EPA (1984-1991); NCDC (all)

Meteorological Projects

- Mixing Height Program
- SAMSON CD - update
- ASOS vs. NWS data analysis

Mixing Height Algorithm

- Based on studies performed by George C. Holzworth (1972)
- Created two front-end programs to accept surface and upper air CD-ROM data
- HOLZI.ZIP file in the Non-EPA Models of the SCRAM website

SAMSON CD - Update

- EPA/NCDC project
- SAMSON update - (1990-1995)
  - ASOS data during this period - starting 1992 (Automated Surface Observation System)
    - cloud data limited to 12,000 feet
  - NCDC will fill temperature/station pressure for 10 or less consecutive missings

ASOS Data Analysis

- ASOS data sensitivity analysis WA
- Analyze affects of limited cloud information on dispersion modeling (12,000 feet limit)
  - ceiling height, sky cover
- Compare concentration estimates using NWS and ASOS data in ISCST3

Electronic Data Transfer

- Support Center for Regulatory Air Models (SCRAM) - latest modeling information available
  - models (user's guides)
  - programs (user's guides)
  - guidance documentation
  - meteorological data
  - state/local modeling contacts

Electronic Data Transfer

- SCRAM - part of the Technology Transfer Network (TTN); 24 technical areas

- URL for SCRAM:
  www.epa.gov/scram001

- URL for TTN:
  ttnwww.rtpnc.epa.gov

Source Attribution Modeling for

☺ DIOXIN ☹

Dioxin = PCDD/PCDF

Term used for any or all of

49 polychlorinated dibenzodioxins

87 polychlorinated dibenzofurans

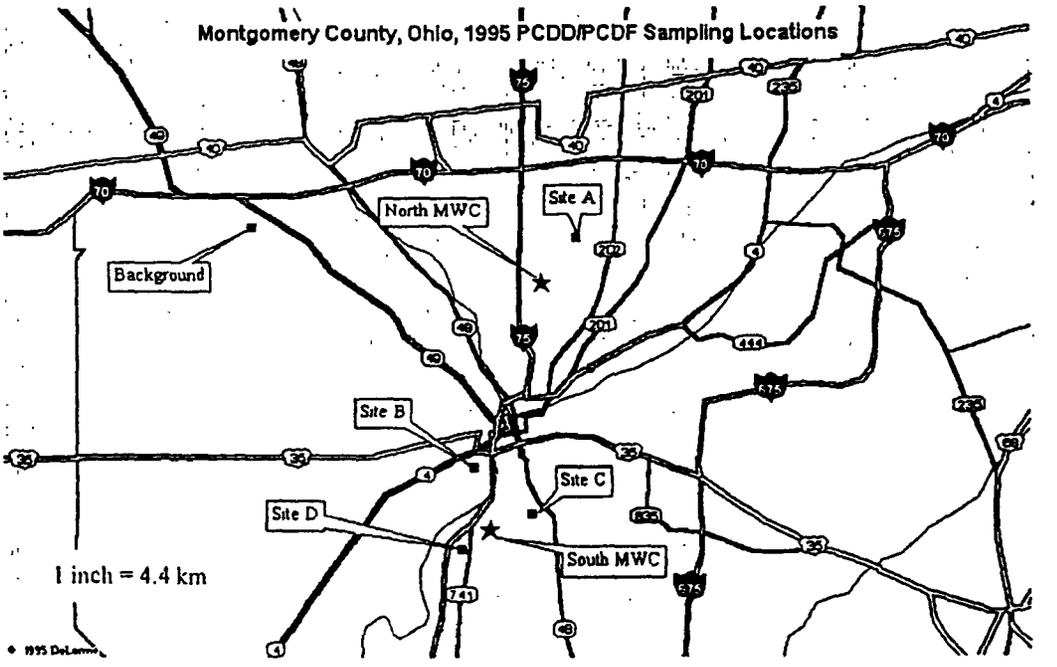
(4 to 8 Chlorine atoms per molecule)

City of Dayton
Montgomery County, Ohio

September, 1995

25 measurements of
PCDD/PCDF concentrations in
ambient air (24-hour samples)

3



4

Measured Total PCDD/PCDF Concentrations, pg/m^3

Sample	Site A	Site B	Site C	Site D
1	1.9	9.4	3.3	2.4
2	1.2	8.6	4.1	1.5
3	1.6	6.3	2.2	2.2
4	1.7	8.2	2.9	2.6
5	4.2	29.7	5.2	22.9
6	2.3	14.0	5.0	5.3

5

Industrial Source Complex (ISC) Dispersion Model

* **stack parameters**...from source tests, permit applications
* **PCDD/PCDF emission rates**...from MWC tested emission rates correlated with ESP temperature
* **receptor grid and elevations**...from USGS topo maps
* **meteorological data**...from National Weather Service (NWS) stations at two Dayton airports

6

ISC Predicted PCDD/PCDF Concentrations, pg/m^3
(due only to the North or South MWCs)

Sample	Site A	Site B	Site C	Site D
1	0	0	0	34.6
2	0	0	4.0	0
3	26.3	0.6	0.5	0
4	13.0	0	4.3	0
5	5.2	0.1	5.6	0
6	1.3	2.3	0.2	1.5

7

SHEESH! Why so bad?!?!

Some possible (extrinsic) sources of error:

1. PCDD/PCDF emission rate estimate was based on log-normal correlation of PCDD/PCDF emission rate and ESP temperature. Testing in 1995, 1994, 1988. Throw out 1988, new estimate ~ 20% of model input.
2. NWS meteorological data consist of short-term readings on the hour. Therefore only 24 met data points per model run/sample period. Not good enough resolution?
3. NWS calms protocol. Any wind speed reading at or below 1.54 m/s (3.0 knots) is set equal to 0 m/s. Ignores dispersion during periods of light winds.

8

Alternative Source Attribution Technique: **Chemical Mass Balance** (CMB) Model

Receptor modeling technique developed for particulate matter source attribution. Instead of source dispersion characteristics, measurements of ambient air particulate concentrations and constituent species (40 elements, organic carbon, sulfate, and nitrate). Library of source emission profiles of particulate matter species are mathematically compared to ambient measurements for source attribution by source type (coal-fired boilers, diesel transportation, road dust, etcetera).

9

United States Environmental Protection Agency
Office of Air Quality Planning and Standards Research Triangle Park NC 27711
EPA-450/4-83-014R May 1987
Air

EPA

Receptor Model Technical Series, Volume III (Revised)

CMB User's Manual (Version 6.0)

Why not PCDD/PCDF?

Grouping PCDD/PCDF congeners by number of chlorine atoms results in a profile with 5 polychlorinated dibenzodioxin congener groups and 5 polychlorinated dibenzofuran congener groups.

Write pairs of simultaneous equations for each PCDD/PCDF congener group pair:

$$x_d = F_{mwc,d}M_{mwc} + F_{os,d}M_{os}$$

and

$$x_f = F_{mwc,f}M_{mwc} + F_{os,f}M_{os}$$

where:

x_d, x_f = measured ambient air concentrations of dioxin and furan congener groups, pg/m^3

$F_{mwc,d}$, $F_{mwc,f}$ = dioxin and furan congener group fractions calculated from North MWC stack test profile

M_{mwc} = ambient total mass PCDD/PCDF contributed by the county MWCs, pg/m^3 (unknown)
$F_{os,d}$, $F_{os,f}$ = dioxin and furan congener group fractions calculated from other source profile
M_{os} = ambient total mass PCDD/PCDF contributed by other source, pg/m^3 (unknown)

"Other source" emission profile???

Conceptual, aggregate, non-county MWC source of PCDD/PCDF. No stack data (of course). Best represented by Site B sample 1. Wind direction, distance from county MWCs, high PCDD/PCDF.

13

CMB Results, pg/m^3 (ambient total PCDD/PCDF from County MWCs)

Sample	Site A	Site B	Site C	Site D
1	1.7	---	4.4	1.6
2	0.9	1.1	4.0	0.8
3	1.0	1.2	1.7	1.8
4	1.2	0.8	2.4	2.3
5	0.2	-2.4	3.4	-9.2
6	0.9	1.7	4.8	2.8

What's it all mean??

14

Site A and Site C: generally low PCDD/PCDF levels, suburban sites - MWCs should be responsible for majority of PCDD/PCDF

Site B: urban industrial location, other PCDD/PCDF sources likely, relatively distant from MWCs, relatively minor contribution from MWCs

15

Site D: commercial area close to South MWC, majority of ambient PCDD/PCDF from MWC, EXCEPT sample 5

SAMPLE 5: Two highest levels measured (out of 25 samples). ISC bombed, CMB bombed. MWC operations normal. Site B and Site D north and south of South MWC.

16

NWS reported calms for 11 (out of 24) readings. No dispersion? Portable met tower - light and variable winds.

Polyvinyl chloride burnoff oven: batch unit, relatively low temperature and oxygen, short capped stack, batch run during sample 5 has evidence of afterburner upset.

...no stack data...

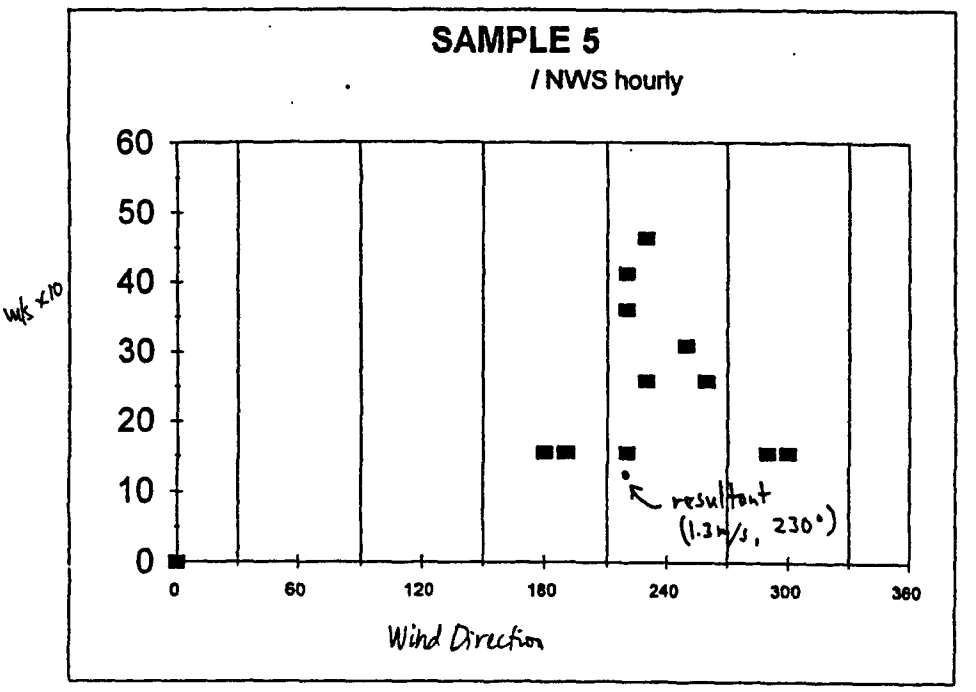
17

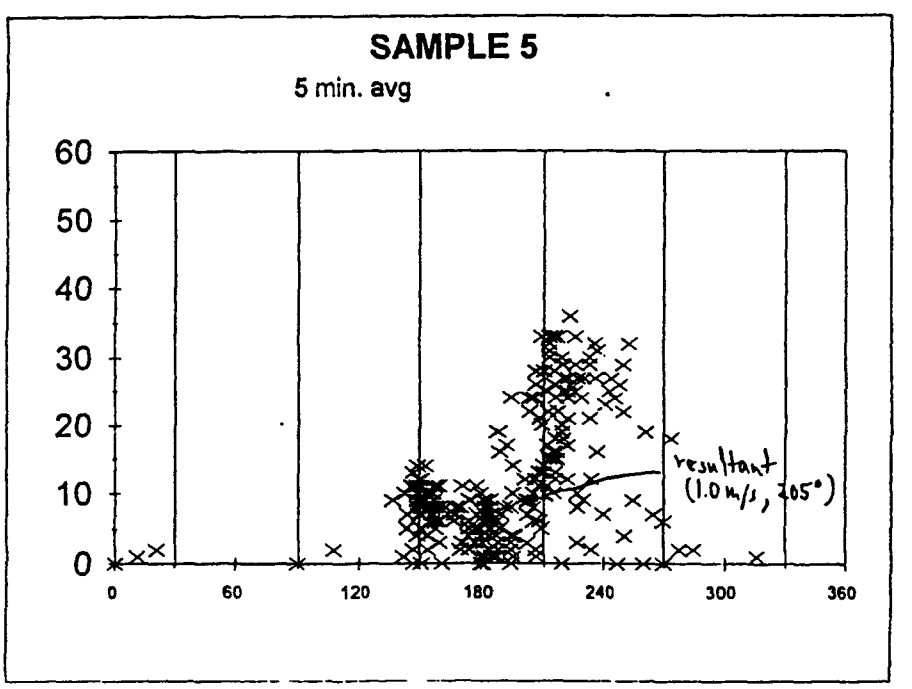
Open Discussion:

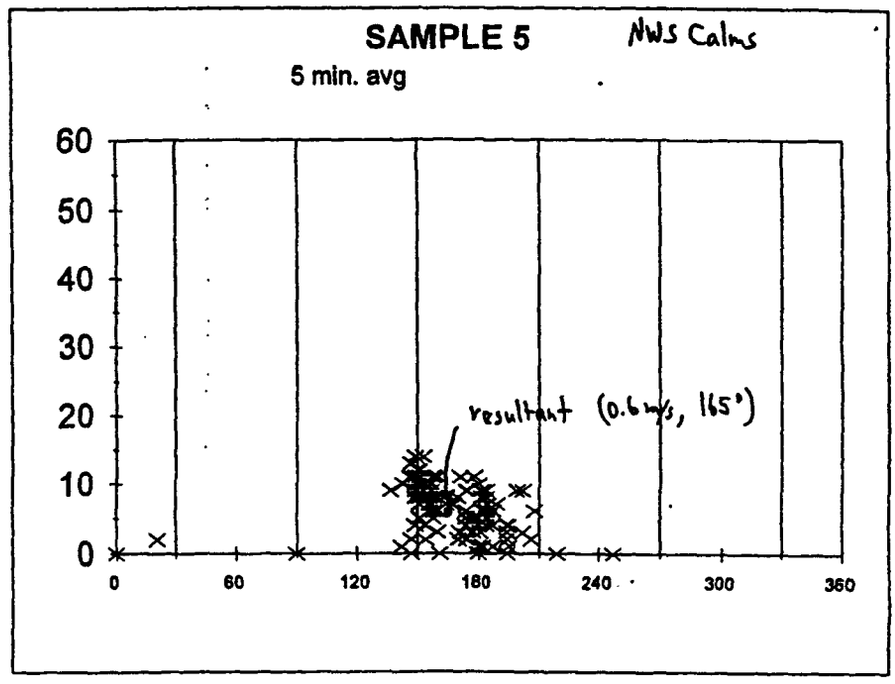
Receptor modeling techniques may help in PCDD/PCDF source attribution studies. Source profile library?

ISC should be modified to employ 5-minute average met data. Availability of portable met towers. Availability of source code.

