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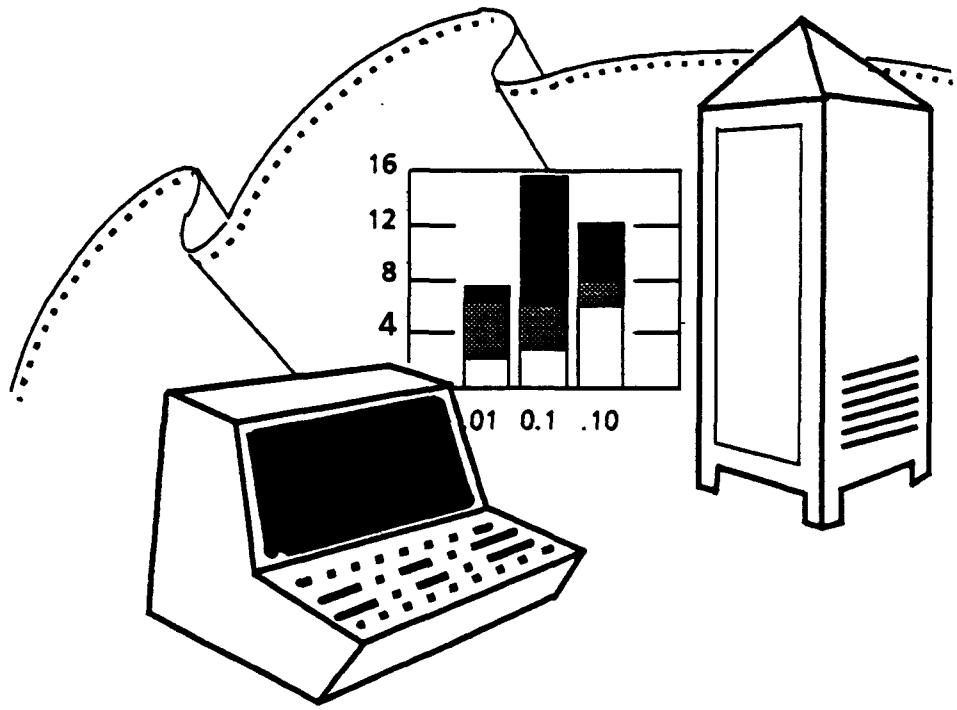
U.S. EPA Workshop to Develop A Simple Model for Acid Deposition

Final Report



U.S. Environmental Protection Agency
Office of Research and Development
Atmospheric Sciences Research Laboratory
Research Triangle Park, NC 27711

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U.S. EPA Workshop to Develop a Simple Model for Acid Deposition

Final Report

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Disclaimer

Although the workshop described in this report has been funded wholly by the U.S. Environmental Protection Agency under Contract 69-02-3839 to Northrop Services, Inc., the report has not been subjected to the Agency's required peer and policy review and therefore does not necessarily reflect the views of the Agency and no official endorsement should be inferred. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Abstract

The Acid Deposition Planning Staff in the Office of Acid Deposition/EPA requested that the Atmospheric Sciences Research Laboratory undertake the development of a low-computational-demanding model suitable for educational use in understanding the linear or nonlinear nature of the acid deposition process and that could assist in constructing a "what if" analysis for a particular situation. In response, ASRL held a workshop, attended by EPA and non-EPA scientists, to discuss the design of such a model. In addition, a five-person working committee of non-EPA scientists was established to write a statement of work for the construction of such a model.

This report summarizes the planning activities that occurred before the workshop, the two days of discussion held at the workshop, and the three days of working committee meetings after the workshop, and includes the resulting statement of work for the creation of a Comprehensive Chemistry Acid Deposition Model (CCADM).

As described in the statement of work, the CCADM should be capable of estimating changes in acid deposition downwind at a receptor site as a function of changes in emissions in a source region. The model would estimate these changes along a fixed trajectory for a fixed set of meteorology-related variables. The model would use the most advanced gas- and aqueous-phase chemistry kinetics modules and an appropriate parameterization of cloud physics. Output from more complex regional-scale Eulerian models could be used as input to establish the context for a CCADM simulation. In addition, the model would include appropriate graphical displays to illustrate and explain acid deposition sensitivity to changes in emissions.

The model is not designed to produce quantitative assessments of acid deposition.

Contents

Acknowledgments

The workshop planners appreciate the time and effort given by the participants and presenters at this workshop. Their contribution made the workshop possible.

This document was written primarily by Harvey Jeffries with significant help from many sources. In producing the meeting background material, Basil Dimitriades, Dennis Trout, Marcia Dodge, Jack Durham and John Clarke, all EPA personnel, participated in several cycles of discussion, review, and revisions of draft material. In addition to Jeffries, the working committee that produced the statement of work consisted of Akula Venkatram, Environmental Research and Technology; Chris Walcek, National Center for Atmospheric Research; Leonard Peters, University of Kentucky; and Hiromi Niki, Ford Motor Co. We are very grateful to the members of this working committee for lending their special expertise and time to this project. In writing the middle chapters of this report, Jeffries used tape recordings of the meeting provided by Barry Mangum, Northrop Services, Inc., as well as extensive notes taken by Marcia Dodge during the meeting. These items were necessary for the accuracy and completeness of the report and we appreciate their availability.

Ms. Linda Cooper, Northrop Services, Inc., made all arrangements for the meeting and with the attendees. Her editorial assistance in producing this report was essential and is greatly appreciated.

Introduction

Origin of Workshop

The Acid Precipitation Act of 1980 (P.L. 96-294) calls for a comprehensive and coordinated program to identify causes and effects of acid precipitation, as well as actions needed to control harmful effects. An Interagency Task Force on Acid Precipitation was established in 1980 to manage this program, with members from 12 Federal agencies, including EPA as a co-chair member. The Task Force has 10 working-level groups, one of which is responsible for Assessment and Policy Analysis research activities. The responsibility of this group includes development of periodic assessments in which available scientific information is focused on policy issues. The information is examined for gaps and uncertainties to identify actions and new research needed. Of crucial importance in such assessments are the availability and use of source-receptor models, that is, models that predict changes in acid deposition from changes in precursor emissions.

Development of source-receptor models for such assessment uses is the responsibility of EPA, and within EPA, of the Atmospheric Sciences Research Laboratory (ASRL) in the Office of Acid Deposition, Environmental Monitoring, and Quality Assurance (OAD). There is a long history of process and receptor model development activities within ASRL that include

- an urban and regional scale three-dimensional Eulerian-type physicochemical model for O_3;
- a simpler, nomogram-type chemical mechanistic model for urban O_3 (OZIPM/EKMA);
- a comprehensive, regional, three-dimensional Eulerian model for acid deposition, and

- an "engineering" model, a simpler three-dimensional Eulerian model for acid deposition.

While the latter two models are intended and expected to fulfill the basic needs of the assessment effort, the EPA-OAD Headquarters staff perceived an urgent need for a simpler, nomograph-type model that would assist in further understanding potential state-level emissions trade-offs for source-receptor relationships in acid deposition assessment issues.

On recommendation from Headquarters, therefore, ASRL undertook the responsibility for completing, by the fall of 1986, an effort that would lead to the development of such a model. This ASRL effort consisted of two tasks. The first, under the direction of Dr. Basil Dimitriades, was to organize and conduct a workshop. In this workshop, alternative development approaches would be identified and discussed with the objective of recommending an approach and producing a scope of work for its implementation. The second ASRL task, under the direction of Dr. Marcia Dodge, was to contract the subsequent development effort for the model.

Workshop Approach

The workshop planning was primarily the responsibility of Dr. Jeffries, a consultant to Northrop Services, Inc., working in conjunction with Dr. Dimitriades, ASRL staff, and members of the Acid Deposition Planning Staff (ADPS) in the Office of Acid Deposition in Washington, D.C. In planning the meeting, Dr. Jeffries chose to follow an approach similar to that in EPA's Data Quality Objectives program, (see EPA Memorandum, 1984, "The Development of Data Quality Objectives") but to adapt these so that they were applicable to the production of Model Quality Objectives.

Model Quality Objectives are qualitative and quantitative statements of the quality of model output needed to support specific decisions or regulatory actions. They are the mechanism for balancing the conflicting demands of time and resource constraints and the need for the model to have acceptable quality and utility.

The objectives development process consisted of a series of exchanges among headquarters decision makers and technical staff to reach an understanding of what was needed and why. In the idealized situation, this process would consist of three iterated phases:

1) the decision maker supplies initial information, from his perspective, in as much detail as possible, about what is needed and why;

2) the technical staff refines the initial concepts through discussion among staff and the decision maker to reach a common understanding of the problem and its constraints; and
3) various approaches are proposed and evaluated for meeting the necessary functions within the constraints.

We began the development process with a verbal explanation of what was desired by ADPS staff. After discussion among ASRL staff, a draft statement was prepared and circulated to all parties. Using a series of written exchanges and discussions, the basic requirements for the model were established. In the latter stages of this process, members of the scientific modeling community were contacted and asked to participate actively in the meeting planning process, and four individuals were selected to form, with the meeting chairman, the working committee. This committee had the primary responsibility for creating the main workshop product, a statement of work for the development of the model.

