



USAGE OF COMPUTER MODELS IN THE HAZARDOUS WASTE AND SUPERFUND PROGRAMS

**REVIEW OF OSWER'S DRAFT
REPORT ON THE USAGE OF
COMPUTER MODELS IN THE
HAZARDOUS WASTE/SUPERFUND
PROGRAMS AND PROPOSED
PILOT STUDY**





UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

EPA-SAB-EEC-91-016

September 6, 1991

OFFICE OF
THE ADMINISTRATOR

Honorable William K. Reilly
Administrator
U.S. Environmental Protection Agency
401 M Street, S.W.
Washington, D.C. 20460

Dear Mr. Reilly:

The Science Advisory Board (SAB) has completed its review of the Office of Solid Waste and Emergency Response (OSWER) draft report entitled "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs," dated November, 1990, and the proposed OSWER pilot study on model management. The report and proposed pilot project were reviewed and discussed in a teleconference review meeting on December 7, 1990, at which time Subcommittee members conveyed comments to representatives of OSWER's Information Management staff, their contractor and personnel from the EPA Office of Research and Development (ORD).

The Subcommittee finds that the study presented in the draft report was well planned and executed, and was very responsive to the issues raised in the SAB Modeling Resolution. The conclusions drawn in the report are consistent with the data and information presented. Needs for some improvements to the draft report were identified; in particular, the OSWER staff should review the list of models for accuracy of classifications and names, especially where some models are known by multiple names. We also recommend that follow-up work be conducted to improve the overall value of the study. This follow-up work should include the following:

- a. Several case studies illustrating how models were used and applied by EPA personnel,
- b. The models listed in the report should be identified and categorized according to their primary function. This would complement the information provided in the report on the use of the various models in different phases of RCRA and Superfund activities, and
- c. Further consideration should be given to the different levels of education and training needed for different modeling tasks, such as model development, model use, and review of modeling results of others.

The pilot study on model management originally proposed by OSWER was to involve soil contamination models. The Subcommittee felt that the science of



processes affecting soil contamination is not well understood, and that corresponding models are still very much in the research phase. Thus, it would be difficult to obtain what constitutes an acceptable model or set of models for soil pollution problems. As an alternative, the Subcommittee suggested that OSWER consider a study on the use of ground water flow models with possible extension to solute transport models applied to the saturated zone. Ground water flow models have been used in a wide range of applications for a number of years, and several good models are widely accepted as standard tools. The Subcommittee believes that such a study would allow a clearer focus to be placed on the administrative aspects of model management, including procedures for determining whether a model is acceptable for use in a particular application, establishing protocols for proper model validation and application, and mechanisms for education, information dissemination and model user support.

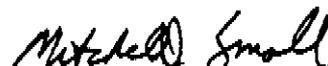
These recommendations are made with the anticipation that OSWER's models management initiative will be encouraged within the Agency. Further, the Subcommittee strongly supports the initiative taken by the OSWER Information Management staff to extend the OSWER activity Agency-wide with a proposed Agency Task Force on Modeling. The SAB views this initiative to be very important, as its proper implementation should lead to the eventual establishment of a formal institutional mechanism with responsibility for review, oversight and coordination of model use within the Agency.