18


SAMPLE 5
/ NWS hourly
wks x10
60
50
40
30
20
10
0
0
60
120
180
240
300
360
resultant
(1.3 m/s, 230°)
Wind Direction


SAMPLE 5
5 min. avg
60
50
40
30
20
10
0
0
60
120
180
240
300
360
resultant
(1.0 m/s, 205°)


SAMPLE 5
NWS Calms
5 min. avg
60
50
40
30
20
10
0
0
60
120
180
240
300
360
resultant (0.6 m/s, 165°)

Sensitivity Analysis Results

PARAMETER	SENSITIVITY	RECOMMENDATION
Elevated vs. Flat Terrain	Severe	Must include terrain < 1-2 km; Hills > stack height only if > 5 km
Rural vs. Urban Air Dispersion Coefficients	Severe	Detailed land use analysis required
Surface Roughness at Application Site	Severe	EPA-required method, or site-specific justification
Watershed Size and Proximity	Severe	Use actual watershed area near source; use representative points > 10 km away
Anemometer Height	Moderate	Under estimates < 1km
Particle Size Distribution and Density	Moderate	Require stack test data for particle size and density
Polar vs. Cartesian Grid nodes	Slight	Applicant selects grid
Terrain Gird File	None	No impact on model results
Minimum Monin-Obukhov Length	Slight	Specify default values
Surface Roughness at Measurement Site	Severe	EPA-required value for NWS site
Noon-Time Albedo	Slight	Specify default values
Bowen Ratio	Slight	Specify default values
Anthropogenic Heat Flux	None	No impact on model results
Fraction of Net Radiation Absorbed	None	No impact on model results
Scavenging Coefficients	Severe	Isolated events 300%, but rare occurrence in Region 6

NEW JERSEY DEP RISK ASSESSMENT PROCEDURES FOR MINOR SOURCES
(since 1989)

MAJOR SOURCES (ex. Municipal Solid Waste, Sewage Sludge, and Hazardous Waste Incinerators; Coal-Fired Power Plants; etc.)

Risk Assessment Responsibility of Applicant

Protocol Ψ Analysis
Inhalation or Multi-pathway

MINOR SOURCES (ex. Chemical Batch Plants, Degreasers, Air Strippers, etc.)

Risk Assessment Responsibility of NJDEP

Level-1/screening ΨLevel-2/refined modeling
Inhalation Pathway Only

APPLICABILITY TO MINOR SOURCE RISK ASSESSMENT PROCEDURES

Air Permit Applications For New or Modified Sources Which Emit One or More of the Following 56 Carcinogens:

Acetaldehyde	Hexachlorobenzene	Heptachlor
Acrylamide	Hexachloroethane	Formaldehyde
Acrylonitrile	Hydrozine	Ethylene Oxide
Allyl Chloride	Lindane	Ethylene Dichloride
Arsenic	Methyl Chloride	Ethylene Dibromide
Asbestos	Methylene Chloride	Ethyl Acrylate
Benzene	4,4-Methylenedianiline	Epichlorohydrin
Benzidine	Nickel	1,2-Diphenylhydrazine
Benzo(a)pyrene	Nickel Subsulfide	1,4-Dioxane
Benzyl Chloride	Nitrobenzene	Vinylidene Chloride
Beryllium	2-Nitropropane	Vinyl Chloride
Bis(2-Chloroethyl)ether	N-Nitrosodimethylamine	2,4,6-Trichlrophenol
Bis(chloromethyl)ether	N-Nitroso-n-methylurea	Trichloroethylene
1,3-Butadiene	N-Nitrosomorpholine	1,1,2-Trichloroethane
Cadmium	Pentachlorophenol	Toxaphene
Carbon Tetrachloride	Polychlorinated Biphenyls	Tetrachloroethylene
Chlordane	Propylene Oxide	Chloroform
Chromium VI	2,3,7,8-TCDD (Dioxin)	Styrene
1,2-Dichloropropane	1,1,2,2-Tetrachloroethane	

NJDEP LEVEL-1 RISK ASSESSMENTS

[Conducted by the NJDEP Air Permit Review Engineer]

1. Calculate the Ton per Year Emission Rate for Each Carcinogen

2. Use NJDEP Nomograph to Obtain Long-Term Ambient Concentration of Each Carcinogen

3. Use NJDEP Unit Risk Factors to Obtain Cancer Risk Factor for Each Carcinogen

4. Add Incremental Cancer Risk of Each Carcinogen

   Total Cancer Risk # 1 in a million ☛ PASS

   Total Cancer Risk > 1 in a million ☛ FAIL

   go to Level-2 Risk Assessment

NJDEP NOMOGRAPHS

ISCLT2 Model -
5-Year Composite STAR Deck
Flat Terrain
Dense Receptor Grid

CONSERVATIVE ASSUMPTIONS:

* No Plume Rise
* Significant Building Downwash
  Stk. Hts.# 30 ft →Building Ht. = 2/3 Stack Ht.
  Stk. Hts.> 30 ft →Building Ht. = 1/2 Stack Ht.
* Higher Impact of Either the Urban or Rural Mode Used
* If More than One Stack, Add Maximum Impacts Regardless of Location

NJDEP LEVEL-2 RISK ASSESSMENTS

[Conducted by the NJDEP Air Modelers]

1. Applicant Must Provide:

~ Detailed Plot Plan

~ Location of All Emission Points

~ Building Dimensions.

~ Location of Nearby Sensitive Receptors (i.e. homes, schools, etc.)

2. NJDEP - GEP Stack Height Analysis with BPIP

3. NJDEP - ISCST3 Modeling with 2-3 Years of Hourly Meteorological Data

4. Review Expanded to Include 121 Carcinogens and 119 Noncarcinogens

NJDEP LEVEL-2 RISK ASSESSMENTS (Continued)

If the Maximum Incremental Cancer Risk of Each Carcinogen:

Step 1

→ less than/equal to 1 in a million ☞ PASS

→ greater than 1 in 10,000 ☞ FAIL (no permit)

→ 1 in 10,000 to 1 in a million ☞ Go to Step 2

Step 2

→ Maximum Cancer Risk less than 1 in a 100,000 and Cancer Risk at All Sensitive Receptors less than 1 in a Million ☞ PASS

→ Maximum Cancer Risk greater than 1 in a 100,000 or Cancer Risk at Any Sensitive Receptors greater than 1 in a Million ☞ go to Risk Management Committee

RISK MANAGEMENT COMMITTEE

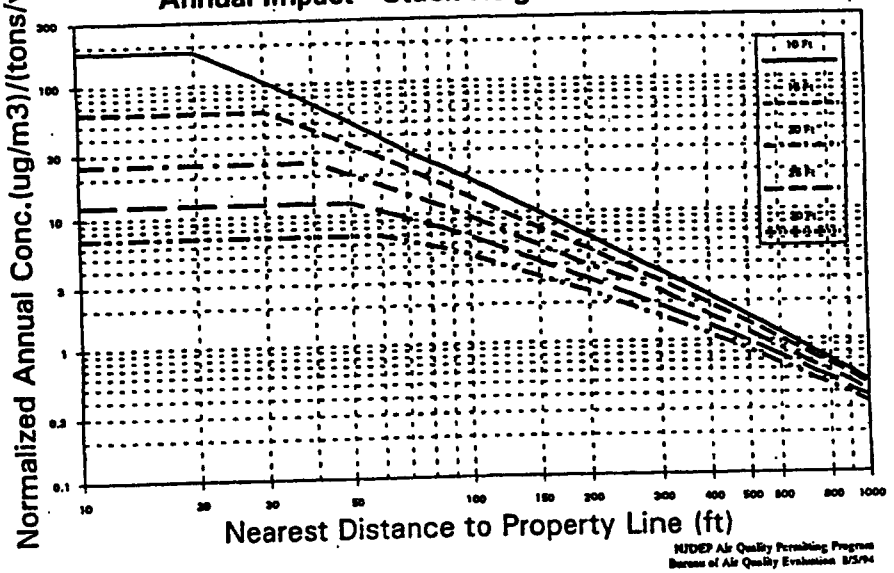
Meeting Attended by: Chief of New Source Review, Chief of Air Quality Evaluation, Air Permit Review Engineer, Modeler, and Regional Enforcement (facility inspector)

EXAMINES FEASIBILITY OF:

* Better Pollution Controls or Refinement in Emission Estimates
* Reduce Proposed Hours of Operation
* Modifying Stack Characteristics for Better Dispersion:
  - Higher Stack Height
  - Change from Horizontal to Vertical Release
* Conduct a More Refined Risk Assessment to Better Define Impacts or Include Other Sources at the facility (applicant or NJDEP)

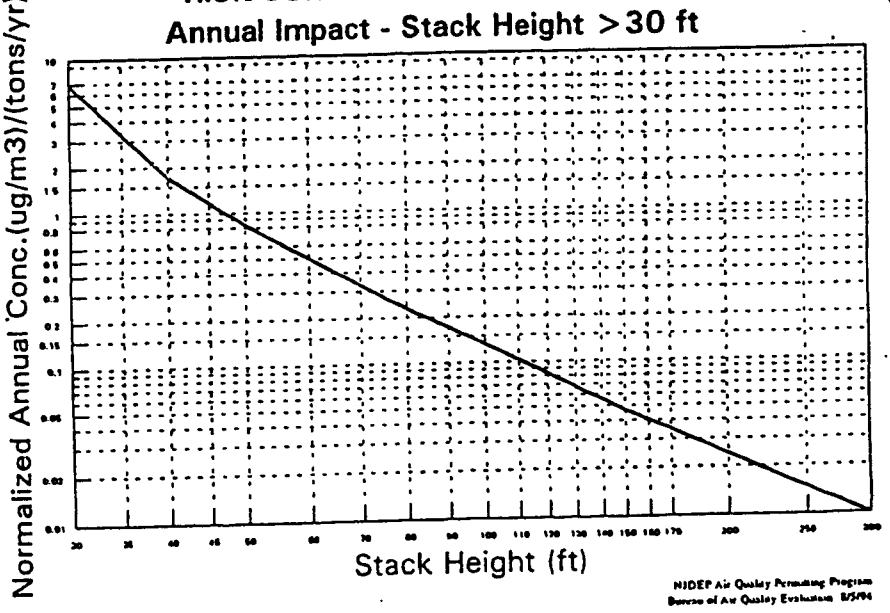
RISK SCREENING NOMOGRAPH A

Annual Impact - Stack Height 10 - 30 ft



RISK SCREENING NOMOGRAPH B

Annual Impact - Stack Height >30 ft



EXPOSURE MODELING: COMPONENTS, STATUS, AND USES

Michael Zelenka
U.S. Environmental Protection Agency
National Exposure Research Laboratory
Research Triangle Park, North Carolina

National Speciality Workshop on Technical Tools
for Air Toxics Assessment
June 19, 1997

PRESENTATION OUTLINE:

1. Brief overview of the structure of laboratories conducting risk assessment work at EPA's Office of Research and Development.
2. Define "*exposure*" and illustrate the "*risk assessment*" paradigm.
3. Illustrate the evolution of approaches to human exposure assessment efforts and human exposure modeling in particular.
4. Overview of the basic construct of exposure models currently in use by the EPA's National Exposure Research Laboratory (NERL).
5. Discuss the needs and directions of future exposure modeling efforts at the NERL.

OFFICE OF RESEARCH & DEVELOPMENT

- **National Exposure Research Laboratory**
  1. Characterize the physical and chemical properties that govern exposures.
  2. Develop, test, evaluate, and demonstrate mathematical models of exposure.

- **National Health and Environmental Effects Research Lab**
  1. Address health and/or ecological effects of exposures to man-made stressors.
  2. Determine the likelihood that these effects will occur under conditions of environmental exposure.

- **National Risk Management Research Laboratory**
  1. Characterize pollutant sources that require management.
  2. Identify, develop, and evaluate tools and technologies for prevention, control restoration, and remediation of environmental problems.

- **National Center for Environmental Assessment**
  1. National resource center for the overall process of risk assessment: integrating hazard, dose-response, and exposure data and models to produce *risk characterizations.*

RELEVANCE OF HUMAN RISK ASSESSMENT RESEARCH AT EPA

The Clean Air Act Amendments of 1990 address human exposures (for example):

Title I, Sec. 103(d):

- The Administrator must prepare environmental health assessments for the hazardous air pollutants listed under Section 112(b).

  ... These assessments shall include an examination, summary, and evaluation of available ... information for the pollutant to ascertain the levels of human exposure which pose a significant threat to human health and the associated acute, subacute, and chronic adverse health effects.

HUMAN EXPOSURE:

- *The contact at one or more personal physical boundaries (skin, lungs, and other organs) between a human and contaminant(s) having a specific concentration for a specified period of time.*

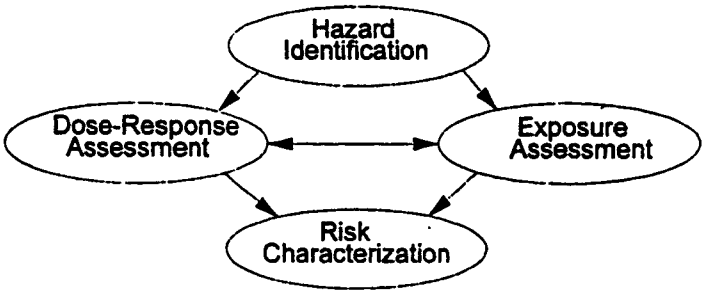
TOTAL HUMAN EXPOSURE:

- *Human exposure that consists of inputs from all media (air, water, food, soil, house dust) that contain the contaminant(s) and all routes of entry into the body (inhalation, ingestion, dermal absorption).*

SCIENTIFIC CONTEXT: HUMAN RISK ASSESSMENT RESEARCH

- Focus of Near-Term Human Exposure Assessment Research:
  - **NERL:**
    - Uncertainties in exposure measurements (particularly, microenvironmental data), measurement-derived exposure models, and activity-pattern data.
  - **NHEERL:**
    - Uncertainties in mechanistic information (e.g., pharmacokinetics) for hazard identification and dose-response assessment.

RISK ASSESSMENT



- Hazard Identification: Describe the adverse health effects that might occur due to exposure to an environmental contaminant.
- Dose-Response Assessment: Determine the toxicity or potency of a contaminant. The dose-response assessment describes the quantitative relationship between the amount of exposure to a contaminant and the extent of injury or disease.
- Exposure Assessment: Describe the nature and size of the population exposed and the magnitude and duration of exposure. Exposure assessment includes a description of the pathways (e.g., air, food, water, house dust) by which the contaminant travels through the environment, the environmental concentrations of the contaminant relative to time, distance, and direction from its source (including transformations), potential routes of exposure (i.e, dermal, inhalation, or ingestion), and information on sensitive subgroups (i.e, children or pregnant women).
- Risk Characterization: Use the information from above steps to predict the effects of exposure to the contaminant. Estimates are made of the likelihood that a population will experience any of the adverse effects associated with the contaminant, under known or expected conditions of exposure.

EVOLUTION: HUMAN RISK ASSESSMENT RESEARCH

- **HISTORIC APPROACH:**
  - Reliance on media-specific legislation, single pathway assessment, individual source emitters, individual (i.e., single) contaminants.
  - Dominated by ambient monitoring and regulations on sources and ambient concentrations.
- **EVOLUTION OF NEW APPROACH DRIVEN BY:**
  - Multimedia legislation.
  - Growing recognition of the importance of multipathway risk assessments.
  - Increased capability to measure multimedia environmental and human exposure metrics.
  - Increased understanding of biokinetics and the use of biological markers of exposure (biomarkers).