The four members of the working committee assisting Dr. Jeffries were

- Dr. Leonard Peters, Department of Chemical Engineering, University of Kentucky, coauthor of the STEM-II, a sulfur transport Eulerian model;
- Dr. Chris Walcek, National Center for Atmospheric Research, a member of the Regional Acid Deposition Model development team;
- Dr. Akula Venkatram, Environmental Research and Technology, a member of the ERT team developing ADOM, the Acid Deposition Oxidant Model, for use in Canadian assessment studies; and
- Dr. Hiromi Niki, Ford Motor Company, a chemistry and kinetics specialist.

Organization of Workshop

The workshop was divided into eight 1.5-hour sessions, and each session had one or more discussion leaders. These discussion leaders supplied background information and introduced proposals, hypotheses, and questions. The leaders facilitated discussion and information exchange among participants and assisted the working committee in introducing information needed to develop a statement of work. The workshop was designed so that, initially, researchers active in the acid precipitation field would present material about existing models and about alternative approaches that might be acceptable for meeting the needs expressed by the model quality objectives. Later in the meeting, the various approaches were debated and discussed. Finally, the strengths and weaknesses of each approach were discussed.

The two-day workshop was followed by a three-day meeting of the working committee. In these meetings, an approach was settled upon and a statement of work for its development was produced.

Need and Purpose

This chapter provides the initial background and setting in which the workshop occurred. It presents material concerning the model objectives process as discussed by the Atmospheric Sciences Research Laboratory staff and Acid Deposition Planning Staff before the meeting. This material was available to all participants before the workshop.

Existing or Planned Acid Deposition Models

Regional Acid Deposition Model (RADM)

This National Center for Atmospheric Research (NCAR) model is

> "an Eulerian regional acid deposition model suitable for assessing source-receptor relationships. It will be a modeling framework that integrates a mesoscale meteorological model with a transport and chemical transformation model. All components of this model system are expected to include state-of-the-art representations of the relevant physical and chemical processes. This model, with its comprehensive description of all the currently recognized major physical and chemical processes, makes RADM a suitable tool for research and a scientifically defensible application model. For policy and assessment studies, however, the RADM would need to be streamlined for computational efficiency and to have the representation of the physical and chemical details suitably simplified. A synthesis of the comprehensive RADM modeling result would be required ... to construct a set of fast-turnaround "engineering" models for application."
>
> — from Jan. 1985 NCAR Status Report on the First-Generation Eulerian Acid Deposition Model

RADM is an episodic model—12 synoptic cases have been selected to represent the annual variations—and statistical techniques are being investigated to construct the annual and seasonal deposition.

NCAR Engineering Models

These "engineering" models are simpler, but still three-dimensional Eulerian models. They are presently described as lower resolution models derived from the RADM by simplification and parameterization of the physical and chemical processes important in acid deposition. These EMs will still be large models, having 3 to 5 vertical levels and 160 to 320-km grids, and requiring a small mainframe or large supermini computer for their solution. These models require a series of technical studies before development, including such subjects as parameterization of the nonlinear chemistry; evaluation of computational costs; evaluation of suitable databases for initialization, execution, and evaluation; and testing of statistical ensemble procedures for generation of seasonal and annual averaged deposition.

Need for A Simple Model

The RADM Eulerian model is expected to provide scientifically credible answers to many source-receptor relationship issues such as the degree to which the entire system is "linear" or "nonlinear," and, in selected scenarios, the response of deposition to changes in emissions.

The engineering models, which are closely coupled in development to the full RADM, have simplified representations of many nonlinear physical and chemical processes and thus will not require the large computer resources of the RADM. Many more assessment strategies can be explored with these models than with the more comprehensive, and presumably more correct, RADM model.

Both of these models will be used by EPA to make assessments for sulfur emissions reduction on a state-wide basis. The ADPS is concerned, however, for the time and space scales "where things are linear or nonlinear" and where the states may have trade-off options among VOC, NO_X, and SO_2 emissions. Understanding how these options work and exploring possible alternatives are highly desirable objectives from the viewpoint of the decision maker.

Thus, a tool is needed that would allow a decision maker to explore "what if" and trade-off options. This tool is not seen as an alternative to RADM or engineering models, rather, these options would be variations upon the reductions of sulfur emissions that were predicted by these larger regional-scale models. The basic goal

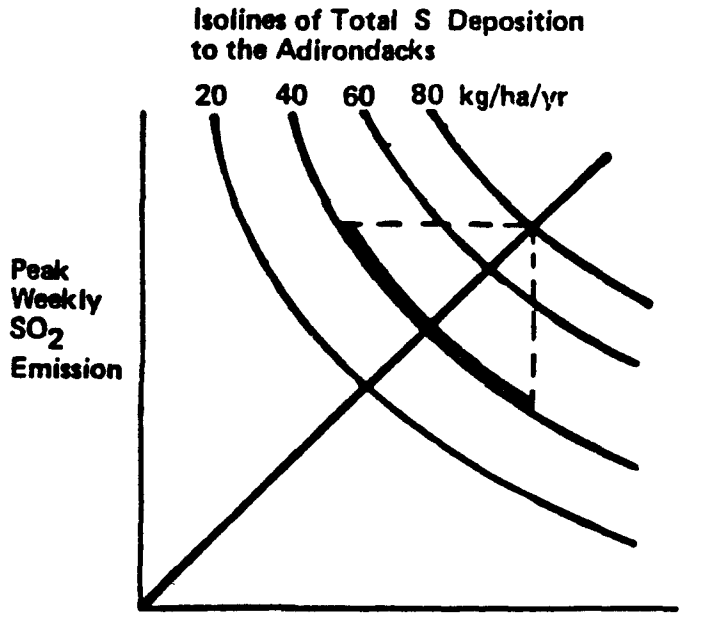

Figure 1.

would be to investigate linearities or nonlinearities in the chemistry, that is, to explore the coupling among NO_X, VOC, O_3, and SO_x chemistry. Ideally, relationships might be portrayed in an EKMA-type nomogram method: one example supplied by the ADPS is shown in Figure 1. The simplicity and intuitive understanding associated with such a pictorial representation of the options is considered highly desirable.

Model Objectives

In pre-meeting discussion among EPA staff and the workshop chairman, a concept of how these different models would be used was described. This concept was further refined into a set of objectives and expected uses for the simple model.

Concept of Hierarchical Application of Models

Each of the models was seen as having a role and scope in its application. The role and scope of RADM follow:

- ▷ to provide complete, state-of-the-art treatment for 12 synoptic events;
- ▷ to be a relatively high resolution regional model;
- ▷ to have intermediately complex chemistry;
- ▷ to be very resource intensive;
- ▷ to calculate seasonal and annual averaged values with statistical ensemble techniques;
- ▷ to be used to verify assessment strategies derived from lower level models; and
- ▷ to provide a foundation for simpler engineering models.

The role and scope of the engineering models follow:

- ▷ to provide faster computation on smaller machines, allowing more strategies to be tested;
- ▷ to be low resolution regional models;
- ▷ to have parameterized chemistry;
- ▷ to be derived from and checked by comparison to full RADM; and
- ▷ to be the primary tools used to calculate state assessments.

The role and scope of the simple model follow:

- ▷ to provide variations of a single state's impact on receptor site for a given episode;
- ▷ to most likely require complex chemistry vs. transport because it must be capable of demonstrating any nonlinearities in local options;
- ▷ to begin with regional model's predictions of needed S-deposition;
- ▷ to provide fast computation on generally available machines;
- ▷ to provide effects of local control on changes in deposition.

Scenario for Assessment

To understand better how these three models might work together, a scenario for a potential assessment was developed for discussion. This scenario has three steps:

- Step 1: an engineering model would be used to calculate regional sulfur deposition. As currently envisioned this would consist of
  - ▷ making calculations for 12 synoptic episode conditions;
  - ▷ computing seasonal deposition by statistical ensemble procedure;
  - ▷ performing cause-and-effect analysis of deposition by
    - ○ analyzing source-receptor relationships for high deposition cases,
    - ○ identifying "worst-case" contributions of sources to key sites, and
    - ○ describing the processes by which each state contributes to sites;
  - ▷ calculating reductions for each state to achieve key site deposition goals;
  - ▷ conducting, and iterating if needed, reduced conditions in the engineering models;
  - ▷ assigning needed sulfur reductions to states.
- Step 2: the simple model would be used to calculate local emissions trade-offs. In this calculation
  - ▷ each key site that would be impacted by state would be treated separately;
  - ▷ conditions would be those giving "worst-case" state contribution;
  - ▷ other states would be assumed to meet their reduction goals; and
  - ▷ the ultimate product would be a set of alternative emissions for VOC, NO_x, SO_2.
- Step 3: the engineering model and/or the RADM model would be used to verify alternatives. In this step:
  - ▷ options for VOC, NO_x, and SO_2 reductions would be input to the regional model;
  - ▷ a new set of calculations would be performed with the RADM or engineering models;
  - ▷ estimated local reductions would be adjusted, if needed, and new values would be calculated.

What Will Be Calculated by the Simple Model?

The model will calculate variations on a *particular* relationship between state emissions and receptor site. In these calculations, the following information would be

obtained:

- The context of the source-receptor relationship would be supplied by regional model data. The initial source-receptor relationship would be supplied to the simple model by the "baseline" run of the regional model. In calculating the possible trade-offs available to a geographical subregion, it would be assumed that the other states or regions that impacted on the site in the same "worst case" episode would reduce their S-emissions as predicted by the EPA assessment.