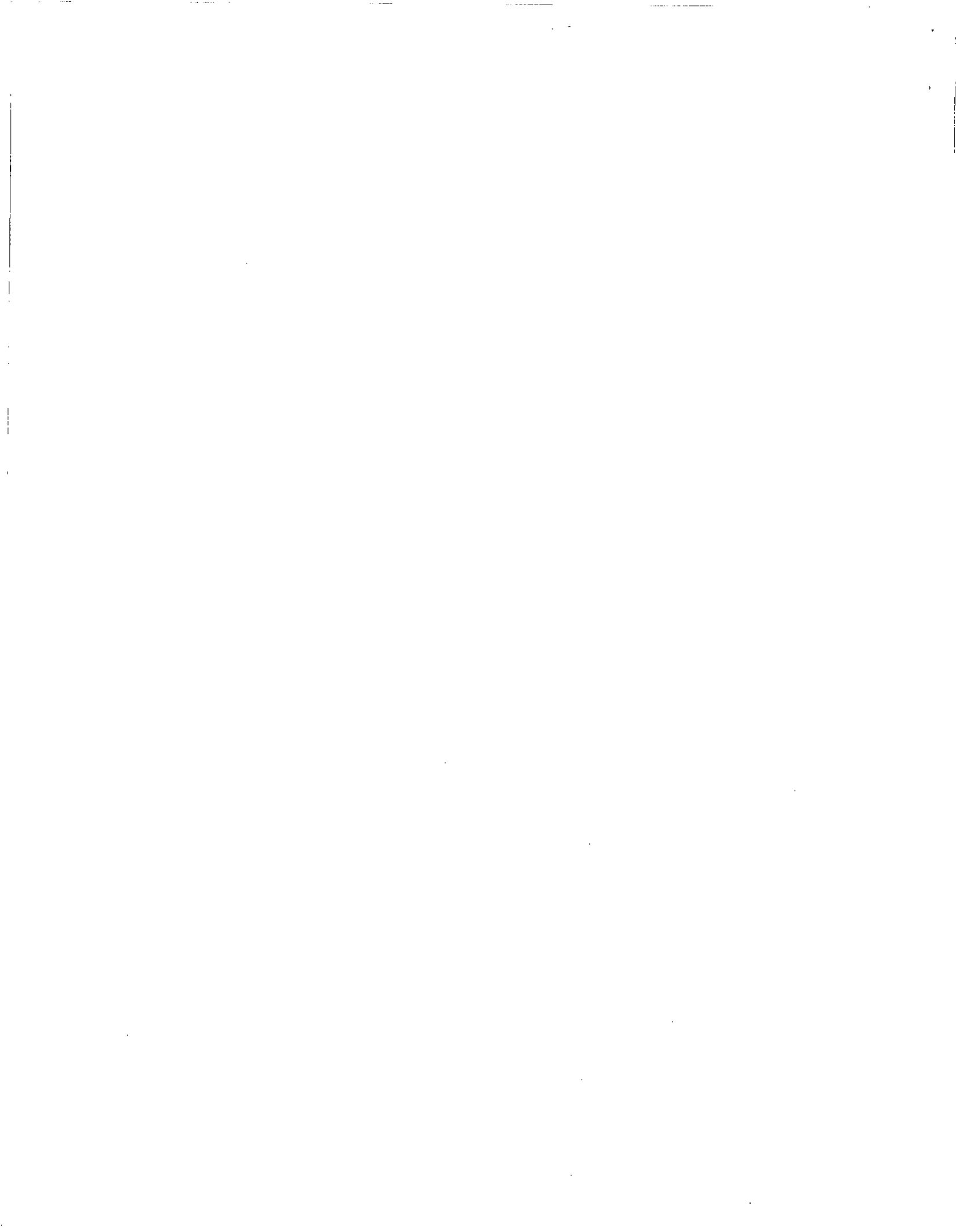
We are pleased to have had this opportunity to be of service to the Agency, and look forward to your response to this report.