EVOLUTION: HUMAN RISK ASSESSMENT RESEARCH

HISTORIC APPROACH	EVOLVING APPROACH
Problem Identification & Investigation	
• Single source of contaminant	• Multiple sources of contaminants
• Single environmental pathway	• Multiple environmental pathways
• Single route of exposure	• Multiple routes of exposure
• Single (presumptive) health endpoint	• Multiple health endpoints
Risk Assessment Decisions	
• Single media focus	• Multi-media focus
• Single pollutant focus	• Multi-pollutant focus

IMPLICATIONS OF RISK ASSESSMENT EVOLUTION ON EXPOSURE MODELING

- *The SAB (EPA-SAB-IAQC-95-005) recommended the following:*

  1. Develop and implement a strategic plan to collect critical input data for exposure models and validate the entire methodology.

  2. Establish a framework to ensure that the entire range of potential risks from multiple sources are addressed holistically within that framework.

- To achieve these goals, exposure model development should:
  a. be linked within comprehensive models that characterize exposure and dose at target sites, and,
  b. include the ability of future exposure models to be used as tools for prioritizing the major routes and media of concern.

EVOLVING APPROACHES TO HUMAN EXPOSURE MODELING AND ASSESSMENT EFFORTS

- **Exposure Pathways:**
  - *HISTORIC APPROACH*: Source emissions and concentrations of contaminants reach a receptor (human) through a single pathway.
  - *EVOLVING APPROACH*: A contaminant can reach humans through multiple routes of exposure.

- **Predictive Models based on Source Emissions and Transport:**
  - *HISTORIC APPROACH*: Exposures assessed by using either source emissions or concentrations of contaminants in media and environmental transport models, along with a limited number of exposure situations (scenarios).
  - *EVOLVING APPROACH*: Time-activity patterns significantly influence exposures and need to be included in modeling efforts in order to include all exposure pathways and account for the large variability across the diverse population of the United States.
    - Much more direct measurement exposure data is needed to validate model assumptions regarding the most significant routes of exposure, and about how contaminants move into or through environmental compartments.

- **Temporal Variability at Specific Locations:**

  - *HISTORIC APPROACH:* The concentration of contaminants in media remains constant over time.

  - *EVOLVING APPROACH:* Contaminants can come from multiple sources whose concentrations can vary greatly, causing responses that are substantially different from those assessed on a "per source" basis.

- **Independence of Exposures to Multiple Contaminants or Sources:**

  - *HISTORIC APPROACH:* Exposures assessed on a chemical-by-chemical basis.

  - *EVOLVING APPROACH:* Effects from multiple contaminants may be other than additive.

- **Infiltration of Outdoor Air into Buildings:**

  - *HISTORIC APPROACHES:* Buildings do not significantly affect exposures to outdoor pollutants.

    a. Building conditions are static, and indoor concentrations of airborne contaminants can be modeled using steady state conditions.

  - *EVOLVING APPROACHES:* Indoor exposures from outside air are affected by factors related to:
    1) the building itself (e.g., type of construction, ventilation method),
    2) environmental conditions (season, temperature differences between indoors and outdoors),
    3) contaminant morphology (reactive or non-reactive, gas or particle), and
    4) human habits and practices (adjustment of windows, sweeping, vacuuming).

    a. Infiltration of outdoor contaminants have substantial inter- and intra-building variability making steady-state conditions less likely.

Human Exposure Simulation Models at NERL

1. ***pNEM/"X"* (probabilistic NAAQS Exposure Model for pollutant "X")**

   ✓ Different versions for different pollutants

   - Currently the "Xs" are: CO*, O_3*, NO_2, SO_2, and particles.
     * Most application has been done with the CO and O_3 versions.

   ✓ pNEM is used by OAQPS when considering NAAQS and for evaluating alternative NAAQS proposals.

   ✓ pNEM provides hourly estimates of the distribution of exposures,

Goal: To simulate the movements of people through zones of varying air quality to approximate the actual exposure patterns of people living in a defined study area.

2. ***HAPEM-MS* (Hazardous Air Pollutant Exposure Model for Mobile Sources)**

✓ This model provides long-term (1 year or more) average exposure estimates for pollutants generally attributed to mobile sources.

- HAPEM-MS uses ambient CO data for input and uses CO-to-chemical Y ratios to estimate exposures to other mobile source pollutants.

✓ HAPEM-MS is used by OMS and program offices -- most recently used for the Motor Vehicle-Related Air Toxics Study* (required under S. 202 of the CAA for motor vehicle air toxics regulation).

*U.S. EPA (1993) *Motor Vehicle-Related Air Toxics Study* (Draft). Office of Air and Radiation, Ann Arbor, MI.

HAPEM-PS

- Outgrowth of 1991 critical evaluation of the Human Exposure Model (HEM).
- Provides annual average estimates of exposures to hazardous air pollutants and resulting cancer incidence for populations residing near point sources.
- Ambient pollutant concentrations are determined by dispersion model using point source emission rates and local meteorology. Census unit centroids are used as dispersion model receptors.
- Model accounts for residential patterns, activity patterns, ME's, and home-work commutes.

Comparison of pNEM and HAPEM

- Ambient Air Quality Data:
  - ***pNEM***: fixed-site
  - ***HAPEM-MS***: fixed-site
  - ***HAPEM-PS***: dispersion model data
- Microenvironmental Concentrations:
  - ***pNEM***: mass balance model
  - ***HAPEM***: regression equations [indoor = (a)(outdoor) + b]
- Time/activity patterns:
  - ***pNEM***: strict time sequence of assignments to ME's, districts, and breathing rates.
  - ***HAPEM***: fraction of time spent in each combination of ME and district. Also, accounts for season and hour of day.

Comparison of pNEM and HAPEM - 2

- Indoor Sources:
  - ***pNEM***: probabilistic algorithms for simulating emission patterns within the mass balance model.
  - ***HAPEM***: treats as additive factor in regression equation.
- Residential Patterns:
  - ***pNEM and HAPEM-MS***: people are assigned to large districts surrounding fixed-site monitors.
  - ***HAPEM-PS***: people are assigned to small census units near point source and larger census units away from source.
- Commuting Patterns (based on census data):
  - ***pNEM and HAPEM-MS***: workers commute between large districts.
  - ***HAPEM-PS***: workers commute between individual census units.

Comparison of pNEM and HAPEM - 3

- Ventilation Estimates:
  - *pNEM*: equivalent ventilation rate estimated for each exposure event (EVR = (vent.rate)/(body surface area).
  - *HAPEM*: does not estimate ventilation rate.

- Microenvironments:
  - *pNEM*: typically less than 10.
  - *HAPEM*: 37 available.

- Time Activity Data:
  - *pNEM*: data base currently contains diary data from 10 studies.
  - *HAPEM*: Cincinnati, Denver, and Washington, D.C. only.

Comparison of pNEM and HAPEM - 4

- Census Data:
  - *pNEM and HAPEM*: use 1990 census data to extrapolate cohort exposures to general population.

- Health Effects Resulting from Exposure:
  - *pNEM*: CO version estimates COHb level resulting from each individual exposure event.
  - *HAPEM*: estimates one-year and 70-year cancer incidence within exposed population.

- Adjustment of Ambient Air Quality Data:
  - *pNEM*: statistical techniques are applied to fixed-site monitoring data to simulate attainment of each NAAQS under evaluation.
  - *HAPEM-MS*: pNEM techniques can be used to adjust input fixed-site monitoring data.
  - *HAPEM-PS*: model is typically used to simulate "as is" conditions -- no adjustment of ambient data. Analysts can change emission rates in dispersion model to simulate point source controls.

Comparison of pNEM and HAPEM - 5

- **Exposure Estimates (model output):**
  - ***pNEM***: model provides pollutant concentration and EVR by exposure event for each population cohort (pNEM/CO also provides resulting COHb level). Output tables list numbers of people exposed and exposure occurrences by concentration range and EVR range for various averaging times.
  - ***HAPEM-PS***: output tables list annual average pollutant concentration and cancer incidence for each population cohort and for total population.
  - ***HAPEM-MS***: produces HAPEM-PS outputs plus tables of average pollutant concentrations by season, hour of day, demographic group, and microenvironment.

- **Current Computer Requirements:**
  - ***pNEM and HAPEM***: IBM main-frame.

REQUIRED OF THE NEXT GENERATION OF EXPOSURE MODELS

EPA's exposure models play an important role in the risk paradigm and therefore must:

1. characterize the full range of the distribution of human exposures that can occur,
2. identify microenvironments that must be considered in exposure assessments to urban air toxics,
3. integrate all pertinent information into a rational human exposure framework,
4. and, ultimately, produce scientifically-based estimates of human exposures with the ability to emphasize sensitive or "at risk" subgroups of the population such as children, asthmatics, and others.

FUTURE NERL HUMAN EXPOSURE MODEL DEVELOPMENT:

KEY ELEMENTS FOR EXPOSURE MODEL DEVELOPMENT:

I. *Basic research:* needed to improve our estimates, including those that are modeled, of exposure.

Examples:
microenvironmental concentrations
activity patterns
dose metrics (e.g., breathing rates)

II. *Improvements to the models:*
- More, and better use of GIS.
- Faster and more user friendly models.
- Additional data (measured and derived) and computing platforms that allow the ease and flexibility of performing human exposure research.
- Develop a modeling "framework" so that:
  a. models that characterize exposure and dose at target sites can be linked, and,
  b. future exposure models will include the ability to be used as tools for prioritizing the major routes and media of concern.

MICROENVIRONMENTAL MODELING ISSUES

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WHAT ISSUES?

- Definition of a Microenvironment
- Assessment Goals
- Modeling "Art" versus "Real" Data
- Perspective on Models
- Examples
- Discussion

DEFINITION OF MICROENVIRONMENT

- Intersection of human presence/activity with a characterizable environment
- The world of our dialy activity takes place in a series of microenvironments
- While all exposure is "local"
  ET(total) = EL(local)+ ER(regional)

Assessment Goals

- Population-distribution of exposure
- Special group and/or special microenvironment
- Effective reduction of exposure
- Residual Risk and/or Relative Risk

Modeling "Art" versus "Real" Data

- Model development/application and measurement studies must intersect
- Statistical science is important in both pre study design and post analyses

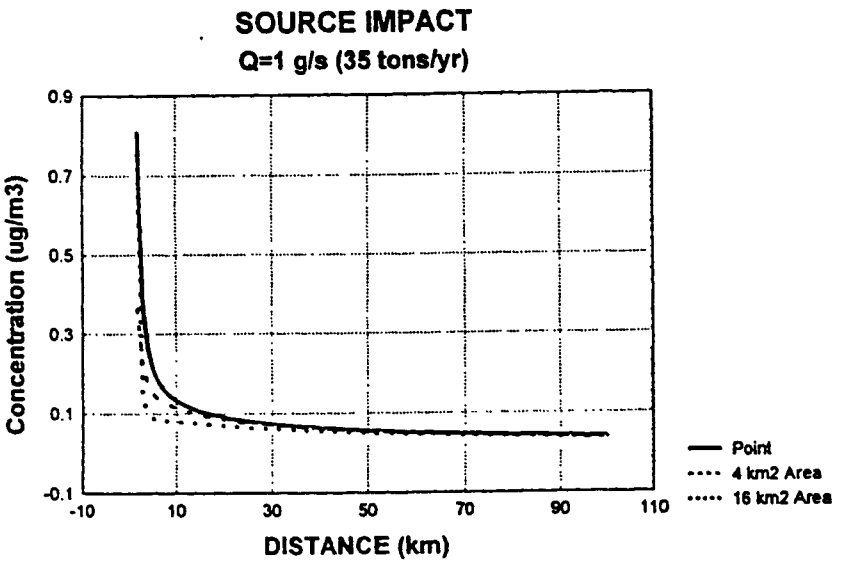
Perspective on Models

- Regional Scale Models and Ambient Air
- Urban Scale Models and Ambient Air
- Local Scale (Microenvironmental) Models
  - where the exposure begins and ends

Characteristics in Model Selection

- Pollutant Emission Sources
- Chemistry of Interest
- Human Activity Patterns for Exposure
- Spactial and Temporal Scales of Interest
- Available Meteorology
- Numerical Methods

ISC3



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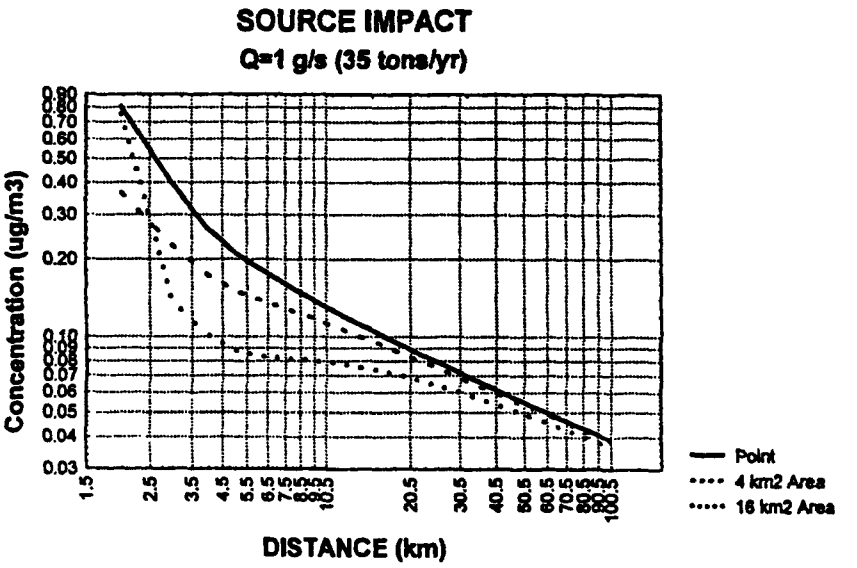
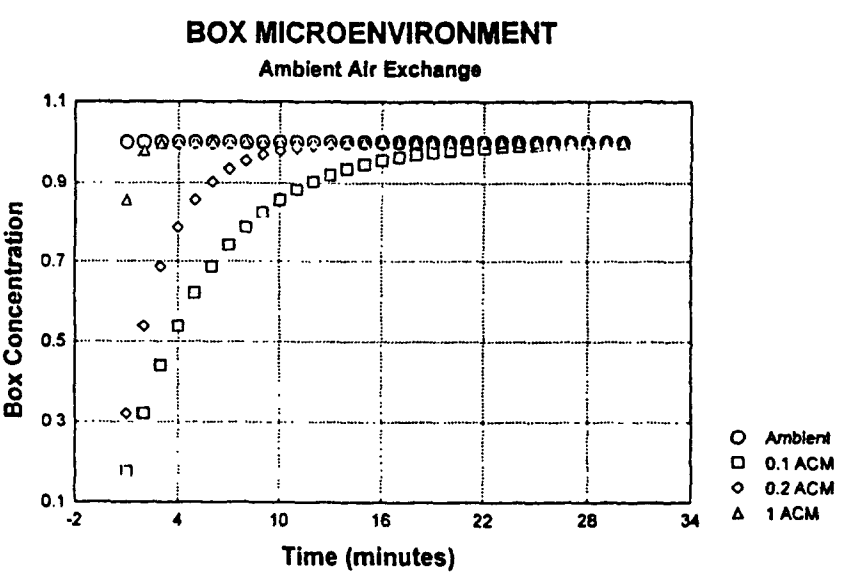
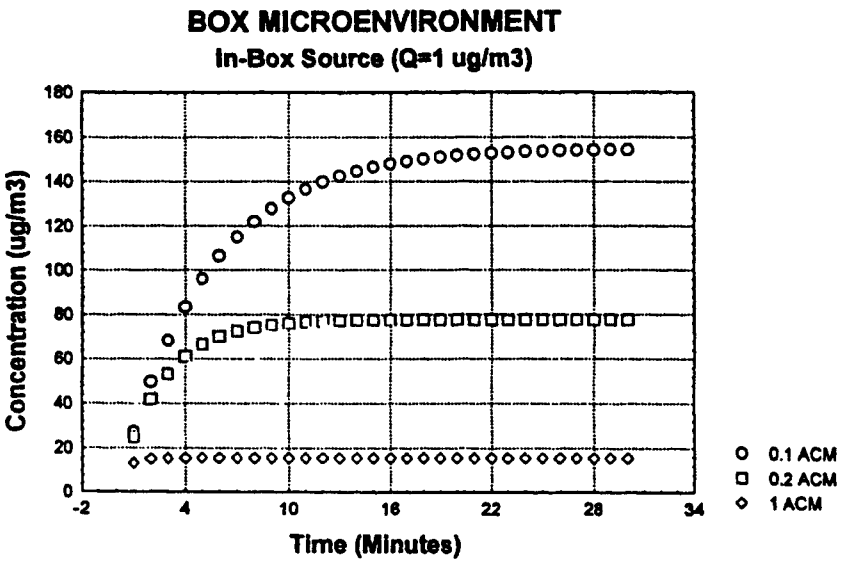