  All other factors, however, would be the same as the "worst case" baseline run of the regional model. That is, the VOC emissions, NO_X emissions, precipitating and non-precipitating cloud conditions, *etc.*, along the path between the state and the receptor site would be exactly the same as those in the engineering or RADM model "worst-case" episode conditions; the S emissions along the path and outside the state, however, would be reduced according to the EPA assessment for that state.
- The model will provide quantitative predictions of total S-deposition at receptor. These would be produced as a function of VOC, NO_X, and S emissions. Ideally, the model would also provide other items such as total acidit, SO_2 and O_3 concentration, nitrate deposition, and ammonia.
- The model would provide a graphical display illustrating effects of emissions changes.

Expected Use of Model Results

The first use of the model results is expected to be as an *educational tool* to illustrate the extent to which source-receptor relationships may be "nonlinear" and the extend to which "emissions trade-off" might be possible. A later use of the model might be to provide *regulatory assistance* in which a decision maker would perform "what if" analysis for individual states or regions. Eventually, depending upon its utility, the model might be to *explore options* for trade-offs available to a given state.

Ultimate Products or Actions Anticipated

By exploring factors affecting S deposition at key target receptors for each subregional area, the ADPS expects that decision makers would gain a significantly increased understanding of the acid deposition problem.

In addition, because there might be many options available for reducing S deposition impact at a distance site, and because the Federal assessment will only be at a whole-state level, tools are needed to assist in fine tuning the control options.

The ultimate products or actions, therefore, are expected to be an improved understanding of the problem and an evaluation of the control options needed, taking into account the individual situations in each subregion under analysis.

Resource and Time Constraints for the Simple Model

There are important resource and time constraints for this model. In routine applications of the model, it should be able to perform 4 to 10 assessments per day with total computer costs for each assessment being between $50 and $200. Constraints in the development of the model are the necessary completion of full documention and peer review by November 1986. The total cost for developing the model should be less than $240,000.

Model Approach

Model Components: Approaches and Problems

In this portion of the meeting, discussion leaders presented information about model components, describing the factors that would need to be treated in various approaches and discussing the problems likely to arise in each approach.

Chemistry

Dr. Allen Lloyd, ERT, led a discussion of the chemistry component. Jeffries asked Lloyd, "Is the chemistry understood well enough to develop a chemistry component for this model?"

Lloyd responded that gas- and aqueous-phase chemistry are very complex problems and may not be well represented by simple models. He listed areas of gas- and aqueous-phase chemistry that may present potential problems in constructing chemical models (see Table 1). Even the chemistry models in RADM may be quite simple compared to the complexities of the actual chemistry. He stated that the only method for assessing the accuracy of a model was to test it against real-world data.

In the case of radical initiation, Lloyd said, "Although O_3 work shows that we have a reasonable understanding of these processes, experimental data, under careful controlled conditions, do not give us very much faith that we *fully* know what is going on." A similar statement could be made for radical termination processes, which are represented only approximately in many mechanisms for O_3. This is because, until now, we have not been concerned about predicting the products that arise from these termination processes. The major source of hydrogen peroxide (H_2O_2) is a termination reaction of $HO_2^{\cdot}$ radicals. Lloyd believes that the ability of mechanisms to predict H_2O_2 concentrations must be tested with real-world data.

Table 1. Potential Problem Areas In Chemical Models.

gas-phase	*aqueous-phase*
radical initiation	role of H_2O_2, O_3, trace metals
radical termination	free radical chemistry
nighttime chemistry	lifetime of droplet
biogenic HC	liquid water content
slowly reacting species	mass transfer
VOC, NO_X, SO_x relationships	temperature–rates and solubilities
temperature and pressure	

Nighttime chemistry also has not been of much concern because of the typical one-day O_3 applications of the models, but for multi-day simulations an adequate representation of nighttime chemistry will be vital. The role of biogenic HC has been seen as small for one-day O_3 predictions. On a regional scale, however, these sources may be very important in producing H_2O_2 or organic peroxides. Thus, they could be very important regional sources of oxidation. Precise information is not known about these processes.

For the most part, many slowly reacting species have been neglected for the O_3 problem and these can be very important in a regional oxidation scheme. These also may not be well represented in the current chemical mechanisms.

With regard to VOC, NO_X, and SO_x relationships, the VOC-NO_X-O_3 relationships are again reasonably well understood, but the relationship of other oxidants to SO_x is not as well defined. There may be major uncertainties that will make the development of trade-off strategies difficult.

Finally, for the gas-phase, pressure and temperature effects vary as a function of altitude, and, for the multi-layer models, may represent potential difficulties.

In the area of aqueous-phase chemistry, Lloyd said, "Many in this room think that these are completely understood—this is not the case. There are very few experimental data to check the assumptions."

The relative roles of H_2O_2, O_3, and trace metals are still undergoing analysis and simulation. O_3 itself, or free radicals for which O_3 may be a surrogate, are only

partially understood. Radical sticking coefficients are needed. Models have to use profiles and assumptions to represent lifetimes of droplets and liquid water content of clouds.

Data are lacking for many parameters such as gas/aqueous-phase mass transfer and the effect of temperature on solubility and reaction rates.

Clearly, the aqueous-phase chemical component of models must be designed for change. A protocol for testing and providing quality assurance (QA) for rapidly developing chemical submodels needs to be developed.

We need a whole range of sensitivity studies to determine effects of uncertainties in the aqueous chemistry components. In addition, mechanism comparison studies are needed. If different mechanisms are used in each of the models and these mechanisms have different sensitivities, how do we know that, in the same scenario, we are going to come up with the same results. A testing protocol and QA guidance are needed to minimize such problems.

Other sources of potential differences in the chemistry are dry deposition velocities, particle size distributions, and biogenic emissions.

Finally, is there a "best approach" to mechanism condensation, and what will be the method used in RADM?

Lloyd concluded by saying, "The tool you design must be able to accommodate change."

Source-Receptor Relationship

Dr. Akula Venkatram, ERT, led a discussion about establishing a source-receptor relationship. Jeffries asked, "Is there a source-receptor relationship that is quantitfiable, and if you had a model that gave you such a relationship, how would you use it?"

Venkatram said that if you defined a source-receptor relationship in an operational manner as "How much does the receptor concentration decrease when the source is removed?", then the concept does not make much sense in a nonlinear system. He argued that in a nonlinear system, deposition may not be very dependent upon SO_2 source strength, but might be oxidant limited. Thus, in an experiment with the ADOM model, when SO_2 emissions were reduced uniformly by 50%, land regions only saw a 10% decrease in wet sulfate ($SO_4^=$) deposition. Far from the

sources, over the ocean, there was a 50% decrease in wet $SO_4^=$ deposition. The reason given was that the system was oxidant limited, not sulfur limited, and there was excess SO_2 to start.

Workshop participants objected to the limited definition of source-receptor relationships proposed and suggested instead that any source-receptor relationship would be highly context sensitive. The desired source-receptor relationship would be determined by "How many molecules of S deposited at the receptor site came from the source?" In the example used by Venkatram, one source-receptor relationship affected other source-receptor relationships. That is, removing S from one source increased the source-receptor relationships for other sources. This is because oxidizing species that were used by the original source were, in its absence, available for use on other sources, and the system was limited by the availability of these oxidizing species. Thus, any particular source-receptor relationship will be influenced by interactions of other sources along the way to the receptor. This is why Eulerian models are used: they are best able to represent this source-source interaction.

Jeffries asked, "Can the engineering model be used to determine source-receptor relationships?" Venkatram replied that if it was done by removing sources and examining effects at receptors, then no. Walcek said that NCAR was "assuming that the engineering model can apportion sources and receptors at each point in the current model framework' and that "we are assuming that we can define a worse case." Walcek went on, "This apportionment will require many repeated runs of the engineering model to determine the effect of a given source on a given receptor. That is, just because you know that Ohio was contributing 20% of the sulfur to New York, does not tell you what reducing emissions in Ohio will do to reduce sulfur deposition in New York. The model must be run over and over."

Lamb pointed out that what was desired was knowing that 20% of the sulfur atoms in New York came from Ohio, not that changing some source resulted in a 20% change in sulfur deposition in New York. Venkatram said, "But knowing that 20% of the sulfur comes from Ohio is not very useful for a control decision. This is because removing Ohio's sulfur emissions may not change the sulfur deposition in New York at all because the transformation process may be highly nonlinear!"

Walcek again stated that many runs of the engineering model would be required to determine needed controls.

Discussion suggested that the parameterization of the chemistry in the engineering model would have to mimic any nonlinearities that occurred in the use of

the full RADM. There were concerns that this might be a very difficult task. Clarke explained that there are several engineering models envisioned, each designed to work for a different range—there could be 8–10 engineering models. In any case, these models are the tools EPA will used to perform apportionment.

Mixing

Dr. Jack Shannon, ANL, led a discussion on the mixing process in models.

Mixing is caused by turbulence and this is represented differently in all models. The treatments range from almost no mixing to instantaneous mixing. Mixing will be very simple no matter which model approach is used.