Sincerely,


Raymond C. Lochr, Chairman
Executive Committee
Science Advisory Board

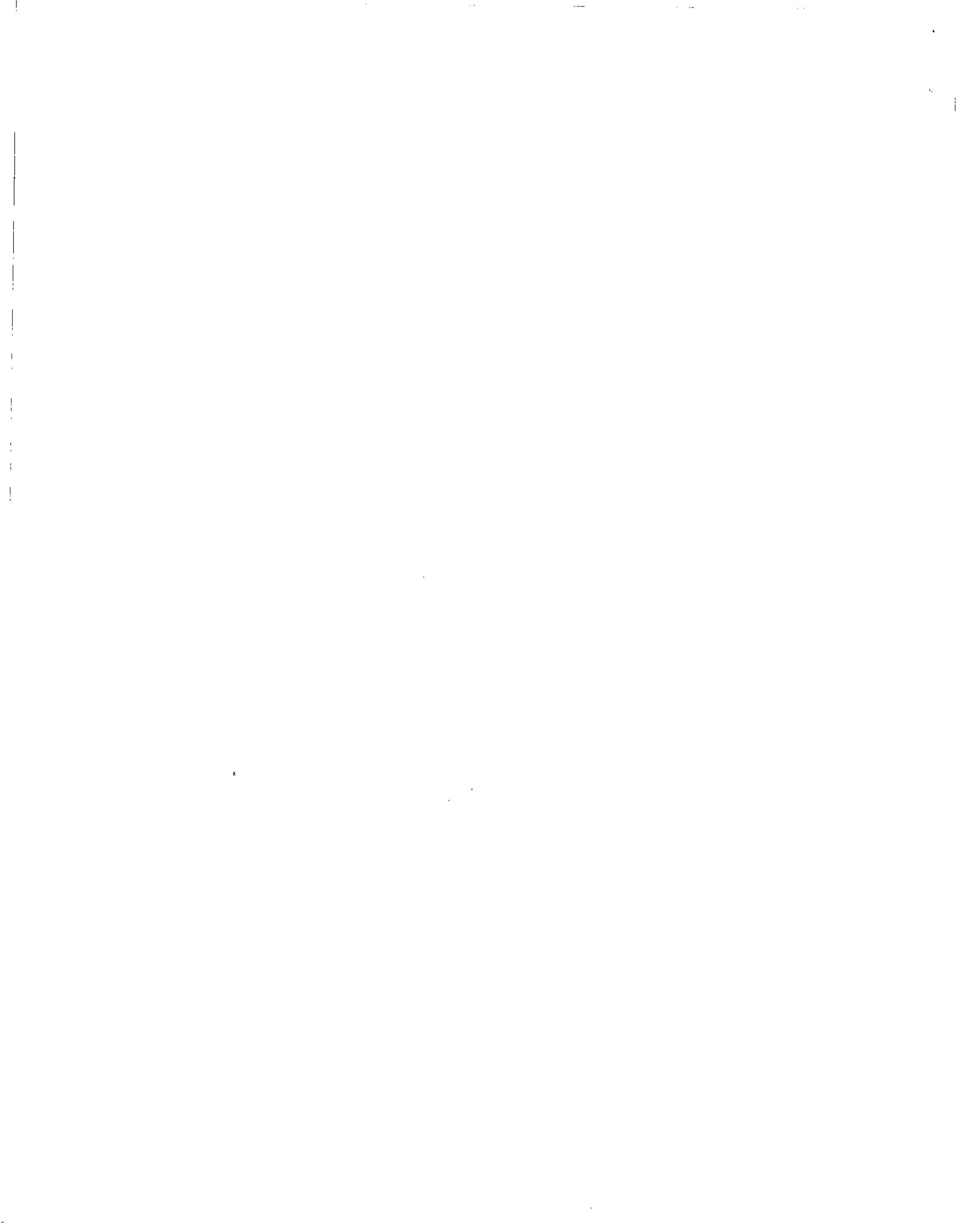

Richard A. Conway, Chairman
Environmental Engineering Committee
Science Advisory Board


Mitchell J. Small, Chairman
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ABSTRACT

The Modeling Project Subcommittee (MPS) of the Environmental Engineering Committee (EEC) of the EPA Science Advisory Board (SAB), has reviewed aspects of the Office of Solid Waste and Emergency Response (OSWER) models management initiative. The review examined OSWER's draft report entitled, "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs," and a proposed OSWER pilot study on model selection and administration.

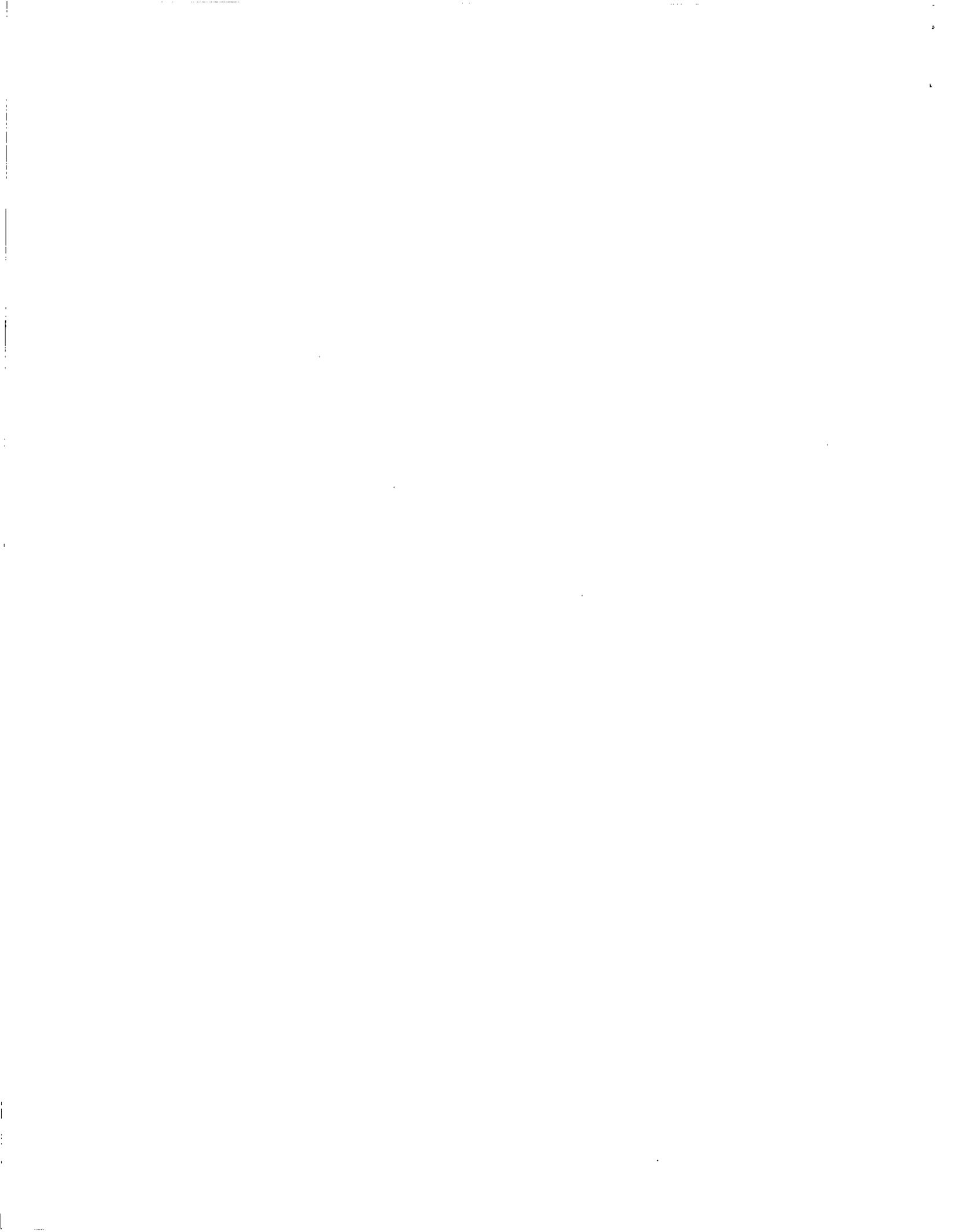
The MPS found that the study presented in the draft report was well planned and executed, and was very responsive to the issues raised in previous SAB reviews and resolutions. The conclusions drawn in the report are consistent with the data and information presented. The MPS suggested a number of improvements to the draft report, particularly regarding the accuracy of models listed and the use of multiple names for a given model.