SOURCE IMPACT
Q=1 g/s (35 tons/yr)
Concentration (ug/m3)
DISTANCE (km)
Point
4 km2 Area
16 km2 Area


BOX MICROENVIRONMENT
Ambient Air Exchange
Box Concentration
Time (minutes)
Ambient
0.1 ACM
0.2 ACM
1 ACM


BOX MICROENVIRONMENT
In-Box Source (Q=1 ug/m3)
Concentration (ug/m3)
180
160
140
120
100
80
60
40
20
0
-2
4
10
16
22
28
34
Time (Minutes)
0.1 ACM
0.2 ACM
1 ACM

Real-Time Monitoring of Polycyclic Aromatic Hydrocarbons

EcoChem PAS 1002i and 2000

- Real-time monitoring of PAH on the surface of fine airborne particles
- Principle of operation:
  - Photoionization of surface-adsorbed PAH
  - Photoelectrons diffuse rapidly to the wall
  - Positively charged particles continue to a collection electrometer
  - Measure the positive current in pA or fA
  - Output to PC or datalogger

Conversion factors, pA to ng/m3

- Depend on the source
- Range from 1000 to 3000 ng/m^3 per pA
- Published work (Burtscher, Niessner, and others) substantiates the utility and range of conversion factors
- Semi-quantitative in ambient air
- Greatest accuracy requires specific calibration

Response

- No response to vapor
- Particles less than about 1 um
- PAH with 3 or more rings
- Highest for 5-7 ring PAH, such as benzo[a]pyrene
- Limit of detection about 10 ng/m^3 for PAS 1002i; much lower for PAS 2000

Differences between PAS 1002i and 2000

- PAS 1002i
  - Ultraviolet lamp, 187 nm
  - 4 L/min
  - LOD 10 ng/m^3
  - PAH, a few metals, and some organics
  - Lamp intensity calibration required
- PAS 2000
  - Excimer laser, 222 nm
  - 2 L/min
  - LOD < 1 ng/m^3
  - PAH, perbromo- and periodo-alkanes
  - Software compensation

Comparisons with integrated sampling (PAS 1002i)

- In more than 40 indoor and outdoor microenvironments, agreement was good, with a conversion factor of 1000 ng/m^3 per pA.
- Agreement was best (R^2 > 0.6) with the sum of the carcinogenic (B2) PAH as determined by GC/MS.

Activity patterns and ambient monitoring

- Rapid response and high sensitivity make the PAS valuable for following activities that generate PAH.
  - Example: PAH at a veterinarian's office
- Ability to collect real-time averages make it valuable for monitoring ambient concentrations of PAH, traffic patterns, other combustion.
  - Example: Ambient monitoring in DC, summer of 1994

Current activities

- Comparison of PAS 1002i, 2000i, and integrated sampling for PAH inside and outside 8-9 RTP homes
  - Denuded and non-denuded integrated sampling to determine phase distributions

"An Indexing System for Comparing Toxic Air Pollutants Based Upon Their Potential Environmental Impacts"

Gregory C. Pratt[1], Paul E. Gerbec[1], Sherryl K. Livingston[1], Fardin Oliaei[1], George L. Bollweg[1], Sally Paterson[2], and Donald Mackay[2]

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2. Institute for Environmental Studies, University of Toronto, Toronto, Ontario M5S 1A4, Canada

The Toxic Air Pollutant Indexing System

- Compares substances emitted to the air based upon potential environmental impacts
- Does not predict actual impacts

$$\text{Index} = \frac{\text{Potential exposure}}{\text{toxicity}} = \text{hazard potential}$$

Potential exposure

- Estimated with Level III Fugacity Model using chemical and physical properties of substance:
  - molecular weight
  - solubility
  - vapor pressure
  - octanol-water partition coefficient
  - melting point
  - food chain multipliers
  - degradation half lives in air, water, soil and sediment
  - air emission rate (10 kg/hr)
- Concentrations estimated in five compartments:
  - Air
  - Water
  - Aquatic biota (fish)
  - Soil
  - Terrestrial biota

Toxicity Indicators

- Human Health
  - Inhalation Reference Concentration (RfC)
  - Ingestion Reference Dose (RfD)
  - Inhalation Cancer Unit Risk (UR)
  - Ingestion Cancer Slope Factor (SF)
  - Threshold Limit Value (TLV)
- Ecological Effects:
  - Aquatic Life Criteria (ALC)
  - Piscivorous Wildlife Criteria (PWC)
- Data Sources:
  - IRIS2
  - HEAST
  - ASQB
  - USEPA Water quality standards and criteria

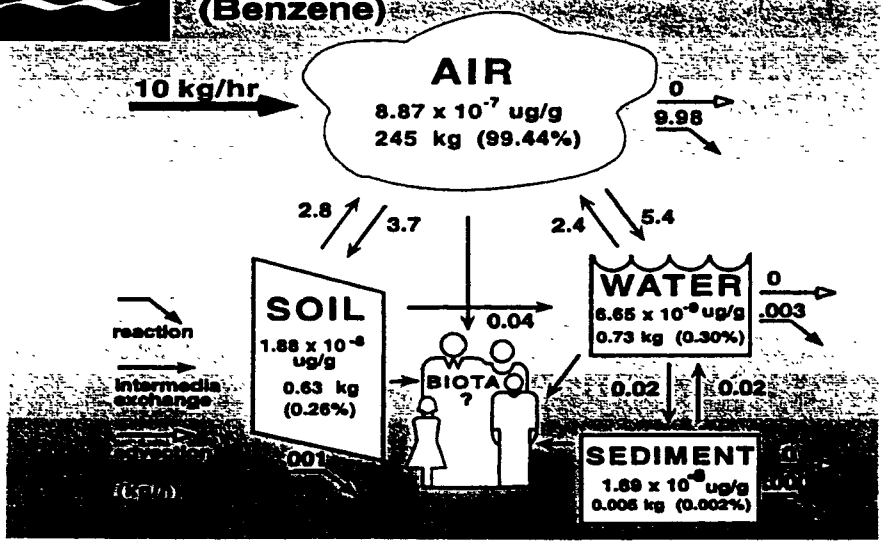
Potential exposure / toxicity combinations:

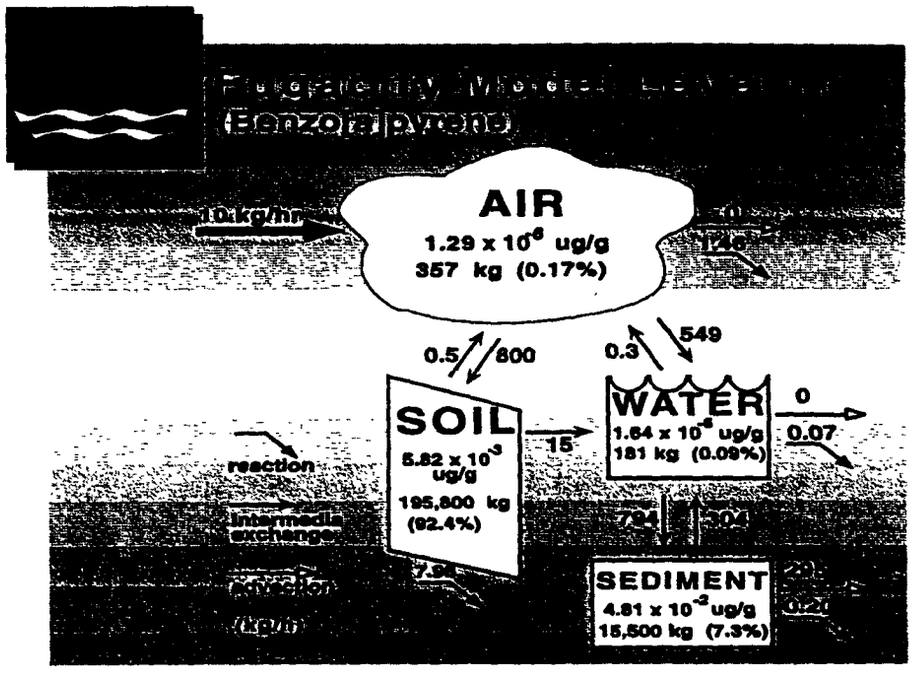
- Air/Inhalation RfC
- Air/Inhalation UR
- Air/TLV
- Water/Ingestion RfD
- Water/Ingestion SF
- Aquatic Biota/Ingestion RfD
- Aquatic Biota/Ingestion SF
- Soil/Ingestion RfD
- Soil/Ingestion SF
- Terrestrial Flora/Ingestion RfD
- Terrestrial Flora/Ingestion SF
- Water/Aquatic Life Criteria
- Water/Piscivorous Wildlife Criteria

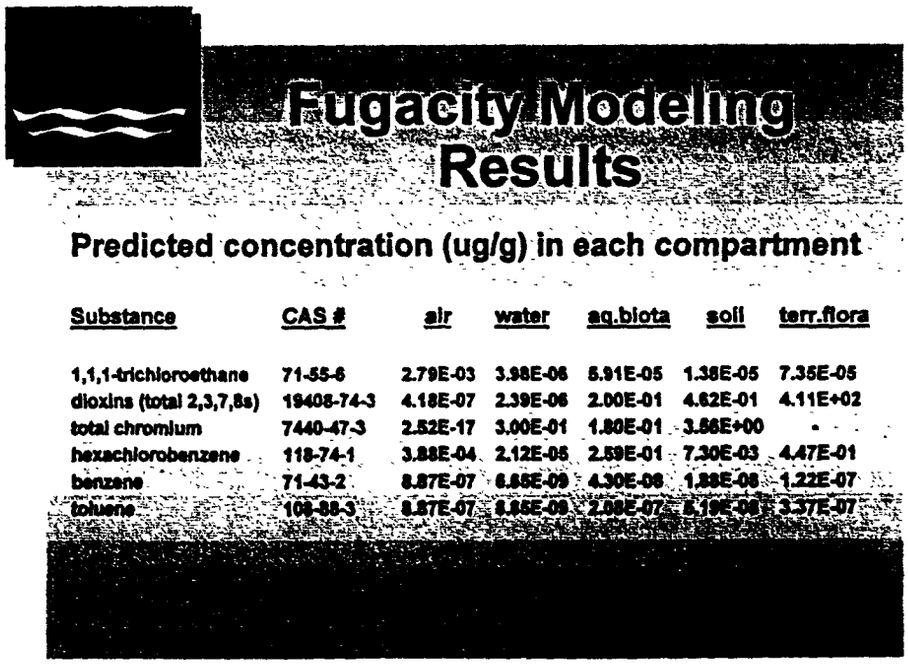
Environmental compartment sizes used in the fugacity modeling

Compartment	area (m2)	depth (m)	volume (m3)	fractionOC	density (kg/m3)
Air	2.178e11	1.0e3	2.178e14	-	1.2
Water	1.380e10	8.0e0	1.104e11	-	1000
Soil	2.040e11	1.0e-1	2.040e10	0.03	1650
Sediment	1.380e10	2.0e-2	2.760e8	0.15	1170
Suspended Sediment	-	-	1.1 e5	0.49	2400
Fish	-	-	1.1 e5	-	1000
Air Parcel	-	-	2.0 e2	-	2400

Fugacity Model Level III (Benzene)







Fugacity Modeling Results

Predicted concentration (ug/g) in each compartment

Substance	CAS #	air	water	aq.biota	soil	terr.flora
1,1,1-trichloroethane	71-55-6	2.79E-03	3.98E-06	5.91E-05	1.38E-05	7.35E-05
dioxins (total 2,3,7,8s)	19408-74-3	4.18E-07	2.39E-06	2.00E-01	4.62E-01	4.11E+02
total chromium	7440-47-3	2.52E-17	3.00E-01	1.80E-01	3.56E+00	-
hexachlorobenzene	118-74-1	3.88E-04	2.12E-05	2.59E-01	7.30E-03	4.47E-01
benzene	71-43-2	8.87E-07	6.85E-09	4.30E-08	1.88E-08	1.22E-07
toluene	108-88-3	8.87E-07	6.85E-09	2.08E-07	8.19E-08	3.37E-07

Fugacity Results Modified By Human Intake

log(intake via indicated compartment in mg/kg/day)

Substance	air	water	aq.biota	soil	terr.flora
1,1,1-trichloroethane	-2.99	-6.94	-7.60	-10.40	-8.64
dioxins (total 2,3,7,8s)	-6.81	-7.16	-4.07	-5.88	-1.89
total chromium	-17.03	-2.07	-4.11	-4.99	[illegible]
hexachlorobenzene	-3.84	-6.22	-3.95	-7.68	-4.85
benzene	-9.49	-9.72	-10.78	-13.27	-11.42
toluene	-9.49	-9.60	-10.05	-12.35	-10.95

Human Health Toxicity Data

Substance	RfC/RfD Inhalation (mg/m3)	RfC/RfD Ingestion (mg/kg/d)	Cancer Unit Risk(Inhal.) 1/(ug/m3)	Cancer Slope Factor(Ingest.) 1/(mg/kg/d)	TLV (mg/m3)
1,1,1-TCA	1.0E+00	9.0E-02			1910.
dioxins			1.3E+00	6.2E+03	
total Cr					0.5
HCB		8.0E-04	4.6E-04	1.6E+00	
benzene			8.3E-06	2.9E-02	32.
toluene	4.0E-01	2.0E-01			[illegible]

Human Health Toxicity Data (log(mg/kg/day))

Substance	RfC/RfD Inhalation	RfC/RfD Ingestion	Cancer-dose (10e-5 risk) Inhalation	Cancer-dose (10e-5 risk) Ingestion	TLV (/100)
1,1,1-TCA	-0.54	-1.05			0.74
dioxins			-8.66	-8.79	
total Cr					-2.85
HCB		-3.10	-5.21	-5.20	
benzene			-3.46	-3.46	-1.04
toluene	-0.94	-0.70			0.03

Environmental Fate/Human Health Combinations (log(intake in mg/kg/day) - log(toxicity in mg/kg/day))

Substance	air/inhal.RfC	air/inhal.UR	air/TLV	water/ingest.RfD	water/ingest.SF
1,1,1-TCA	-2.44			-5.90	
dioxins		1.85			1.63
total Cr			-14.19		
HCB		1.36		-3.12	-1.01
benzene		-3.02			-6.26
toluene	-5.54			-8.90	

Environmental Fate/Human Health Combinations

(log(ug/kg/day) - log(toxicity in mg/kg/day))