Sub-grid processes are very difficult to represent and are very important from a chemical viewpoint. Lamb said that, in the Regional Oxidant Model, the results are entirely different depending upon whether 18-km or 80-km grids are used. (RADM will use 80-km grids.) For example, Shannon said that, in the real world, a point source of SO_2 and a point source of VOC might never meet, but in the model they will meet if they are in the same grid, as illustrated in Figure 2 from a 1983 NCAR report.

A second mixing problem is with representing the effects of vertical mixing and vertical shear. Walcek said that tests on the meteorology model in RADM showed that vertical mixing was critical to the correct calculation of multi-day trajectories.

Clouds and Storms

Dr. Chris Walcek, NCAR, led the discussion on cloud and storm processes.

Walcek said that clouds have four important effects on regional processes:

1) they are very effective vertical mixers of pollutants,
2) they have important radiative effects for photochemical reactions,
3) they provide an aqueous chemical reaction system, and
4) they are effective at scavenging pollutants.

The spatial scale of processes for clouds covers about seven orders of magnitude from microns for droplets to several kilometers for whole clouds. The effects of clouds can be nonlinear.

In describing clouds as vertical mixers of pollutants, Walcek said that the updraft velocities in clouds are several orders of magnitude larger than free air velocities, thus clouds can mix emissions (lower layers) with oxidants (upper layers).

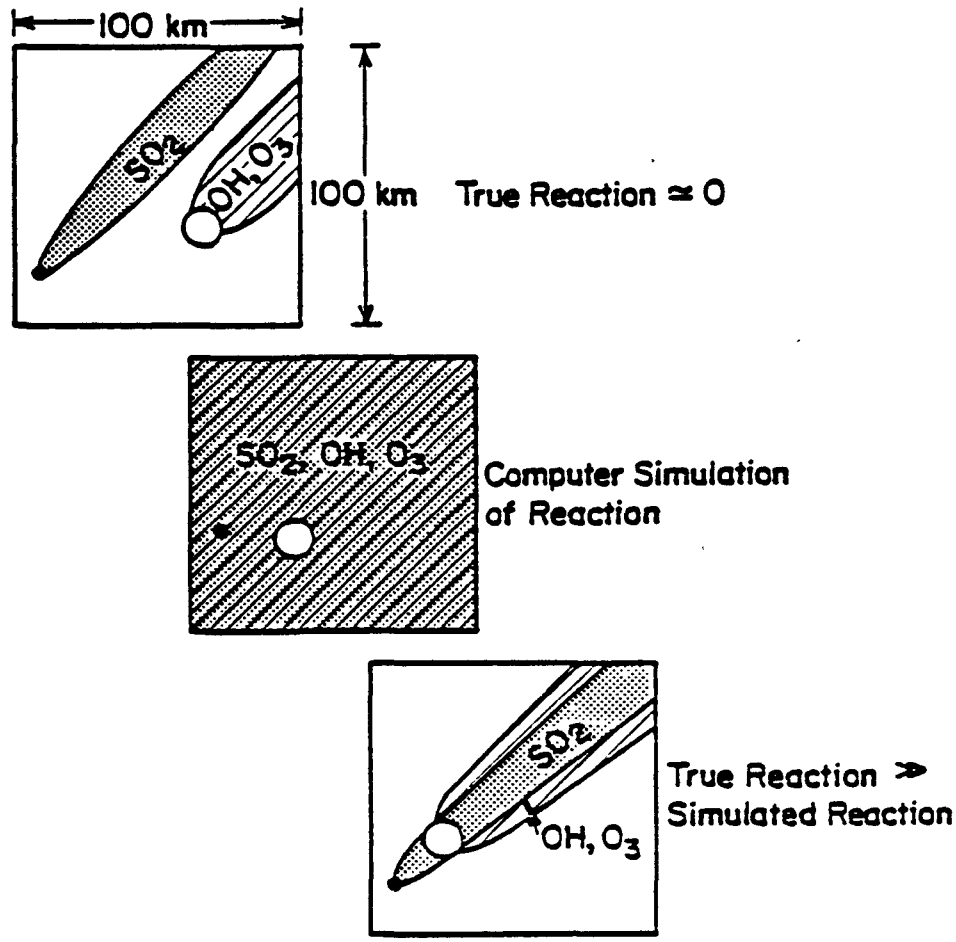

Figure 2. Effect of Grid Size on Chemical Reactions (ADMP, NCAR, 1983).

In the aloft layers, horizontal transport occurs quickly compared to the boundary layer.

Clouds represent a sizable volume of water and thus they can provide an aqueous chemical reactor system. Figure 3 is a summary of the RADM cloud processes routine. Figure 4 is an example calculation of the effect of an individual convective cloud on the distribution of sulfur. It represents one hour of processing of a 6-km deep cloud that covered about 10% of a grid cell area. The numbers attached to the boxes are percent of total sulfur originally below the cloud base. About 25% of the sulfur was processed by the cloud, about 5% was deposited, and 10% was vented above the mixed layer.

In the aqueous chemistry in the cloud, the production of $SO_4^=$ is limited by the oxidant present. Because of oxidant limitations, there can be a very nonlinear relationship between sulfur and oxidant concentration.

At present, most of the cloud physics must be highly simplified or parameterized. For example, cloud vertical velocities may have to be specified based on rainfall rate being slow, medium, and fast. These models generally ignore any feedback effects between the cloud chemistry and the gas chemistry (other than photochemical rate changes).

Although simplifications of cloud processes may be possible, Peters pointed out that, in the VENTEX experiment in 1984, the conversion rates in very similar clouds varied from 2 to 36% per hour.

Emissions

Dr. Leonard Peters, University of Kentucky, led the discussion on emissions information for the simple model.

Peters stated that, based on the desired application of the simple model—to examine potential emissions trade-offs, this model may need more detailed emissions data than RADM, and on a smaller grid than 80 × 80 km. Although we can identify major individual sources, there are many smaller and area plume sources that will be important. Plume interactions become more important, and diurnal variability of emissions is more important for the application of this model.

Lamb described model experiments with the Regional Oxidant Model, which had an urban plume only 10 km wide. In the two-day simulation, a reduction of 32% in HC and 8% in NO_X emissions had a much greater effect on the peak O_3 than

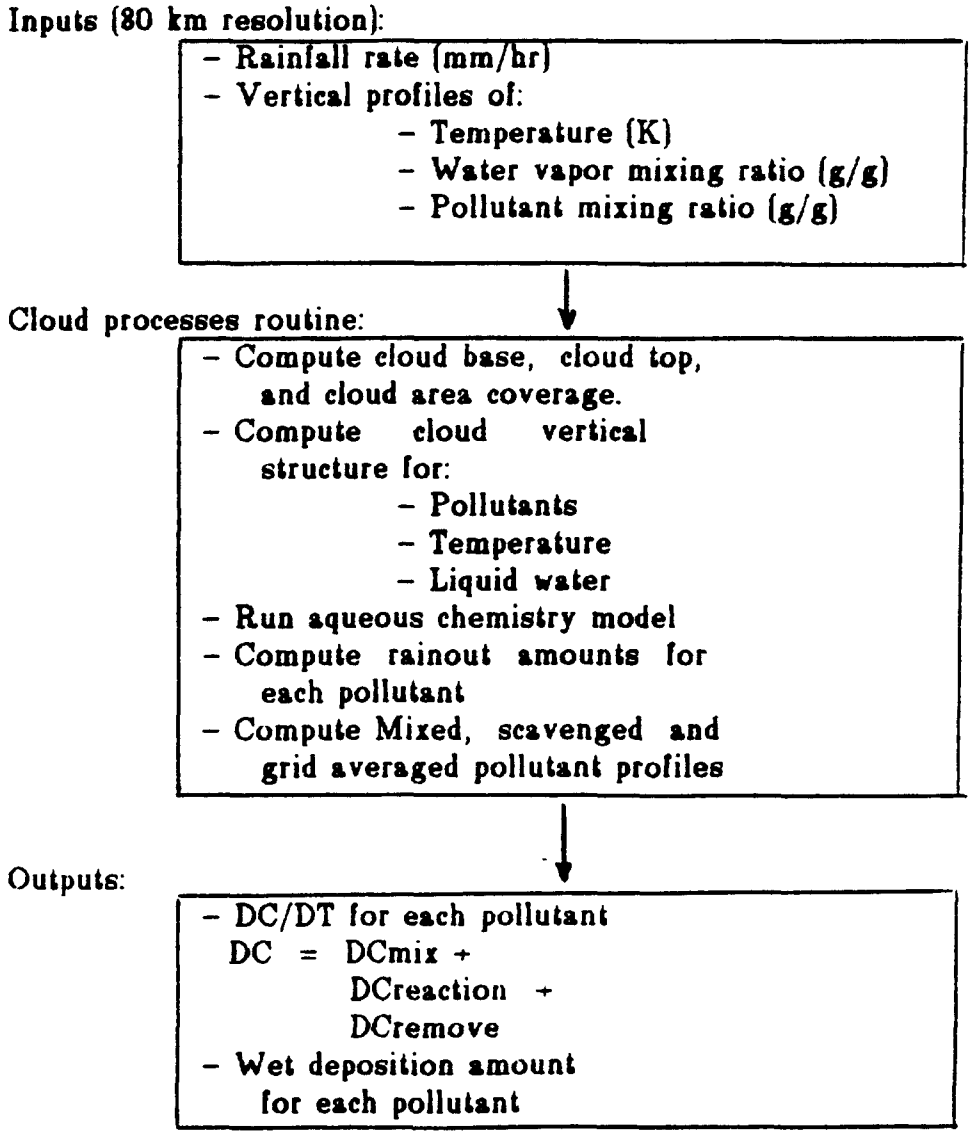

Figure 3. Summary of Cloud Processes in RADM.