Substance	aq.biota/ Ingest.RfD	aq.biota/ Ingest.SF	soil/ Ingest.RfD	soil/ Ingest.SF	terr.flora/ Ingest.RfD	terr.flora/ Ingest.SF
1,1,1-TCA	-6.55		-9.36		-7.59	
dioxins		4.73		2.91		6.90
total Cr						
HCB	-0.86	1.25	-4.58	-2.48	-1.76	0.35
benzene		-7.27		-9.81		-7.96
toluene	-9.35		-12.13		-10.2	

Ecological Toxicity Data

Fate/ecological toxicity combos (log(ug/g)-log(ug/g))

Substance	Aquatic Life Criterion(ug/l)	Pisc.Wildlife Criterion(ug/l)	water/ALC	water/PWC
1,1,1-TCA	263.0		-4.82	
dioxins		8.50E-09		5.45
total chromium				
hexachlorobenzene	0.02		0.02	
benzene	114.0		-7.23	
toluene	253.0		-7.45	

The Bottom Line

Substance	maximum of combinations	scaled max (= log index)	Fate/Toxicity Index (10^(scaled max))	Index basis
1,1,1-TCA	-2.44	9.03	1.08E+09	air/RfC
dioxins	6.90	21.09	1.23E+21	terr flora/SF
total Cr	-14.19	0.00	1.00E+00	air/TLV
HCB	1.36	15.55	3.54E+15	air/UR
benzene	-3.02	11.16	1.46E+11	air/UR
toluene	-5.64	8.84	7.10E+08	air/RfC

Results

183 substances indexed so far

Values range over 21 orders of magnitude:

Substance	Index (log)	Basis
dioxins	21.09	terr flora/SF
mercury	19.80	water/PWC
PCBs	16.92	water/PWC
silver	16.12	water/ALC
benzo(a)pyrene	16.05	terr flora/SF
cadmium	16.00	water/ALC
dibromochloropropane	15.94	air/UR
chromium (VI)	15.63	water/ALC
lead (Pb)	15.55	water/ALC
hexachlorobenzene	15.55	air/UR
antimony	15.53	aq biota/RfD
carbon tetrachloride	15.30	air/UR
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]

Results (cont'd)

Substances with the lowest index values

Substance	Index (log)	Basis
nitrotoluene (2-)	6.81	water/RfD
benzoic acid	6.53	terr flora/RfD
phthalic anhydride	6.03	terr flora/RfD
dichlorobenzidine (3,3'-)	5.75	terr flora/SF
cyclohexanone	5.02	water/RfD
anthracene	4.05	water/ALC
biphenyl (diphenyl)	3.97	aq biota/RfD
methyl methacrylate	3.79	water/RfD
diethanolamine	2.71	air/TLV
chromium (total)	0.00	air/TLV

Uses of the Indexing System

- Set thresholds for reporting requirements (registration, inventory, environmental monitoring, and enhanced emission estimates)
- Set air emission fees using hazard-based fee rates (rather than flat rate)
- Identify persistent and bioaccumulating substances that require further study
- Refine environmental monitoring needs
- Identify emission reduction goals
- Set priorities for facility review

Interfacility Comparison

		Facility 1		Facility 2	
	index value	emissions lb/y	weighted emissions	emissions lb/y	weighted emissions
acetone	7.16	0	0.00E+00	3,285,000	4.75E+13
benzene	11.16	0	0.00E+00	3,522	5.09E+14
chlorophenol	8.31	9,240	1.89E+12	800	1.63E+11
mercury	18.99	77	7.52E+20	0	0.00E+00
vinyl acetate	8.79	5232	3.23E+12	0	0.00E+00
sum		[illegible]	[illegible]	[illegible]	[illegible]
			2038		1.79

Conclusions

- A system for ranking chemicals by their environmental hazard potential
- Combines human and ecological toxicity data with environmental fate (fugacity) modeling of potential exposure
- Hazard Potential = potential exposure/toxicity
- Ranges over 21 orders of magnitude
- 195 substances indexed to date
- Many uses for resulting quantification of potential for environmental hazard

The Mercury Study: An Integrated Risk Assessment

Martha H. Keating
Risk and Exposure Assessment Group
Office of Air Quality Planning and Standards

Background

The Clean Air Act as amended in 1990 required the U.S. Environmental Protection Agency (EPA) to prepare a report to Congress on mercury emissions. The study was to identify the sources, rate and mass of mercury emissions from utility boilers, municipal waste combustors and all other sources, the public health and environmental impact of such emissions, technologies available to control such emissions and the costs of such technologies. Two major features of the requirement are that 1) there are no direct regulatory requirements, and 2) environmental effects must be considered. This is in contrast to the requirements of the Utility Air Toxics Study which addresses all pollutants from utilities, including mercury.

In 1992, the Office of Air Quality Planning and Standards and the Office of Research and Development began a collaborative effort to design and prepare the Mercury Study. The culmination of this effort is a seven-volume report which covers in considerable depth a national emissions inventory, fate and transport of mercury in the environment, exposure analyses, human health effects, wildlife impacts, risk characterization, and control technologies and costs. While the main "customer" for the study is Congress, it was also recognized that State and local agencies could benefit from a compendium of the subject. In addition, the Mercury Study broke new ground with a number of analyses which necessitated thorough and extensive documentation.

Mercury is a pollutant that is emitted from many industries and sources, including natural sources. It's persistence in the environment and propensity to be transported globally and cycle through all of the various environmental compartments in various chemical forms, makes assessment and characterization of the problem extremely difficult. The potential public health impacts of such contamination involve certain segments of the U.S. population, particularly women and children. Wildlife impacts are already being observed in loons, mink and the endangered Florida panther. Control of this elusive pollutant, while demonstrated and cost-effective for some industrial processes, has not been demonstrated and is extremely costly for others.

Given the complexity of this issue, EPA's policy decisions regarding control of mercury have the potential to impact numerous industries, other program offices and federal and state public health policies. Because of these potential impacts, the Mercury Study Report to Congress has come under intense scrutiny and evaluation. In particular, the exposure assessment and risk characterization have been characterized

as both "state of the science" and completely off base.

The study had a statutory deadline of November 1994 for submittal to Congress but has yet to be submitted. Currently the EPA is awaiting the final written report of the Science Advisory Board which reviewed the study in February 1997. It is hoped a Mercury Study will be released by the end of 1997.

This paper is intended for state and regional agencies who may wish to design a multimedia risk assessment. The discussion does not focus on specific models or results. The intent is to describe the approach which was used to model and characterize the problem, how limitations in the assessment were described and the lessons learned from applying these tools to a problem that has far-reaching policy implications.

Design of the Mercury Study

The Mercury Study was designed to integrate a number of different (but linked) types of information:

* Data on type, sources, and trends in emissions;

* evaluation of the atmospheric transport of mercury to locations distant from emission sources;

* assessment of potential impacts of mercury emissions close to the source;

* identification of major pathways of exposure to humans and wildlife;

* identification of the types of human health consequences of mercury exposure and the amount of exposure likely to result in adverse effects;

* evaluation of mercury exposure consequences for ecosystems and for wildlife species;

* identification of populations especially at risk from mercury exposure due to innate sensitivity or high exposure; and

* estimates of control technology efficiencies and costs.

Because of the paucity of monitoring data for mercury, particularly around source types of particular interest, the Mercury Study exposure assessment relied on a number of models to predict mercury fate and transport in the atmosphere, watershed, water body and aquatic and terrestrial food chains. Quantitative modeling analyses examined the following ; (1) the long range transport of mercury from emission sources through the atmosphere; (2) the transport of mercury emissions through the local atmosphere;

(3) the aquatic and terrestrial fate and transport of mercury at hypothetical sites; and (4) finally the resulting exposures to hypothetical humans and animals that inhabit these sites. Exposure to mercury from seafood was estimated using a cross sectional survey with a three day sampling period and central tendency estimates of mercury concentrations in the tissues of seafood.

Figure 1 illustrates how the various exposure models were combined to estimate both human and wildlife exposure.

Describing the Limitations of the Assessment

Each facet of the Mercury Study has it's own set of uncertainties - either due to uncertainties inherent in the approach (e.g., using emission factors for the emissions inventory) or uncertainty related to the models themselves or the parameters used in the model.

The approach used to describe the limitations of the analysis was to list and discuss what the factors were that created uncertainty, the effect of these factors on the analysis (e.g., over- or underestimation), and the means by which the uncertainties were addressed. It is extremely important that the researcher understand the data - their derivation, quality and how a change might influence the overall results.

For example, the emissions inventory was the basically the input for the long range transport analysis. The quality of the emissions data for each of the source categories varied. It was important to know what the basis for the emissions estimate was (e.g., stack test data or engineering judgement), how the estimate compared to other estimates in the published literature or provided by industry, whether the estimate was current or how it might change over time and most importantly how changes in the emissions estimate (either lower or higher) would affect the results of the modeling analysis.

For the exposure analysis, a table of factors important for estimating mercury exposure was provided along with how important they were and how they were handled in the analysis. Some were addressed by sensitivity analyses, different scenarios were used for others and quantitative uncertainty analyses were performed for those where the data were sufficient.

Limitations in the assessment should be acknowledged and considered when drawing conclusions. It is also helpful to list areas of research or further study or analyses needed to reduce the uncertainty and variability of the data.

Lessons Learned

1. "Science guides, but policy decides". The risk assessment is only one piece of the information needed by the risk manager. Other risk management factors such as economic considerations, technical feasibility and other non-risk related factors are always part of policy considerations.

2. Extensive justification and documentation of model parameters is essential for a "transparent" analyses. The downside is that there is much information for critics to challenge.

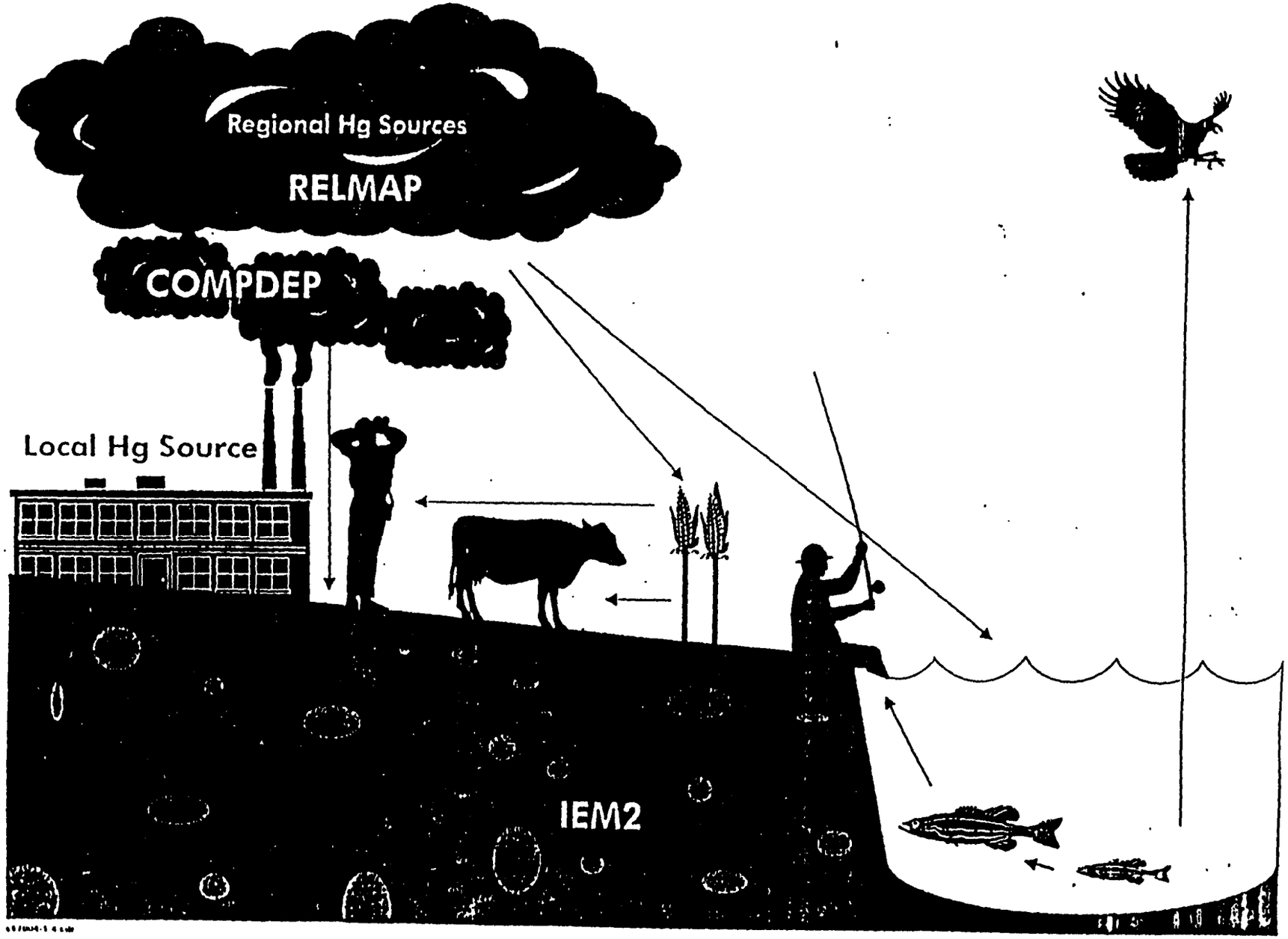
3. A discussion of uncertainty, even if it's qualitative is required. Describe the limitations of the assessments. Know your models.

4. Sensitivity analyses are useful to test a range of possibilities when there is no one correct answer (always!). Using a range is more defensible than point estimates.

5. Use measured data as much as possible to test, and hopefully corroborate, modeled predictions.

6. Qualify conclusions, if necessary, with statements about the level of confidence in the results.

Figure 1
Fate, Transport and Exposure Modeling Conducted in the Combined COMPDEP and RELMAP Local Impact Analysis



Evaluation of the Screening Risk Assessment (SRA) for the Anniston Army Depot

LEIGH BARB BACON
STATE OF ALABAMA- DEM

OVERVIEW

- Background
- Facility Layout
- Elements of a HHRA
- Dispersion Modeling
- Electronic Spreadsheet
- Summary

SRA'S ARE COMPRISED OF:

- A multi pathway human health risk assessment (HHRA)
- An ecological risk assessment (ERA)

THE ADEM AIR DIVISION'S ROLE IN THE HHRA

- Verification of the emissions rates used in the chronic and acute HHRA's.
- Verification of the modeling methodology, model options, stack parameters and resulting media concentrations.
- Verification of the methodology used in determining the pollutant specific ambient concentrations and depositions.
- The ADEM- Air Division was not responsible for the health effects assessment.

HHRA'S INCLUDE:

- Estimated risks and hazards from direct exposure through inhalation of emissions.
- Estimated risks and hazards from indirect exposures through soil, water and food products exposed to emissions depositions.

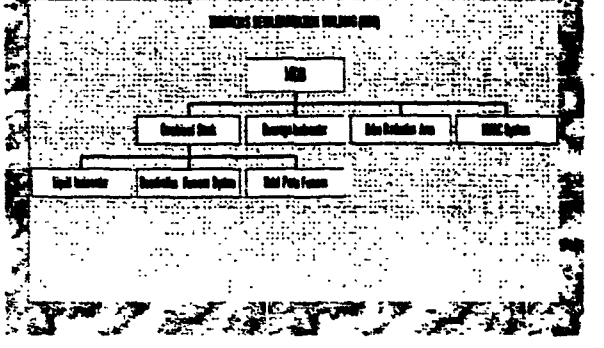
BACKGROUND

- The U.S. Department of Defense (DOD) currently stores lethal unitary chemical agents at the Anniston Army Depot.
- These include the blister agents HD and HT and the organophosphate nerve agents GB and VX.