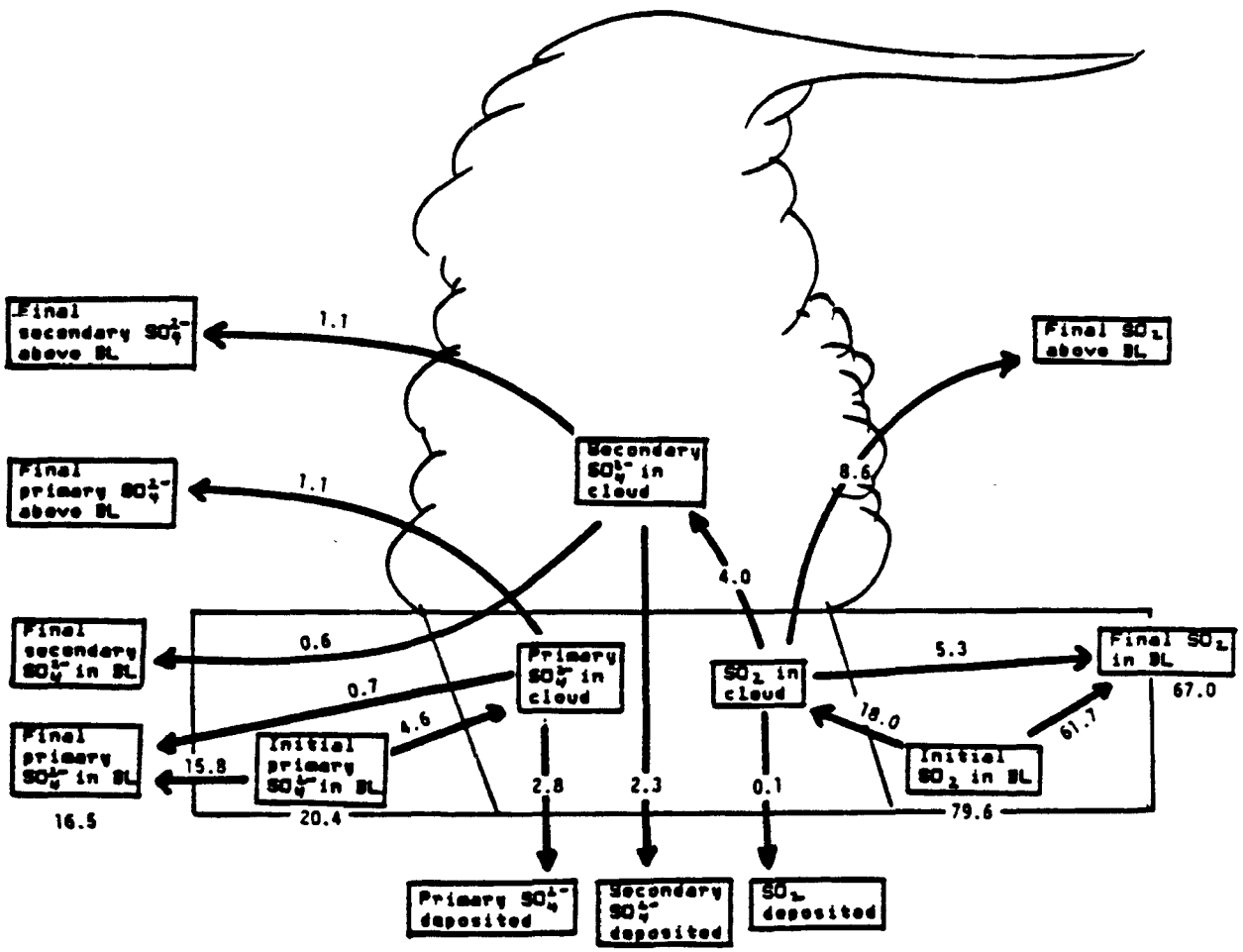

Figure 4. Effect of Cloud Processes on Sulfur Distribution.

on the area wide O_3 average. So, Lamb suggested that, because of the nonlinearity of the chemistry and because large grids smear oxidants out, the grid resolution must be about the size of the urban plumes in the areas under study.

Boundary Conditions

Dr. Venkatram also led the discussion on boundary condition issues for the simple model.

In the pre-meeting material, it was stated that the meteorological and boundary conditions would be supplied by a model external to the simple model, such as the RADM or engineering models. Venkatram saw potential problems in this approach. He questioned whether a box model would work on the scales needed in the simple model. He felt that a critical factor would be the entrainment of material through the sides and top of a simple box model. A good representation must consider vertical motion and wind shear. He felt that to get the initial conditions for the control simulations with a simple box model, the engineering model would have to be run in several specific situations, adopting a state-by-state emissions control, resulting in hopeless combinations of conditions to even approximate the necessary boundary conditions.

Johnson questioned why the simple model had to tie to RADM under any circumstances. Why not have a total stand-alone model? Jeffries replied that the simple model had to give up something to be simple, and if the same emissions, wind fields, and other operational conditions of RADM were not used in the simple model, then extraneous causes of differences in predictions may be introduced. A complex model would be needed to predict transport correctly.

Display of Output

The original request from the ADPS in Washington suggested that some type of "nomograph" display technique be used to illustrate the possible control options (see Figure 1).

Although not seen as directly applicable to this simple model, the manner in which the O_3 isopleth diagram is produced was thought to be of interest. Dr. Gary Whitten, SAI, described how multiple simulations—about 65 individual simulations along the same trajectory—are used to produce an O_3 isopleth diagram.

Although the concept of some type of a graphical display for acid deposition was appealing, no one could describe what would be displayed as a function of what.

Would $SO_4^=$ deposition at a single site be displayed for variations in source VOC and NO_X emissions at constant SO_2 emissions? How would the deposition that occurred in this episode be related to the annual acid deposition at the receptor site?

Approach to the Simple Model

Jeffries presented some observations about likely model approaches based upon pre-meeting discussion. He offered the following observations:

- The simple model most likely will be a derivative of some existing modeling approach. That is, because of time and money constraints, the model will be some form of a statistical-based approach or a process-based approach. Empirical-based approaches most likely are not acceptable because of the limited data on which to base such an approach. Statistical-based approaches might include frequency distributions based on a large number of RADM runs. Process based approaches might include simple Eulerian-type models, such as a two-dimensional approach operated from a three-dimensional database (*e.g.*, STEM II run in x-y mode or in z-x mode). Or they might include a Lagrangian-type model (single cell or vertically resolved trajectory model) operated from a three-dimensional database.
- Statistical approaches applied to engineering model results are probably not adequate as options for simple models because of inadequate treatment of *local* chemistry and details of state emissions in the model.
- In process-based models, chemistry is responsible for $> 80\%$ of the costs.
- The simple model will need a general, large-number-of-species, chemistry module to be able to correctly represent the trade-offs among VOC, NO_X, and SO_2 emissions.
- A process-based simple model must have fewer dimensions than the engineering model because the need for more complex chemistry and because the restriction on size and cost of computer time limit how complex the total representation can be. Even two cells of chemistry will cause significant computation time.

From these considerations, Jeffries proposed that the approach should consist of some type of a process-based, two- or three-dimensional model with most of the meteorological inputs supplied from a complex regional-scale model such as the engineering model or RADM. The model will have to have the ability to deal with fairly complex chemistry.

Participants and working committee members presented various other approaches, including the following:

- because of source-receptor relationship problems, a low resolution engineering model with a reduced domain;
- a Lagrangian model, but not tied to engineering model (because it does not exist), instead the model would be tied to observations, that is, calibrated to observations;
- a trajectory-based Eulerian model, 3 cells wide by 3 cells deep by 10 cells long;
- nomographs derived from hundreds of engineering model simulations;
- a complex chemistry model because acid deposition is really a full oxidants issue and its appropriate treatment would need more than just S transport and deposition.

These proposals will be examined further in the next chapter.

Refinement of Approach

Discussion of Problems

Niki felt that parameterizing the chemistry—which has never been done—was very difficult for the purpose of addressing sensitivity to reduction in VOC, NO_x, and SO_2. Others in the workshop felt that most of the "nonlinearity" was in the gas- and aqueous-phase chemistry and that this would have to be as complex as possible to capture these nonlinear elements. The simple model would not be repeatedly tuned against the RADM, as would the engineering models, and thus it would have to have the ability to utilize the RADM chemistry or other chemistry directly.

It appeared from the resource and computer limitations, that only one cell of chemistry could be accommodated in the simple model, because the nature of the trade-off and nonlinearity issues seems to require a comprehensive, and therefore expensive, chemistry treatment.

Venkatram, Walcek, and Peters argued that boundary condition problems would greatly compromise any realistic assessment performed with a Lagrangian cell model. That is, the source region of interest influences the chemistry of adjacent sources to modify the ultimate impact. The specifications of the one-cell boundary conditions, that is, specifying the inflow of sulfur and oxidants into the cell over a three-day period, would be a very difficult task.