BACKGROUND (cont.)

- They are stored at the Depot as bombs, cartridges, mines, projectiles, rockets, and ton containers.
- The AAD is located in Calhoun County, approximately 4 miles west of Anniston, AL.

FACILITY LAYOUT



HHRA

- Definition of the study area
- Definition of the exposed individuals
- Determination of the concentration of each substance in the environmental media
- Estimation of the amount of substance each individual is exposed to.
- Assessment of the toxicity of media concentrations.

LIFE EXPECTANCY OF INCINERATION ACTIVITIES

- Chronic
  - Operational duration of 6 years.
- Acute
  - Operational duration of 1 hour.

AAD STUDY AREA

- For the chronic portion of the HHRA, it was limited to all the acreage within 50 kilometers.
- For the acute portion of the HHRA, it was limited to all the acreage within 10 kilometers.

CHRONIC EXPOSURE SCENARIOS

- Adult Resident
- Child Resident
- Subsistence Farmer
- Subsistence Fisher-
  - Logan Martin/Neely Henry Lake
  - Eastaboga Fish Hatchery
  - Abandoned Catfish Farm

ACUTE EXPOSURE SCENARIOS

- Adult Resident living on the AAD
- Onsite Worker at the AAD

METHOD OF EXPOSURE

- Particulate Concentration
  - Air
- Vapor Concentration
  - Air
- Dry Deposition
  - Food, Soil
- Wet Deposition
  - Water

ESTIMATION OF EMISSIONS

- Emission Rates for the AAD sources were established from data at the Johnston Atoll Chemical Agent Disposal System (JACADS).
- Maximum lifetime incinerator/source specific emissions were determined for the chronic assessment.
- Maximum short term emissions were used for the acute assessment.

UPSETS- Chronic

- To account for increased emissions due to startup/shutdown, upsets or malfunctions, upset factors were applied to the emission estimates for each pollutant.
- Upsets were assumed to occur 5% of the time for metals and 20% for organics.
- Emissions were scaled by 2.8 and 1.45 for organic and metal emissions, respectively.

UPSETS- Chronic

- Example- Metals
  - $(0.95)(1) + (0.05)(10) = 1.45$
- The only exception is the BRA, which can right itself, or be shut down within 10 minutes.
- Example- BRA
  - $(10/60)(10) + (50/60)(1) = 2.5$

UPSETS- Acute

- To account for increased emissions due to startup/shutdown, upsets or malfunctions, upset factors were applied to the emission estimates for each pollutant.
- Assumed that only one source would be in upset at a time.
- The source in upset is scaled up by a factor of 10, while all other processes run under normal conditions.

AIR DISPERSION MODELING

- For the chronic portion of the HHRA, modeling was completed with the COMPDEP model to predict ambient vapor and particulate concentrations, wet and dry depositions.
- For the acute portion of the HHRA, modeling was completed with the BEEST-X model to predict ambient vapor and particulate concentrations.

AIR DISPERSION MODELING

- In addition to the chronic and acute modeling, the COMPLEX I model was run for all areas for complex terrain to ensure maximum predicted concentrations.
- Modeling was completed with a unit emission rate for all sources at the facility.

AIR DISPERSION MODELING

- In lieu of on-site data, 5 years of surface, upper air and precipitation data from the Birmingham, Alabama municipal airport was used in the modeling.
- Three receptor grids were generated for the HHRA.
  - Chronic- polar receptor grid
  - Acute- polar receptor grid, and a fenceline grid
  - Chronic/Acute- discrete receptors

ELECTRONIC SPREADSHEET

- USACHPPM
- Based on the exposure scenario, media concentrations can be verified for a specific pollutant for a specific year.

ELECTRONIC SPREADSHEET CHRONIC HHRA

- Using the unit emission rate maximum predicted concentration for each source, the pollutant specific emission rate is applied to the unit concentration for each individual source.
- All sources are upset and the maximum predicted concentration is the greatest of these scenarios.

ELECTRONIC SPREADSHEET ACUTE HHRA

- Using the unit emission rate maximum predicted concentration for each source, the pollutant specific emission rate is applied to the unit concentration for each individual source.
- Each source is upset individually, while the other sources are run under normal conditions. The maximum predicted concentration would be the greatest of these.

CONSERVATIVE ASSUMPTIONS OF THE AAD HHRA

- All incinerators assumed to run 6000 hours per year.
- All ambient concentrations assumed to be co-located.
- The AAD life expectancy increased by 50% from 4 years to 6 years.

CONSERVATIVE ASSUMPTIONS OF THE AAD HHRA

- Chronic upset conditions assumed to occur 5% of the time for metals, and 20% for organics. Actual data shows less than 2% upset time.
- JACADS data based on fuel oil; the AAD will fire natural gas with LPG backup.
- Conservative stack parameters.

CONSERVATIVE ASSUMPTIONS OF THE AAD HHRA

- Non detect substances are assumed to be present at the detection level for regulated pollutants, and at 1/2 the detection level for unregulated pollutants.

SUMMARY

- The U.S. Army submitted a SRA for the proposed demilitarization activities at the Anniston Army Depot.
- Through dispersion modeling and the use of an electronic spreadsheet, the ADEM Air Division was able to verify media concentrations used in the health effects portion of the SRA.

EPA's AIR PROGRAM TRAINING OPPORTUNITIES

Howard Wright
Education and Outreach Group

WHAT IS EOG?

- THE EDUCATION AND OUTREACH GROUP (*EOG*)
- ACKNOWLEDGES THE IMPORTANCE OF EDUCATION, OUTREACH, AND TRAINING (APTI) TO THE AIR PROGRAM
- MERGED INTO ONE GROUP IN NOVEMBER, 1994
- MULTI-DISCIPLINARY GROUP OF ENVIRONMENTAL ENGINEERS, SCIENTISTS, SPECIALISTS, AND EDUCATORS

WHAT ARE EOG's MISSIONS?

- PROVIDE TECHNICAL AIR POLLUTION TRAINING TO PRIMARY CLIENTS (*State and local air agency personnel*)
- PROMOTE ENVIRONMENTAL EDUCATION TO TEACHERS AND STUDENTS, WITH A FOCUS ON K-12
- ENHANCE OUTREACH ACTIVITIES BY FORGING NEW PARTNERSHIPS AND STRENGTHENING EXISTING ONES
  - Small Business Support
  - Air Quality Learning Centers
  - Public Information Officers

HOW ARE YOUR TRAINING NEEDS DETERMINED?

- JOINT NEEDS ASSESSMENT SURVEY
- STAPPA/ALAPCO/EPA TRAINING COMMITTEE
- COURSE EVALUATIONS
- ANNUAL TRAINING CONFERENCE

HOW IS TRAINING DELIVERED TO YOU?

- SELF INSTRUCTIONAL MATERIALS (obtained from EOG and air quality learning centers)
- CLASSROOM COURSES (taught at area training centers and academies)
- SATELLITE BROADCASTS (on the Air Pollution Distance Learning Network)

WHAT'S AVAILABLE? (more)

- SELF INSTRUCTIONAL COURSES

SI: 400 Introduction to Risk Assessment/Risk Management

SI: 404 Urban Air Toxics

SI: 422 Air Pollution Control Orientation

SI: 458 Hazardous Waste Calculations

WHERE TO FIND EOG TRAINING INFORMATION?

- OAQPS HomePage on INTERNET
- APTI BBS on TTN (dial 919-541-5742)
- WESTAR Homepage
- EPA's LAN Services Menu
- APTI 1997 Classroom Schedule
- S/L Site Coordinators and Training Contacts

Unified Air Toxics Web Site

www.epa.gov/oar/oaqps/airtox/

Dr. Nancy B. Pate
EPA/OAQPS/ITPID
Information Transfer Group
919-541-5347
pate.nancy@epamail.epa.gov

Basic Facts

EPA Rules and Implementation

Pollutants and Sources

Technical Resources

EPA Programs

State and Local Agency Programs

Basic Facts

Why "Unified"?
What are Air Toxics?
What are the Health Effects?
"Criteria" vs "HAP"
Citizen Guides
Links to more health info

EPA Rules and Implementation

List of all Air Toxics Rules and related rules

Links to all Preamble and Rule texts

Policy Guidance

Implementation Resources

Pollutants and Sources

List of 112(b)(1) HAP's

Modifications

Current Source Category List

Technical Resources

Hotlines

Hotlinks

Document Information Resources

Selected List of Documents

EPA Programs

Alphabet Soup

Road map to EPA Offices

Functional Statements

State and Local Agengy Programs

Describes the Partnership

Links to State and Local Web Sites

Share Library

Unified Air Toxics Website
Purpose of website - To provide the general public, federal, state and local governments and emitting facilities, comprehensive air toxics information (from basic to very technical) in a centralized location on the internet. To encourage sharing of information in order to reduce duplication of effort.

Website address: **http//www.epa.gov/oar/oaqps/airtox/**

Brief description of the 6 areas of information either presently or soon to be on this website:

1. **Basic Facts**
   - describes Unified Air Toxics Website
   - briefly explains what are air toxic pollutants and their effects
   - provides links to citizen guides and brochures on health risks of air toxics and other basic sources of information

2. **EPA Rules and Implementation**
   - lists all air toxics rules and closely related rules
   - provides links to all preamble and rule texts, related policy guidance and access to implementation materials produced by federal, state or local agencies

3. **Pollutants and Sources**
   - lists the 188 toxic air pollutants regulated by the EPA
   - defines types of air toxic pollutant sources
   - lists 174 source categories of industrial and commercial sources of air toxics

4. **Technical Resources**
   - lists telephone information resources (such as hotlines) and internet technical information resources (such as centers, clearinghouses) with air toxics information
   - gives access to select published technical documents and links to document information resources

5. **EPA Programs**
   - describes air toxics program and its major components
   - lists all EPA offices with air toxics responsibilities and describes their roles

6. **State and Local Agency Programs**
   - describes federal, state and local air toxics program partnership
   - lists state and local air agency program websites
   - provides a "sharing library" for states and local agencies without websites to display work products in one centralized location

National Speciality Workshop on Technical Tools for Air Toxic Assessment

EPA Environmental Research Center
Research Triangle Park, NC
(June 17- 20, 1997)

Education and Outreach Panel Group Summary

Panel Members:

Brian Haugstad: Chair (Iowa)
Dr. Ellen Morris (Connecticut)
Samuel Bell (Jefferson County, AL)
Leigh Bacon (Alabama)
Jimmy Johnson (Georgia)

EPA Coordinators:
Jim Dicke (EPA-EOG)
Ron Townsend (EPA-EOG)
Howard Wright (EPA-EOG)

PART ONE:

When are present technical tools adequate in helping you do your job?

1. In providing staff training on specific air toxics standards or procedures, and in providing information on general air toxics issues.
2. In providing education, outreach and training to the regulated community.
   - Printed training and outreach materials, and live or taped educational videos are helpful, when provided in a timely manner.
3. Telecourses filmed at regulated facilities, that demonstrate regulated compliance.

PART TWO:

When are technical tools inadequate?

1. When the training focuses not on the regulatory requirements, but instead upon the general operations of the facility, or upon other methods by which the facility reduced air pollution.
2. When training is not provided in a timely basis.
   - This happens frequently.
3. When telecourse speakers provide vague information, and are unable to answer specific questions or details.
4. When communicating risk assessment to the public.
5. When there are no viewing sites equipped to receive satellite courses.
   - When local network sites are not available, otherwise interested participants must either travel to more distant sites, or otherwise not participate.

PART THREE:

What recommendations may solve these identified problems?

1. Training should focus upon the needs of the regulatory agencies implementing the regulations, while clearly understanding who is the target audience.

- Different target audiences have different training needs. (i.e. permit writers v. compliance staff v. the public)

Recommendations:

A. EPA should coordinate with STAPPA/ALAPCO and make greater use of **annual and special interest surveys**, to more clearly identify target audiences and their training needs.

B. STAPPA/ALAPCO has a **listing of state air toxics contacts**.
   - State and local agency staff should review these contact lists, to ensure correct staff are listed.

C. Survey the targeted audience well **prior** to developing the training materials.

D. Different state and local regulatory agencies have **different goals** and training needs. Surveys should identify these differences.

E. Survey STAPPA/ALAPCO, EPA Regions, and Trade Associations, to determine what type of training is needed, and to specifically identify **when** the training is most needed.

F. Surveys should include long-term **strategic goals** and these long-term ideas should be forwarded toEPA. This will force state and local agencies to actively think and prioritize their training needs long-term.

G. States and local agencies should **actively solicit** and **prioritize** the training needs from their identified targeted groups, and this information should be forwarded to EPA.

H. Training goals should be identified for specific **regulatory standards**.

I. Develop written surveys for distribution to state and local agencies that identify and prioritize **requisite and required training**.

J. Local and state agencies should **conduct** their **own surveys** of their agency staff, to determine their agency's training needs.

K. Identified training needs could be shared through the use of **regional** air toxics **conference calls**.

L. Newly released educational materials should be **screened** early after receiving it, to insure it is useful for targeted groups.

2. Many of the video materials available to states and local agencies are out-of-date.

Recommendations:

A. A quarterly update on **all current available training materials** should be provided to primary state and local agency air toxics contacts.

B. Do not rely upon the state educational coordinator to pass on training updates to air toxics staff. Primary air toxics coordinators should be **contacted directly**, or informed where to find this information on the Unified Web Site.

C. References to all written and video materials should include a **date of publication, and a** brief **synopsis**.

D. New training materials should be developed by EPA as **soon after** surveys are received and significant training needs are identified.

E. Videos should **not** be **repetitive**, but should reflect current policies and procedures.

F. **Remember**... it is difficult for state and local agency staff to provide industry with training, until state and local program staff first are provided a clear understanding themselves.

3. Make EPA training and outreach materials more accessible.

Recommendations:

A. Provide an **on-line clearinghouse** of all available course materials, including video tapes, training courses, and other training resource materials, by accessing the Unified Air Toxics Web Site.

B. Continually (or quarterly) **update** course materials on-line, as these materials become available, so that most current training materials are always up-to-date.

C. Separate training materials by **discipline** or **MACT standards**, to more easily locate resource materials.

D. EPA and STAPPA/ALAPCO should **contact** state and local air toxics staff contacts **directly**, as opposed to strictly through state/local educational coordinators.

E. Solicit input from **trade associations**, and have trade associations **co-sponsor** training programs.

F. Provide a means whereby training materials already developed by state and local programs may be **shared electronically** on the Unified Web Site.

G. Provide an easily identified on-line heading (ie. **"air toxics education"**), so that on-line browsers may more easily locate educational training materials.

H. Greater **publicize** the Unified Air Toxics Web Sites.
- Promote its use among state and local air toxics contacts, and among state and local air directors.

I. For regional EPA updates, state and local agencies should greater utilize EPA's **regional web sites**.
- Provide regional EPA contacts with suggestions on how regional EPA web sites may be improved.

J. Make better use of **fiber-optic satellite feeds**, to involve government agencies, regulated facilities and the general public.

K. To improve training attendance, EPA and state sponsored informational meetings should require **minimal** long distance **travel**.

L. Use **more conference calls**.
- It is cheap and convenient.

M. Workshops are **not** commonly well **attended by the public**.
- Suggestions are needed to improve public participation.
- Use state/federal **advertising** and **marketing** resources?

N. Establish additional **automatic e-mailing** methods, sent to air toxics contacts.
- ie. Similar to Federal Register notices, and Mobile Source e-mailings.