After long discussion, the choice appeared to be between complex chemistry in a single Lagrangian cell using highly parameterized transport or a multibox, but "confined" Eulerian model that treats transport in a more realistic manner, but must use highly simplified chemistry.

The basis of the choice was "What is it going to be used for?"

Venkatram said, "The only way to find the boundary conditions for the one cell would be to run RADM for every source reduction to determine the effect on the boundary condition." Others disagreed. Johnson, for example, cited puff model results. He said, "It has not been shown that there are enough heterogeneities—spatial non-uniformity—in the emissions field to create major problems. There are isolated point sources, but how much non-uniformity do you have to have for it to be a problem? This has not been looked at."

Venkatram seriously questioned that any such simple model would be useful in "calculating control options," and many were concerned that it would be abused. Lamb suggested that the present NCAR engineering models might be the simplest viable model that could be developed.

Jeffries asked, "Do we believe that? That there is no possibility to put together a model simpler than the engineering models that still have utility?"

Kleinman said, "There are two problems: getting the transport right and following the fate of the emitted pollutants. In simple Lagrangian models, you pick a trajectory and in doing so you ignore certain components in the transport, for example, vertical wind shear and vertical motion. But you may indeed have a 'representative' trajectory, although not a trajectory that applies to any one situation. On any particular realization, you are going to be in error. So granted, there are difficulties with the transport. As far as following the chemistry, if you can average the chemical conditions, then your calculations will be satisfactory, except that they will not apply to any particular realization. This is because, if averaging over a domain of influence of emissions is an acceptable procedure, then you will have results which are of interest, although not pertaining to a particular situation. The issue is to demonstrate whether or not you can do that averaging."

Venkatram replied, "The simple approach may be satisfactory for educational purposes, for determining qualitative effects, but as soon as you use it for assessment, these uncertainties become very important."

Johnson added, "If the model suggests big controls, then people want the 'best we can.'"

Jeffries concluded, "In that case, we will compromise. We will take, as a first approximation, the boundary conditions from the baseline run of the RADM and assume that those are the correct numbers. This is better than having to make up the numbers. If we are willing to give up the actual calculation of any control

values using the simple model's predictions, then what difference does it make that these boundary conditions will change slightly when I do my calculation?"

Venkatram commented, "As an educational tool that demonstrates qualitative effects, the approach is satisfactory."

Jeffries added, "It is important for us to decide that if this is a limitation to the approach then we say so. That is, we say 'The approach is satisfactory for this purpose and is not satisfactory for that purpose.'"

Walcek stated, "The purpose is primarily educational and to study and learn about potential trade-offs. This suggests a qualitative type of model that might be used to generate, for example, isopleths of deposition. It is not possible to combine, in one model, both the rigorous, numerically accurate calculation of trade-off effects—which implies high complexity—and an educational and learning tool based on a simple model. We can all learn a great deal from a simple framework."

Kleinman said, "One way to make a model simpler is to ask simpler questions of it. For example, you may get the overall geography wrong, but you might get the overall transformation, mass balance, and nonlinearity correct. You need to be careful of the questions being asked of the model."

Trout added, "The user's guide must put limitations on the simple model applications so that its abuse is decreased."

Summary and Conclusions

The working committee had two potential approaches to consider:

- complex chemistry in a single Lagrangian cell using highly parameterized transport; or
- multibox, but "confined" Eulerian model that treats transport in a more realistic manner, but must use highly simplified chemistry.

In addition, there was a general consensus that it would be highly questionable to use such a simple tool to perform quantitative control calculations. In an absolute sense, the tool will not likely agree with the RADM or observations, but it might be very good in a qualitative sense.

The simple model, however, has a good potential to be an excellent educational tool, not only for the policy maker, but also for the scientist.

Working Committee Meeting

The five-person working committee met for three days immediately after the workshop. This committee debated and discussed the approaches, selected a general approach, and wrote a statement of work for its implementation. The statement of work appears in the next chapter and provides detailed specifications for the model. This chapter provides general insight into the creation of the specifications.

Evolution of the Simple Model Description

The committee chose to stress that the primary use of this tool was educational and not to perform assessments in competition with the engineering models and RADM.

Initial discussion was directed at deciding on the basic approach. The committee discussed, and attempted to draw, isopleths of deposition as functions of various variables. They concluded that this was a difficult task and perhaps did not really illustrate the transformation factors and issues adequately. The committee decided that it was unreasonable to require the contractor to produce such specific diagrams, but that the contractor should spend effort developing adequate display techniques that were suitable for the role of the model as an educational tool. The details of these requirements are given in the statement of work in the next chapter.

The committee felt that, from an educational point of view, there are three areas that must be well represented for the model to be acceptable to scientists:

1) gas-phase chemistry,
2) aqueous-phase chemistry, and
3) cloud physics.

Committee members drew upon their experience with models to estimate that

- cutting the Eulerian STEM model from 10,000 cells to 100 cells would still require 30 minutes to 1 hour for calculations with a small chemical module; and
- one cell in the RADM, with its gas- and aqueous-phase chemistry, requires 30 minutes of VAX time.

These factors, plus points made in the workshop discussion, led the committee to decide that the approach should be based on a simple meteorological, comprehensive chemistry framework. The most likely form of such an approach would be a one-cell Lagrangian model, although other approaches that had similar computational requirements could be proposed in response to the statement of work.

In view of the emphasis, the model was named the Comprehensive Chemistry Acid Deposition Model (CCADM).

Inclusion of Important Factors

Figure 5 is a pictorial representation of the important components of the model. This is a conceptual figure and is not meant to portray the actual elements in the final model. As described in the statement of work,

> "...the model will most likely treat atmospheric transport in a highly simplified, yet reasonable manner. It is also likely that the source-receptor relationship would be established external to the model. Similarly, model inputs along the pathway would most likely be established external to the model."

In addition, the transport processes used in the model must account for lateral and vertical fluxes of material.

In the box, gas-phase chemistry, emissions, and dry deposition occur. To incorporate the cloud processes, we envisioned that the box top would sometimes be in contact with clouds that could extract material from the box, process it (by aqueous chemistry), and return it as rain, or the cloud could vent the material above the box, causing permanent loss of the material. Clouds could also entrain material from above the box as well. In addition to these external clouds, sub-box-scale clouds could also occur within the box. These clouds would process material and return it to the box.

Although described as a "simple model," this model is actually very complex. In addition to creating and exercising the model, the exploration of display methods

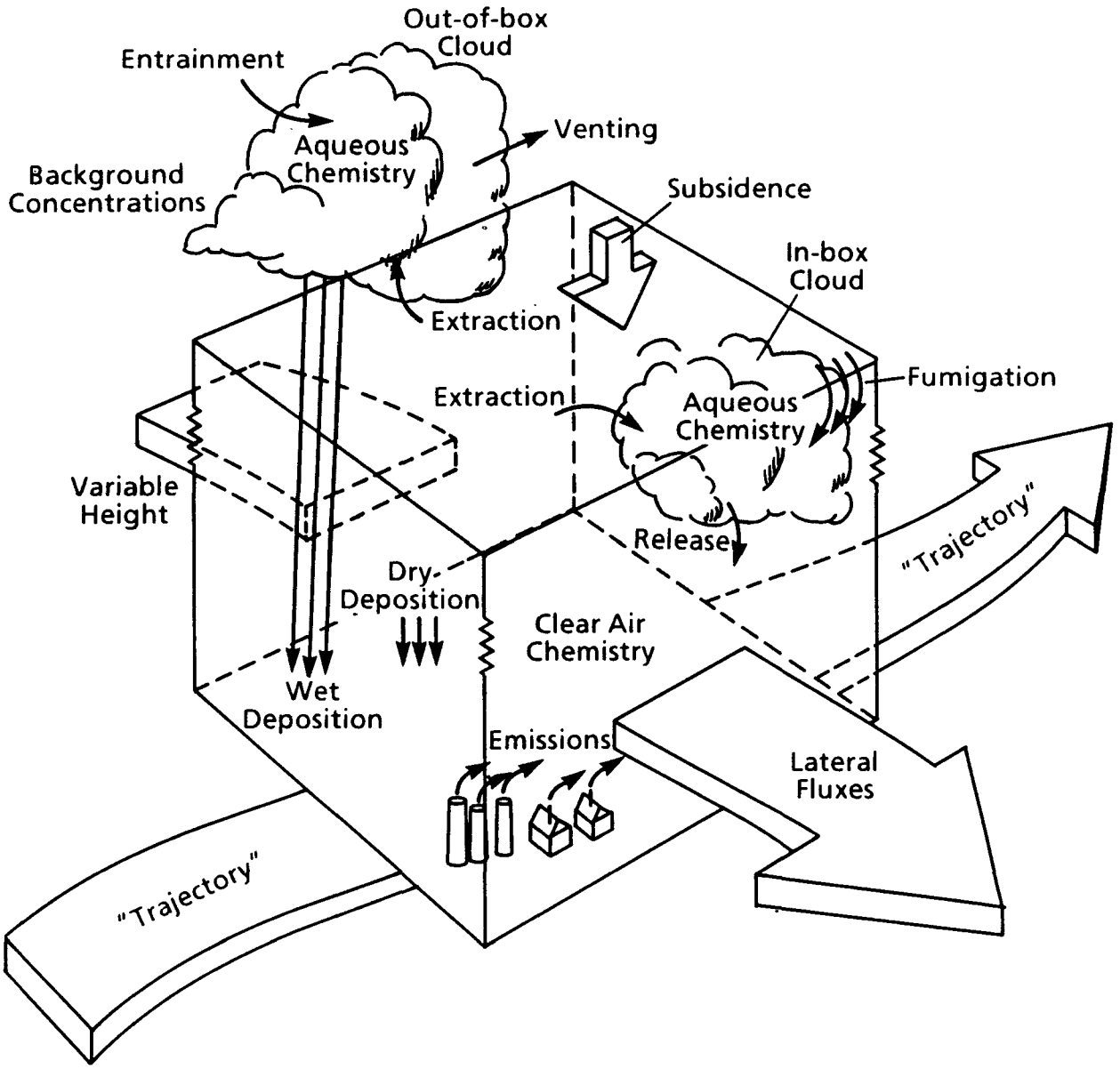

Figure 5. Major Components of the CCASM.

and derivation of long-term deposition estimates from an inherently short-term model were added to the requirements. The total project was seen as being at the upper limit of the time and funds available for the project.