O. **Link** other good **web sites** to the Unified Air Toxics Web Site, for easy access.

P. The Unified Air Toxics Web Site should have a **comments section**, for agency staff to comment upon education materials, and to make further suggestions.

4. Publications such as quarterly newsletters, fiber-optic television links throughout the state (for state specific education and outreach programs), and informational brochures mailed to regulated facilities to aid in MACT compliance, are helpful in educating regulated facilities.

Recommendations:

A. Newsletters may be used to educate and provide **all types** of compliance standard information to regulated facilities.
B. EPA written materials can be **modified and simplified** by state/local agencies for state agency instructional purposes. (ie. Brochures and newsletters)
C. Publications should be **clearly written**, in shortened form.
D. Don't include **needless language** and too much detail.
E. If materials are **too long or detailed**, often regulated facilities don't bother reading them, and the effort is wasted.
F. Use **"catchy and colorful graphics"** that bring attention to the publication or brochure, and prioritize the ideas that you wish to relay to the reader.
G. In addition to regulator news, newsletters should also include **health risk data** based upon health studies, that draws the reader further into the article.
H. To **reduce duplication of efforts**, EPA and state agencies should contact each other when significant communications are forwarded to regulated facilities.
I. Video training should **not** include **extraneous** details.

5. Small Business Assistance Groups are often helpful in providing confidential, on-site assistance with regulatory compliance and educational materials to regulated facilities.

Recommendations:

A. Examples of the nation's most highly effective programs should be summarized and **shared nationally**.
B. STAPPA/ALAPCO should survey **how many** small business assistance groups are currently active nationwide.
   - Investigate their effectiveness.
C. Small Business Assistance Programs should be **expanded**, by increased funding of these sources, and by further sharing of technical ideas between regulated facilities and government agencies.
D. An **alternative** to directly interacting with government regulatory agencies.
   - Regulated facilities often call upon Small Business Assistance Groups, rather than interacting with government agencies.
   - Improved compliance of MACT standards.

6. A Plain English Guidance Document is needed to instruct agencies on how to effectively collect, analysis and present data.

Recommendations:

A. **Statistical analysis training** is needed.
B. More training opportunities provided on the **Education and Outreach home page**.
C. Risk Assessment.
   - More training needed for **Training the Trainers** target groups.
D. Training materials should use **non-technical instruction**, whenever possible, to keep training as simple as possible and easy to understand.

7. Make training materials and specifically satellite/video training more interactive.

Recommendations:

A. **Question and answer** format.
B. Provide additional **MACT standards** satellite/ video training.
   - One MACT standard per video.
C. When possible, **film on-site** at regulated facilities, to demonstrate how to perform required MACT compliance activities.
D. Make video presentations **more interesting**, by using state-of-the-art, **color graphics**.

Appendix E

Contacts List
Participants in the National Specialty Workshop on Technical Tools for Air Toxics Assessment

CONTACTS LIST FOR THE PARTICIPANTS IN THE
NATIONAL SPECIALTY WORKSHOP ON TECHNICAL TOOLS FOR
AIR TOXICS ASSESSMENT

June 17-20, 1997

Name	Agency	Phone	Fax	Email	Area of Expertise*
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Brian Haugstad	IA DNR	515-281-4927	515-242-5094	bhaugst@max.state.ia.us	Air Toxics Policy Development Rules Writing, Education and Outreach
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Alan Huber	EPA NERL	919-541-1338	919-541-1338	huber.alan@epamail.epa.gov	Human Exposure Air Toxic Models

Name	Agency	Phone	Fax	Email	Area of Expertise*
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Peter R. Kahn	Region 1	617-860-4392	617-860-4397	kahn.peter@epamail.epa.gov	Air Toxics Monitoring
Aimee C. Kennedy	WV DEP	304-558-1213	304-558-1222		Air Emissions from Hazardous Waste Combustion
Steve Kish	MI DEQ	517-335-4794	517-335-3122	kish@deq.state.mi.us	Modeling
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Thomas McCurdy	US EPA	919-541-5774			Exposure/Intake Modeling
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Michael Pokorny	MD DEP	410-631-3232	410-631-3202		Air Toxics Regulation/Implementation/ Modeling/Inventories
Greg Pratt	MN PCA	612-296-7664	612-297-8701	gregory.pratt@pca.state.mn.us	Dispersion Modeling, Exposure Assessment, Environmental Fate of Air Pollutants
Bob Ragland	Forsyth County	910-727-8060	910-727-2777	raglanre@co.forsyth.nc.us	Point Source Emission Inventories and Point Source Modeling

Name	Agency	Phone	Fax	Email	Area of Expertise*
Tom Rogers	FL DEP	904-921-9554	904-922-6979	rogers_t@dep.state.fl.us	Air Dispersion Modeling
Andrew J. Roth	RAPCA	937-225-4118	937-225-3486	rothaj@rapca.org	MACT/Air Toxics/Modeling
Dom Ruggeri	TNRCC	512-239-1508	512-239-1123	druggeri@tnrcc.state.tx.us	Air Pollution Meteorology, Dispersion Modeling
Tom Shanley	MDEQ/AQD	517-335-7056	517-335-3122	shanleyt@deq.state.mi.us	Deposition Modeling
Thomas Shoens	Wayne County	313-833-3596	313-833-3561	tshoens@co.wayne.mi.us	Air Toxics, Source Sampling, Air Monitoring
Jeffrey Sprague	IL EPA	217-524-4692	217-524-4710	epa2102@epa.state.il.us	Dispersion Modeling, Receptor Modeling
William K. Steinmetz	NCDEHNR AQ	919-715-7713	919-733-1812		Ambient Monitoring
Andrew Stewart	WI DNR	608-266-5499	608-267-0560	stewaa@dnr.state.wi.us	Air Toxics Policy Development, General Point of Contact Engineering Evaluation
Stanley C. Tracey	DC Air Resources	202-645-6093	202-645-6102	tracey@mail.environ.state.dc.us	Title V/112(r) Regulations
John White	NC DEHNR AQ	919-715-6285	919-733-3340	john_white@aq.ehnr.state.nc.us	Dispersion Modeling
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Appendix F

Workshop Evaluation Summary

Workshop Evaluation Form

National Specialty Workshop on Technical Tools for Air Toxic Assessment, June 17-20, 1997

Please take a few minutes to complete this evaluation of the workshop. We will use your feedback to improve workshops in the future. Thank you!

1. Overall, I found the workshop to be:

circle one

1	2	3	4	5
very beneficial		somewhat helpful		a waste of time

2. The workshop sessions that were most helpful are:

   These sessions were better than others because:

3. The workshop sessions that I liked the least were:

   These sessions were not very helpful because:

4. I found the duration of the workshop to be:

circle one

1	2	3	4	5
too long		about right		too short

Comments:

5. If I were in charge of this workshop, I would have done the following differently:

6. The role of the panel discussions in the workshop was:

circle one

1	2	3	4	5
very beneficial		somewhat useful		not very useful

Comments:

7. Job Title/Specialty: _____ Years of experience: _____

8. Please add any additional comments or suggestions you wish to share:

Workshop Evaluation Form

National Specialty Workshop on Technical Tools for Air Toxic Assessment, June 17-20, 1997

1. Overall, I found the workshop to be:

circle one

1	2	3	4	5
very beneficial		somewhat helpful		a waste of time

↑

Average Response: 2

2. The workshop sessions that were most helpful are:
   These sessions were better than others because:

- All workshop sessions were helpful. The most helpful speakers were those that addressed specific tools or specific projects that were done.
- The most helpful information included how different stated do their own studies and policies and what they have done to apply/respond to air toxics issues and air toxics regulations.
- Those speakers presenting new and unreleased information, i.e., EFIG, TOOLS, AERMOD, were helpful because they provided fresh information to keep ours heads up about in the future. In particular, dispersion modeling and exposure assessment sessions were educational and gave an idea of what is coming down the pipe and who are experts in the field.
- The emissions inventory, exposure assessments, and dispersion modeling sessions were the most helpful sessions. The speakers were better able to communicate their information. Also, the problems/deficiencies were brought out in the open and discussed somewhat.
- The exposure assessment session was helpful because it provided for shorter, but concise discussions. The discussions were more coherent than others. The technical presentations were clear and informative. Mike Zelenka's presentation was helpful because he gave the basic tenets of the field so those not in the field could gain a basic understanding.
- The dispersion modeling session was helpful because the discussion was more general. It was easy to relate their strong and weak points.
- Presentations made by John Irwin, Greg Pratt, Anne Pope, Martha Keating, and Mike Zelenka were exceptionally helpful.

3. The workshop sessions that I liked the least were:
   These sessions were not very helpful because:

- The least helpful sessions were those that were general overview topics. The Elements of OAQPS air toxic program was not helpful because it was shallow. It should either have been shortened or removed, as it was not very helpful.
- The ambient air modeling session was not as helpful because the material presented (i.e., listing methods) was not clearly explained and should have been presented as a handout instead. Some presentations were too technical. There did not seem to be any issues that need immediate attention.
- Some sessions were not as helpful because they got very technical and were bogged down with very specific details that did not have wide encompassing themes that applied to States. The very technical sessions and panel sessions used terms that are not familiar and were often less organized and informational.
- The air toxics emission inventories sessions seemed to start in the middle.

4. I found the duration of the workshop to be:

circle one

1	2	3	4	5
too long		about right		too short

↑

Average response: 2.7

Comments:

- Perhaps a bit too long.
- Needed to schedule in breaks!
- We have brought out a lot of issues. Is there a plan, other than submitting comments to upper management, to seriously address these issues?
- The length of the workshop totally (3½ days) was good.
- I think the next workshop could be only two days. An additional two days could be used for information transfer.

5. If I were in charge of this workshop, I would have done the following differently:

- Had more breaks, sessions with out breaks were too long.
- Not a thing - very well organized.
- Better organization of panel discussions, provide more time for open discussion.
- The panel conference calls needed to be more focused with the product in mind and the intent/needs clearly defined and implemented.
- Fewer but more detailed talks.
- Shorten the length of time for speakers to 20-30 minutes.
- After workshop social functions - not necessarily formal, but dinner or a ball game would help to increase interaction.

- I would have preferred more time allotted for "give and take" between the panels and the audience. It might have been helpful if each panel had more time for internal discussion.
- Direct focus of presentations on State roles or new air toxics policies.
- Would have each State/local give status of current toxics program. .
- Have the meeting at a hotel to avoid transportation issues. Plan a ice breaker meeting the evening before the formal meeting begins or the first evening of the meeting.

6. The role of the panel discussions in the workshop was:

circle one

1	2	3	4	5
very beneficial		somewhat useful		not very useful

↑

Average response: 2.7

Comments:

- Panels could have more focused on brainstorming or long term goal setting/improvements/action (follow up).
- Panel discussion sessions were not very helpful because we could read the summaries.
- Panels were a lot of work for State and local participants. Please improve communication about goals.
- The panel discussions are essential to a dialogue between feds and States. State opinions should be voiced.
- The panels need more mix so that all the experts are not on the same panel. This defeats the purpose of having comments from the audience.
- They were helpful to open lines of communication between States. Gets you more involved and interested.
- The panels turned out to be just additional individual presentation. A panel that actually debates an issue among themselves may have been better.
- Seemed to bring up many issues that related to all State and local situations. Would like to see a summary in writing of panel discussions.

7. Job Title/Specialty, Years of experience:

- Permits Manager, 19
- Chemist/AirTox, 25
- Engineer, 11
- Modeler/Engineer, 15
- EPS/Permits SMACT, 5
- EI, 20+
- Research Scientist/Dispersion Modeling, 15
- Emissions Inventory, 6

- Environmental Engineer, 5
- Staff Epidemiologist, 3
- Modeling, 2
- Engineer, 3
- Modeling, 5
- Environmental Engineer, 1
- Environmental Scientist/Modeler, 5
- Hazardous Air Pollution Analyst, 6
- Hazardous Waste Combustion Engineer for Air, 3
- A.Q. Modeling, 17
- Engineer/Ambient Air Monitoring, 14
- A.Q. Modeling, 5
- Envt. Prot. Spec III/Modeling, 9
- Environmental Engineer, 9
- Toxics Unit Manager/Regulatory Implementation, 11

8. Please add any additional comments or suggestions you wish to share:

- It would have been helpful to have time set aside before the meeting began for the panel members to meet and finalize their comments. It was too much of a push to have a meeting in the day. Policy issues would be good for the next meeting. Some talks were too technical (jargon). The greatest benefit of the workshop was the opportunity to network with others with different expertise/responsibilities. Perhaps consideration should be given to smaller breakout sessions.
- Appreciated opportunity to attend and see other's viewpoints.
- This is the most productive workshop I've attended so far.
- I hope the issues raised and communication and dialog between the various disciplines can be kept alive until resolution and not allowed to fizzle after this conference and the communication lines remain open.
- Overall, an excellent forum for discussing and evaluating the available tools for air toxics assessment. I learned a great amount about this area and welcomed the opportunity to relay my concerns and experiences to other people working in this field.
- Overall, I found the workshop to be worthwhile. With a few minor changes, it should become an ongoing workshop/training session.
- The workshop was well organized and appeared to be well attended by the State and local agencies.
- A fairly successful workshop. I came to gain information and feel like I've gained quite a bit.

Appendix G

Contacts List
EPA Air Regulations and Enforcement and Compliance Assurance

CONTACTS LIST FOR THE EPA AIR REGULATIONS
AND ENFORCEMENT AND COMPLIANCE ASSURANCE
(current as of June 1997)

Phone #	OAQPS Contact	Regulation	OC Contact	Phone #
919-541-2452	Jim Szykman	NSPS Subpart A: General Provisions	Sally Mitoff Belinda Breidenbach	(202) 564-7012 (202) 564-7022
919-541-2837	Steve Fruh	NSPS Subpart CC: Glass Manufacturing		
919-541-5264	Walt Stevenson	NSPS Subpart Ca: Emission Guidelines for Large MWC Units		
919-541-5264	Walt Stevenson	NSPS Subpart Cb: Sulfuric Acid Plants		
919-541-5264	Walt Stevenson	NSPS Subpart Cbb: MWC Rules		
919-541-2421	Martha Smith	NSPS Subpart Cc: Emission Guidelines & Compliance Times for MSW Landfills		
919-541-5265 919-541-5426	Rick Copland Jim Eddinger	NSPS Subpart D, Da, Db, Dc: Boilers	Chris Oh	(202) 564-7004
919-541-5251	Fred Porter	NSPS Subpart E: Incinerators	Joyce Chandler	(202) 564-7073
919-541-5264	Walt Stevenson	NSPS Subpart Ea: Municipal Waste Combustors	Joyce Chandler	(202) 564-7073
919-541-5264	Walt Stevenson	NSPS Subpart Ebb: Municipal Waste Combustors		

Phone #	OAQPS Contact	Regulation	OC Contact	Phone #
919-541-5446	Joe Wood	NSPS Subpart F: Portland Cement	Scott Throwe	(202) 564-7013
919-541-5435	Bill Neuffer	NSPS Subpart G: Nitric Acid Plants	Jeff Kenknight	(202) 564-7033
919-541-		NSPS Subpart H: Sulfuric Acid Plants	Dawn Banks-Waller	(202) 564-7034
919-541-5025	Mary Johnson	NSPS Subpart I: Hot Mix Asphalt Facilities	Scott Throwe	(202) 564-7013
		NSPS Subpart J: Petroleum Refineries	Tom Ripp Dan Chadwick	(202) 564-7003 (202) 564-7054
919-541-5416	Mark Morris	NSPS Subpart K, Ka, Kb: Storage Tanks	Everett Bishop	(202) 564-7032
919-541-2364	Kevin Cavender	NSPS Subpart L: Secondary Lead Smelters	Jane Engert	(202) 564-5021
919-541-0881	Eugene Crumpler	NSPS Subpart M: Brass & Bronze	Jane Engert	(202) 564-5021
919-541-5289	Phil Mulrine	NSPS Subpart N, Na: BOF	Maria Malave	(202) 564-7027
919-541-0881	Eugene Crumpler	NSPS Subpart O: Sewage Treatment Plants	John Dombrowski	(202)564-7036
919-541-0881	Eugene Crumpler	NSPS Subpart P: Primary Copper Smelters	Jane Engert	(202) 564-5021
919-541-5602	Al Vervaert	NSPS Subpart Q: Primary Zinc Smelters	Jane Engert	(202) 564-5021
919-541-2364	Kevin Cavender	NSPS Subpart R: Primary Lead Smelters	Jane Engert	(202) 564-5021

Phone #	OAQPS Contact	Regulation	OC Contact	Phone #
919-541-2837	Steve Fruh	NSPS Subpart S: Primary Aluminum Reduction	Jane Engert	(202) 564-5021
919-541-5515	David Painter	NSPS Subpart T, U, V, W, X: Phosphate Fertilizer	Cletis Mixon Steve Howie	(202) 564-4153 (202) 564-4146
919-541-1084	Juan Santiago	NSPS Subpart Y: Coal Preparation	Chris Oh	(202) 564-7004
919-541-1512	Conrad Chin	NSPS Subpart Z: Ferroalloy Production	Jane Engert	(202) 564-5021
919-541-5289	Phil Mulrine	NSPS Subpart AA: Steel Plants, EAF	Maria Malave	(202) 564-7027
919-541-5289	Phil Mulrine	NSPS Subpart AAa: Steel Plants, EAF & AOD	Maria Malave	(202) 564-7027
919-541-5427	Jeff Telander	NSPS Subpart BB: Kraft Pulp Mills	Maria Eisemann	(202) 564-7016
919-541-2837	Steve Fruh	NSPS Subpart CC: Glass Manufacturing	Scott Throwe	(202) 564-7013
		NSPS Subpart DD: Grain Elevators	Ken Harmon	(202)564-7049
919-541-2379	Mohamed Serageldin	NSPS Subpart EE: Surface Coating, metal furniture	Scott Throwe	(202) 564-7013
919-541-5263	Sims Roy	NSPS Subpart GG: Stationary Gas Turbines	Chris Oh	(202) 564-7004
919-541-5446	Joe Wood	NSPS Subpart HH: Lime Manufacturing	Scott Throwe	(202) 564-7013

Phone #	OAQPS Contact	Regulation	OC Contact	Phone #
919-541-2364	Kevin Cavender	NSPS Subpart KK: Lead Acid Batteries	Jane Engert	(202) 564-5021
919-541-5435	Bill Neuffer	NSPS Subpart LL: Metallic Mineral Processing	Keith Brown	(202) 564-7124
919-541-0859	Dave Salman	NSPS Subpart MM: Surface Coating, Auto	Suzanne Childress	(202) 564-7018
919-541-5515	David Painter	NSPS Subpart NN: Phosphate Rock	Cletis Mixon Steve Howie	(202) 564-4153 (202) 564-4146
919-541-5515	David Painter	NSPS Subpart PP: Ammonium Sulfate Manufacturing	Scott Throwe	(202) 564-7013
919-541-0859	Dave Salman	NSPS Subpart QQ: Graphic Arts, Rotograve Printing	Ginger Gotliffe	(202) 564-7072
919-541-5305	Dan Brown	NSPS Subpart RR: Pressure Sensitive Tape & Label Coating	Seth Heminway	(202) 564-7017
919-541-2379	Mohamed Serageldin	NSPS Subpart SS: Surface Coating, Large Appliances	Scott Throwe	(202) 564-7013
919-541-5261	Gail Lacy	NSPS Subpart TT: Surface Coating, Metal Coil	Scott Throwe	(202) 564-7013
919-541-1084	Juan Santiago	NSPS Subpart UU: Asphalt Roofing	Andrew Cherry	(202) 564-5011
919-541-0837	Dave Markwordt	NSPS Subpart VV: VOC leaks, SOCMI	Jeff Kenknight	(202) 564-7033
919-541-5261	Gail Lacy	NSPS Subpart WW: Surface Coating, Beverage Cans	Scott Throwe	(202) 564-7013

Phone #	OAQPS Contact	Regulation	OC Contact	Phone #
919-541-5397	Steve Shedd	NSPS Subpart XX: Bulk Gasoline Terminals	Julie Tankersley Peter Bahor	(202) 564-7002 (202) 564-7029
919-541-5427	Jeff Telander	NSPS Subpart AAA: Woodstoves	Robert Marshall	(202) 564-7021
919-541-5439	Tony Wayne	NSPS Subpart BBB: Rubber Tire Manufacture	Maria Malave	(202) 564-7027
919-541-5608	Bob Rosensteel	NSPS Subpart DDD: Polymer Manufacture	Sally Sasnett	(202) 564-7074
919-541-5305	Dan Brown	NSPS Subpart FFF: Flexible Vinyl and Urethane	Ginger Gotliffe	(202) 564-7072
919-541-0837	David Markwordt	NSPS Subpart GGG: Equipment Leaks, Petroleum Refineries	Tom Ripp	(202) 564-7003
919-541-5608	Bob Rosensteel	NSPS Subpart HHH: Synthetic Fiber	Belinda Breidenbach	(202) 564-7022
919-541-5124	Warren Johnson	NSPS Subpart III: SOCMI, Air Oxidation	Jeff Kenknight	(202) 564-7033
919-541-5397	Steve Shedd	NSPS Subpart JJJ: Dry Cleaning	Joyce Chandler	(202) 564-7073
919-541-0837	David Markwordt	NSPS Subpart KKK: Equipment Leaks, Onshore Natural Gas	Dan Chadwick	(202) 564-7054
919-541-0837	David Markwordt	NSPS Subpart LLL: Onshore Natural Gas	Dan Chadwick	(202) 564-7054
919-541-5124	Warren Johnson	NSPS Subpart NNN: SOCMI Distillation Operations	Jeff Kenknight	(202) 564-7033

Phone #	OAQPS Contact	Regulation	OC Contact	Phone #
919-541-5435	Bill Neuffer	NSPS Subpart OOO: Non metallic Mineral Processing	Keith Brown	(202) 564-7124
919-541-5435	Bill Neuffer	NSPS Subpart PPP: Wool Fiberglass Insulation	Scott Throwe	(202) 564-7013
919-541-5402 919-541-5499	Randy McDonald Elaine Manning	NSPS Subpart QQQ: VOC from Petroleum Wastewater	Tom Ripp Dan Chadwick	(202) 564-7003 (202) 564-7054
919-541-5124	Warren Johnson	NSPS Subpart RRR: SOCMI Reactor Processes	Jeff Kenknight	(202) 564-7033
919-541-5261	Gail Lacy	NSPS Subpart SSS: Surface Coating, Magnetic Tape	Steve Hoover	(202) 564-7007
919-541-5408	Ellen Ducey	NSPS Subpart TTT: Surface Coating, Plastic Parts for Business Machines	Maria Malave	(202) 564-7027
919-541-5435	Bill Neuffer	NSPS Subpart UUU: Calciners and Dryers	Keith Brown	(202) 564-7124
919-541-5305	Dan Brown	NSPS Subpart VVV: Polymeric Coating of Supporting Substrates	Maria Malave	(202) 564-7027
919-541-2421	Martha Smith	NSPS Subpart WWW: MSW Landfills		
919-541-4516	Mary Tom Kissell	NSPS Subpart YYY: VOC Emissions from the Synthetic Organic Chemical Manufacturing Industry Wastewater		

Phone #	OAQPS Contact	Regulation	OC Contact	Phone #
919-541-2452	Jim Szykman	NESHAP Subpart A: General Provisions	Belinda Breidenbach	(202) 564-7022
202-233-9370	ORIA (Office of Radiation & Indoor Air)	NESHAP Subpart B: Radon from underground Uranium Mines	Dan Chadwick	(202) 564-7054
919-541-5602	Al Vervaert	NESHAP Subpart C: Beryllium	Jane Engert	(202) 564-5021
919-541-5602	Al Vervaert	NESHAP Subpart D: Beryllium Rocket Motor Firing	Virginia Lathrop	(202) 564-7057
919-541-0881/ 919-541-5308	Eugene Crumpler/ Illiam Rosario	NESHAP Subpart E: Mercury	Jane Engert	(202) 564-5021
919-541-5124	Warren Johnson	NESHAP Subpart F: Vinyl Chloride	Jeff Kenknight	(202) 564-7033
202-233-9370	ORP	NESHAP Subpart H: Radionuclides from DOE	Joanne Callahan Virginia Lathrop	(202) 564-5009 (202) 564-7057
202-233-9370	ORP	NESHAP Subpart I: Radionuclide Emissions	Joanne Callahan Virginia Lathrop	(202) 564-5009 (202) 564-7057
919-541-5254, 919-541-5262, 919-541-0837	*Jan Meyer, **Rick Colyer, Dave Markwordt	NESHAP Subpart J: Benzene Leaks	Rafael Sanchez	(202) 564-7028
202-233-9370	ORP	NESHAP Subpart K: Radionuclide from Elemental Phosphorous	Joanne Callahan Virginia Lathrop	(202) 564-5009 (202) 564-7057
919-541-2910	Lula Melton	NESHAP Subpart L: Coke	Maria Malave	(202) 564-7027

Phone #	OAQPS Contact	Regulation	OC Contact	Phone #
919-541-5167	S. Fairchild-Zapata	NESHAP Subpart M: Asbestos ·	Tom Ripp	(202) 564-7003
919-541-2837	Steve Fruh	NESHAP Subpart N: Inorganic Arsenic From Glass Manufacture	Scott Throwe	(202) 564-7013
919-541-0881	Eugene Crumpler	NESHAP Subpart O: Arsenic from Primary Copper Smelters	Jane Engert	(202) 564-5021
919-541-5602	Al Vervaert	NESHAP Subpart P: Arsenic	Jane Engert	(202) 564-5021
202-233-9370	ORP	NESHAP Subpart R: Radon from Phosphogypsum Stacks	Joanne Callahan Virginia Lathrop	(202) 564-5009 (202) 564-7057
202-233-9370	ORP	NESHAP Subpart T: Radon from disposal of Uranium Mine Tailings	Joanne Callahan Virginia Lathrop	(202) 564-5009 (202) 564-7057
919-541-5254, 919-541-5262, 919-541-0837	*Jan Meyer, **Rick Colyer, Dave Markwordt	NESHAP Subpart V: Equipment Leaks,	Rafael Sanchez	(202) 564-7028
202-233-9370	ORP	NESHAP Subpart W: Radon from Operating Mill Tailings	Joanne Callahan Virginia Lathrop	(202) 564-5009 (202) 564-7057
919-541-5416	Mark Morris	NESHAP Subpart Y: Benzene Storage Vessels	Rafael Sanchez	(202) 564-7028
919-541-0837	David Markwordt	NESHAP Subpart BB: Benzene from Transfer Operations	Rafael Sanchez	(202) 564-7028
919-541-0884	Bob Lucas	NESHAP Subpart FF: Benzene Waste Operations	Rafael Sanchez	(202) 564-7028

Phone #	OAQPS Contact	Regulation	OC Contact	Phone #
919-541-0164	Barbara Driscoll	NESHAP Subpart GG: Aerospace Man and Rework Facilities		
919-541-2452	Jim Szykman	MACT Subpart A: General Provisions	Belinda Breidenbach	(202) 564-7022
919-541-5254	Jan Meyer	MACT Subpart F-H, The HON	Jeff Kenknight	(202) 564-7033
919-541-5268	Amanda Agnew	MACT Subpart L: Coke Oven Batteries	Maria Malave	(202) 564-7027
919-541-1549	George Smith	MACT Subpart M: Perc Dry Cleaners	Joyce Chandler	(202) 564-7073
919-541-5420/ 919-541-5289	*Lalit Banker / **Phil Mulrine	MACT Subpart N: Chromium Electroplating	Scott Throwe	(202) 564-7013
919-541-0837	David Markwordt	MACT Subpart O: Ethylene Oxide Sterilizers	Karin Leff	(202) 564-7068
919-541-5289	Phil Mulrine	MACT Subpart Q: Industrial Process Cooling Towers	Mimi Guernica	(202) 564-2415
919-541-5397	Steve Shedd	MACT Subpart R: Gasoline Distribution	Julie Tankersley	(202) 564-7002
919-541-0283	Paul Almodovar	MACT Subpart T: Halogenated Solvent Cleaning	Tracy Back	(202) 564-7076
919-541-5608	Bob Rosensteel	MACT Subpart U: Polymers & Resins Group I	Sally Sasnett	(202) 564-7074

Phone #	OAQPS Contact	Regulation	OC Contact	Phone #
919-541-5402	Randy McDonald	MACT Subpart W: Epoxy Resins & Non-nylon Polymides	Sally Sasnett	(202) 564-7074
919-541-2364	Kevin Cavender	MACT Subpart X: Secondary Lead Smelters	Jane Engert	(202) 564-5021
919-541-0837	David Markwordt	MACT Subpart Y: Marine Vessel Loading	Virginia Lathrop	(202) 564-7057
919-541-5672	Jim Durham	MACT Subpart CC: Petroleum Refineries	Tom Ripp	(202) 564-7003
919-541-2363	Michele Aston	MACT Subpart DD: Off-Site Waste & Recovery Operations	Ann Stephanos	(202) 564-7043
919-541-5261	Gail Lacy	MACT Subpart EE: Magnetic Tape Manufacture	Seth Heminway	(202) 564-7017
919-541-2452	Jim Szykman	MACT Subpart GG: Aerospace	Suzanne Childress	(202) 564-7018
919-541-2379	Mohamed Serageldin	MACT Subpart II: Ship Building and Repair	Suzanne Childress	(202) 564-7018
919-541-0283	Paul Almodovar	MACT Subpart JJ: Wood Furniture Manufacturing	Robert Marshall	(202) 564-7021
919-541-0859	Dave Salman	MACT Subpart KK: Printing and Publishing	Ginger Gotliffe	(202) 564-7072
919-541-5608	Bob Rosensteel	MACT Subpart JJJ: Polymers & Resins Group IV	Sally Sasnett	(202) 564-7074

***Indicates the Primary Project Lead**
****Indicates the Secondary Project Lead**

TECHNICAL REPORT DATA

(Please read Instructions on reverse before completing)

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16 ABSTRACT

This report is the final report documenting proceedings and recommendations from the National Specialty Workshop on Technical Tools for Air Toxics Assessment. The workshop was held from June 17 through June 20, 1997 in EPA's Administration Auditorium, 79 Alexander Drive, Research Triangle Park, NC. The purpose of the workshop was to provide a forum for discussion on the technical tools developed by OAQPS, Regional Offices, State and local agencies for meeting the goal of the air toxics program. This interactive workshop included half-day sessions devoted to Emission Inventories, Dispersion Modeling, Ambient Monitoring and Data Analysis, Exposure Assessment, Case Histories, and Education and Outreach as related to supporting the air toxics program.

17 KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air Toxics Program Emission Inventories Dispersion Modeling Exposure Assessment Monitoring and Data Analysis Education and Outreach		

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