Statement of Work

Title

Development of a Comprehensive Chemistry Acid Deposition Model (CCADM).

Period of Performance

Approximately 12 months.

Background

EPA is sponsoring the development of Eulerian, regional-scale acid deposition models. The Regional Acid Deposition Model (RADM), under development at the National Center for Atmospheric Research (NCAR), is expected to provide scientifically credible answers to many issues related to source-receptor relationships. The completeness and complexity of RADM, however, results in a very large requirement for computer resources, and therefore a series of Eulerian "engineering" models are also under development at NCAR. These will be derived from RADMand designed to use approximations of the complex processes in RADM, especially the chemistry, to produce a simpler, less computationally demanding model for more routine assessment purposes. These models will be the primary tools for assessment of acid deposition issues.

EPA/ORD staff requested that an even less computationally demanding model be designed. This model would be suitable for educational use in understanding the linear or nonlinear nature of the acid deposition process and could assist in conducting a "what if" analysis for a particular situation. It might also be used to design control scenarios for testing in the more complex RADM and engineering models. A workshop, attended by EPA and non-EPA scientists, discussed the design issues for two days. A five-person steering committee of non-EPA workshop

attendees wrote this statement of work for producing a model to meet the majority of the needs originally expressed by EPA staff.

Purpose

The purpose of this work is to produce a computer model that estimates changes in acid deposition downwind at a receptor site as a function of changes in emission in an upwind source region. The model would estimate these changes along a fixed trajectory for a fixed set of meteorology-related variables. The model should use state-of-the-art gas-phase and aqueous-phase chemistry kinetics modules and an appropriate parameterization of cloud physics. It also should include auxiliary programs to convert information from external sources, such as output from more complex regional-scale Eulerian models, into input needed for this model. The model shall be exercised in a series of representative scenarios. Appropriate graphical displays shall be designed to illustrate and explain acid deposition sensitivity to changes of emissions. Some attention should be given to techniques for demonstrating the role of short-term or episodic deposition in producing monthly, seasonally, or annually averaged deposition. A comprehensive user's guide, including test cases that illustrate the processes of producing inputs, running the model, and creating graphical displays shall be produced. In addition, a second document that describes the development of the model and the procedures that should be followed to test and evaluate the model shall be produced.

Specifications of Model

Conceptual Framework

The objective of this effort is to develop a computationally feasible tool for educational use and "what if" analysis related to linearity or nonlinearity of the acid deposition process. To achieve this goal, the model will most likely treat atmospheric transport in a highly simplified, yet reasonable manner. It is also likely that the source-receptor relationship would be established external to the model. Similarly, model inputs along the pathway would most likely be established external to the model. Because nonlinearities of the transformation process are of great interest in the application of this tool, comprehensive chemistry is needed. One concept thought to be adequate for the task is based upon a one-cell Lagrangian framework; other alternative approaches are acceptable if they have similar computer resource requirements. The basic elements of the concept include the following:

- Lagrangian box or column model
- one cell, no vertical shear
  - instantaneously mixed, vertical extent determined by boundary layer height
  - boundary layer should be modeled realistically including nighttime behavior
- box or column area should not exceed 50 km x 50 km
- box top will sometimes be in contact with clouds
  - clouds extract material from box, process it, return it as rain
  - clouds extract material from box, vent it, causing permanent loss of material
- sub-box-scale clouds can occur within box cell
  - clouds incorporate material from box, process it, eventually return material to the box
- gas-phase chemical reactions take place in the box
- aqueous-phase chemical reactions take place in the clouds
- mass transfer occurs between phases
- emissions are added to box as a function of time
- wet deposition occurs from rain in clouds, dry deposition results from uptake of gases and aerosols by the surface
- material is entrained into box from aloft and from sides

Processes To Be Represented in Model

The minimum principal processes to be included are described below.

Chemistry

Both gas- and aqueous-phase processes must be treated.

- Gas-phase photochemical transformation of VOC, NO_X, and SO_2

  The mechanism selected for use should

  - ◇ be comprehensive and state-of-the-art
  - ◇ be fully tested and documented
  - ◇ include temperature-dependent reactions
  - ◇ include important nighttime processes
  - ◇ treat biogenic hydrocarbons

  Suitable candidate chemical kinetics mechanisms include

  a) SAI expanded Carbon Bond Mechanism
  b) ERT Acid Deposition and Oxidant Model mechanism.

- The aqueous phase chemical transformation of SO_2 and NO_X

  - ◇ should be comprehensive and state-of-the-art,
  - ◇ should include mass transfer between gaseous and aqueous phases,
  - ◇ should treat free radical chemistry,
  - ◇ should include oxidation/reduction reactions,
  - ◇ should be updated as new information from laboratory kinetic studies becomes available, and
  - ◇ must predict cloudwater and rainwater composition.

  Suitable candidate aqueous phase kinetics mechanisms are

  a) ERT detailed aqueous-phase mechanism
  b) NCAR RADMmechanism
  c) SAI cloud chemistry mechanism
  d) STEM II cloud chemistry

Deposition

- Dry Deposition

  The approach should use a resistance model framework. That is,

  a) surface resistance values should be derived from the values available in the literature; and

  b) atmospheric resistance, which must be expressed as a function of height, should be derived from micrometeorology.

- Wet Deposition

  Wet deposition can be derived from rainfall rate and predicted rain water composition.

Emissions

Emission inputs are expected to come from existing emissions inventories supplied externally, for example, from the EPRI inventory (1982) or the EPA inventory (1983). In addition,

- the model should have capacity to treat
  - ◇ NO, NO_2,
  - ◇ VOC as up to 10 species and CO,
  - ◇ SO_2,
  - ◇ NH_3,
  - ◇ Soil dust (Fe, Mn, CO_3),
  - ◇ Cl,
  - ◇ biogenic emissions; and
- emissions should be represented as two types:
  - ◇ those associated with the source area, and
  - ◇ those external to the source area along the pathway to the receptor.

Cloud Processes

The model should

- treat at least stratus and cumulus clouds,
- allow precipitating and non-precipitating clouds,
- account for venting by large clouds, and
- include a method for treating the effects of patchiness of clouds.

Entrainment and Dilution Processes

The model should allow:

- diurnally varying boundary layer thickness (box height) including
  - entrainment of material from aloft due to rise of mixed layer,
  - entrainment of material from the sides of the box, and
  - dilution of material in box due to rise of mixed layer;
- for time variable side entrainment; and
- for teh inclusion of entrainment of background air into clouds.

Boundary Processes

The model should include time-variable boundary values aloft and laterally.

Model Inputs

Chemistry Related Inputs

To the extent possible, the chemical mechanism input module should allow the gas-phase and aqueous-phase mechanisms to be changed or replaced in a relatively simple operation, as re-linking modules. Coupling to the emissions input and to the meteorological inputs should be done in as general a manner as is possible.

Meteorological Related Inputs

The minimum meteorological inputs should be

- locations and time of year,
- photolysis rates for the photolyzing species in the chemical mechanism,
- time varying mixing height,
- air temperature,
- time varying boundary conditions aloft and lateral to the box, and
- cloud parameters (inputs to aqueous phase reactor).

  For these cloud parameters, the following parameters must be self consistent and some of the parameters cannot be varied independently:
  - time of occurrence
  - lifetime of cloud
  - lifetime of cloud droplet

- ◇ liquid water content of cloud
- ◇ temperature of cloud
- ◇ freezing level
- ◇ venting or updraft velocity
- ◇ cloudiness, patchiness
- ◇ entrainment
- ◇ rainfall rate
- ◇ vertical and horizontal extent

Emissions Related Inputs

Emissions inputs should be time varying.

Control Inputs

The mimimum control inputs should include beginning and ending simulation times and the range of variation for VOC, NO_X, and SO_2 emissions.

Model Outputs

The normal model output should include displays of deposition of selected species over the pathway and displays of concentrations of selected species over the pathway. In addition, the output should include displays illustrating the importance of processes at selected times.

The model must also include diagnostic output, such as data files for subsequent processing and details of intermediate calculations for QA purposes.

Statement of Work

Task 1–Develop and Submit Detailed Work Plan

Create complete project plan and submit within two weeks after award. Identify algorithms, strategies, and approaches to be used and work needed to implement them. Outline or flowchart major code components. Estimate computer resource requirements both to produce the model and, separately, to run the model in a representative scenario. Identify and plan quality assurance steps. Review and approval by project officer required before proceeding to Tasks 2 and 3. The approved project plan will be incorporated into the work plan.

Task 2–Develop and Test Major Model Components

- ▷ Create model component subroutines
- ▷ Demonstrate correct functioning of model subcomponents

  Each major subcomponent of the model (*e.g.* the cloud chemistry submodel) must be numerically tested and the contractor must demonstrate correct functioning by showing test cases in progress reports. The results of major intermediate calculations must also be demonstrated, *e.g.*, dilution rate profile, NO_2 photolysis rate. Review and approval by project officer required before proceeding to Task 3 and Task 4.

Task 3–Integrate Model Components and Develop Input Processor

- ▷ Create main model computer program
- ▷ Must produce auxiliary programs to assist in calculating inputs

  Create a "user friendly" input processor to assist users in selecting from a collection of "worst case" situations and in modifying the input parameters in a consistent manner. Inputs to this program may come from analysis of Eulerian regional models output (*e.g.*, RADM output), or from observations, or they may be created from climatological/statistical data.

  - ○ Must use a method to assure cloud parameters are consistent by basing the treatment of clouds on one or more of the following methods:
    - ◇ look-up tables consistent with observations and/or
    - ◇ cloud models
- ▷ Project officer's approval needed before proceeding to Task 4.

Task 4–Exercise Model

- ▷ The chemical mechanisms selected for use in these tests must be approved by the project officer
- ▷ Perform limited sensitivity studies:
  - ○ *e.g.*, assess effects of including/excluding side entrainment of material, and
  - ○ *e.g.*, assess effects of excluding the uptake of free radical species by the aqueous phase droplet.
- ▷ Scenarios should include at least the following factors:
  - ○ travel time 1/2 day to 3 days
  - ○ summer and winter seasons
  - ○ path mostly rural and path mostly polluted
  - ○ wet path and dry path
  - ○ non-precipitating and precipitating clouds
  - ○ high background and low background
  - ○ initial starting times varyed.
- ▷ Based on the results for the above scenarios, determine the situations and time scales over which the acid deposition process appears to be linear or nonlinear

Task 5–Assess Feasibility of Deriving Long-term Deposition Estimates

Although the basic model will only provide short averaging time (1–3 hr) estimates of outputs such as S deposition, the contractor should assess the feasibility of producing estimates averaged over episodes (1 to 5 days), months, seasons, and years. This may not be feasible given the nature of the model and its computational requirements, but the contractor is encouraged to investigate the feasibility of deriving such estimates.

Task 6–Develop Display Technique

A graphical display technique should be developed that will demonstrate, in a straightforward manner, the deposition and concentration of sulfur, nitrate, and oxidant at selected points (*e.g.*, day one, day two, day three) in the pathway as a function of VOC, NO_X, and SO_2 emissions from a particular source area. Since these deposition estimates are expected to be highly variable, it would be desirable to see numerous "representative" trajectories analyzed for meteorological conditions associated with dry and wet periods during several seasons. It would also be useful to see estimates of deposition and concentrations along the path of a given trajectory.

Results should be presented in a fashion allowing the user to assess the contribution of the source area of interest to the total deposition in the receptor area and allowing any "nonlinearity" in the process to be readily perceived.

Task 7–Propose Procedures for Testing and Evaluating Model

Propose procedures for testing and evaluating the model against observations and/or regional Eulerian model output (*e.g.*, RADM output) to uncover limitations in model. Such a testing/evaluation would be conducted by an by independent contractor not involved in original development. Testing and evaluation procedures should include testing and examination of the computer code.

Task 8–Documentation of Model

- ▷ Technical Support Document contents
  - ○ Describe the model
    - ◇ Describe all known assumptions and limitations
    - ◇ Describe procedures and algorithms used to produce calculations; include references to sources of algorithms
  - ○ Describe the results of simulations run under Task 4 to exercise the model
  - ○ Describe the time and space scales over which the acid deposition process appears to be linear or nonlinear
  - ○ Describe followup procedures that should be undertaken to test and evaluate the model
- ▷ User's Guide contents
  - ○ Provide instructions on how to run the model
  - ○ Describe procedures to extract the appropriate information from regional models like RADM for use as input information in the CCADM
  - ○ Describe, by example, how a RADM run might be designed based on results obtained with the CCADM
  - ○ Describe computer resources required to run the programs
  - ○ Provide instructions for installing programs on computers
  - ○ Provide block diagrams, flow of control diagrams
  - ○ Provide a definition of every variable in every common statement
  - ○ Provide fully commented code listing

Technical Proposal Instructions

Minimum Qualifications

Experience in acid deposition modeling, cloud chemistry modeling, gas- and aqueous-phase chemistry modeling.

Key Personnel

The on-site personnel must include at least one chemist with experience in gas- and aqueous-phase chemical model development and who will be available to the project on a routine basis. The project team must include expertise in cloud physics, meteorology, and Lagrangian acid deposition modeling.

Computer Programs

Contractor must have existing in-house code for chemical kinetics modeling of the gas- and aqueous-phase chemistry.

Computer Programming Requirements

The model must be supplied to EPA in ANSI standard FORTRAN, preferably FORTRAN77, and it must be designed and coded to run on different machines, at a minimum, the machines are:

- EPA UNIVAC
- IBM 4300-type machines
- DEC VAX

Appendix

A. Discussion Leaders and Topics

B. List of Participants

Discussion Leaders and Topics

Session 1 : Introduction

- Open Workshop
  - ▷ B. Dimitriades (20 min)

    Describe why the workshop is being held, how it was organized. Name the main groups of participants and what role they play.

    Introduce the participants one by one. Each describes affiliation, background.
- Introductory Remarks by ADPS, Washington
  - ▷ D. Trout (15 min)

    Upper level decision maker has broader perspective. Describe, from a policy maker's viewpoint, the type of model needed and why.
- Introductory Remarks by Working Committee
  - ▷ H. Jeffries and Working Committee (20 min)

    Describe the workshop purpose and approach.

    Describe the expected products.

    Describe organization and timing of discussion.

    Individual WC member comments.
- Model Descriptions (35 min)

  This material will provide general information about models that will be discussed frequently in later sessions. For each model, describe
  - ○ Purpose
  - ○ Formulation basis
  - ○ Development process
  - ○ Application methodology
  - ○ Operational Status
  - ○ Costs
  - ▷ NCAR Regional Models (10 min)
    - ○ C. Walcek, NCAR
  - ▷ Canadian Regional Models (8 min)
    - ○ A. Venkatram, ERT
  - ▷ Other Regional Models (8 min)
    - ○ L. Peters, UK
  - ▷ EKMA-type models (8 min)
    - ○ G. Whitten, SAI

Session 2 : Description of Model Objectives

- Concept of Hierarchieal Application of Models (10 min)
  - ▷ D. Trout, ADPS/EPA
- A Scenario For Assessment (20 min)
  - ▷ H. Jeffries, UNC & D. Trout, ADPS/EPA
- What Will Be Calculated by the Simple Model? (30 min)
  - ▷ H. Jeffries, UNC & J. Durham, ASRL/EPA
- Expected Use of Model Results (10 min)
  - ▷ D. Trout, ADPS/EPA
- Resource and Time Constrains (2 min)
  - ▷ H. Jeffries, UNC
- Summary of Background Information (8 min)
  - ▷ H. Jeffries, UNC

Session 3 : Development of Approach

- Assumptions about Approach to Simple Model (10 min)
- Approaches for Model Components (80 min)
  - ▷ Chemistry (10 min)
    - ○ A. Lloyd, ERT
    - ○ H. Niki, Ford
  - ▷ Meteorology (40 min)
    - ○ source-receptor relationship (20 min)
      - ◇ A. Venkatram, ERT
    - ○ mixing (10 min)
      - ◇ J. Shannon, ANL
    - ○ clouds and storms (10 min)
      - ◇ C. Walcek, NCAR
  - ▷ Emissions (10 min)
    - ○ L. Peters, UK
  - ▷ Boundary Conditions (10 min)
    - ○ A. Venkatram, ERT
  - ▷ Display/Analysis of Output (10 min)
    - ○ G. Whitten, SAI

Session 4 : Refinement of Information Needed

- Information Needed in Each Component (90 min)
  - ▷ Working Committee

Session 5 : More Refinement

- Linkage with Regional Model (90 min)
  - ▷ Working Committee

Session 6 : Limitations on Approaches

- What can the model not calculate?
  - ▷ C. Walcek, NCAR
- Are there situations in which results will be poor?
  - ▷ H. Niki, Ford
- What is the range of appliabilty?
  - ▷ A. Venkatram, ERT
- What are estimates of uncertainty?

Session 7 : Performance Criterial and Testing

- What Should the Performance Criteria and Test Procedures Be?
  - ▷ L. Peters, UK

Session 8 : Summary

- Working Committee

Appendix B

EPA Workshop on Development of a Simple Model for Acid Deposition

List of Participants

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