Also, follow-up studies were recommended, involving case studies of model use in OSWER programs and further consideration of the types of training and education that are appropriate for different modeling activities.

The MPS found that the proposed OSWER pilot study on soil contamination models, while addressing an issue of great concern to the Agency, was probably not well suited as a test case for examining issues in model administration, due to the significant scientific uncertainty and research nature of these models. Rather, a project in a more established modeling domain, such as ground water flow models, was suggested to allow the study to focus better on administrative issues related to model selection and use at EPA.

The MPS strongly supports the model management initiative taken by the OSWER Information Management staff, and endorses extension of the activity Agency-wide through an Agency Task Force on Modeling.

Key Words: Mathematical Models, Superfund, CERCLA, RCRA, Computer Model Validation, Ground Water Models, Soil Contamination



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1. EXECUTIVE SUMMARY

This report provides a review of the EPA Office of Solid Waste and Emergency Response (OSWER) draft "Report on the Usage Of Computer Models in Hazardous Waste/Superfund Programs," and consultative comments on a proposed OSWER pilot study on model management. The proposed pilot study will identify a group of models which serve a particular function and determine the criteria which would qualify them as acceptable for use in EPA programs. This review was conducted by the Modeling Project Subcommittee (MPS) of the Environmental Engineering Committee (EEC) of the EPA Science Advisory Board (SAB).

The MPS found that the draft "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs," represents a very well-planned and executed study of model use in OSWER Programs. Recommendations to improve particular aspects of the report were made, including: inclusion of a summary of the Phase I report (the MPS reviewed only the second phase of the OSWER study); review of the list of models in the report for accuracy of classifications and names of models; and, clarification of the assertion that there is some, though little, model misuse in the OSWER programs. Suggestions were also made for additional work to enhance the study, including: presentation of extended case studies of model use in the OSWER programs; and, further consideration of the types of training and education that are appropriate for different modeling activities, including model development, model use, and review of modeling results developed by others.

Recommendations on the proposed pilot project were made with the understanding that these would depend on the goals and priorities of OSWER in conducting the study. These goals required further clarification. The initial proposal to study soil contamination models addressed a problem area of great interest to the Agency, but required a focus on scientific rather than administrative issues. Important administrative issues that should be addressed in the pilot study include the development of procedures to determine whether a model is acceptable for use in a particular application, establishing protocols for proper model validation and application, and mechanisms for personnel education, information dissemination and model user support. An alternative project in a more established modeling domain, such as ground water flow models, was thus suggested by the MPS to allow the study to focus better on these administrative issues related to model selection and use at EPA.

The MPS and the EEC is pleased to see this effort to study and improve model use and management in OSWER programs, and endorses the eventual extension of the proposed pilot project to consider model use throughout the EPA.

2. INTRODUCTION

The U.S. Environmental Protection Agency (EPA), Office of Solid Waste and Emergency Response (OSWER), has undertaken a study of the use of computer models by EPA. The objective of this study was to identify administrative approaches for promoting a more effective and consistent use of models by the Agency. The OSWER study was motivated, in part, by the U.S. EPA Science Advisory Board (SAB), Environmental Engineering Committee (EEC) "Resolution on Use of Mathematical Models by EPA for Regulatory Assessment and Decision-Making" (EPA-SAB-EEC-89-012) (U.S. EPA, 1989), and focused primarily on model use in OSWER programs. The study results to date are summarized in the draft "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs" (U.S. EPA, 1990). In addition, OSWER has proposed a pilot study on model management that would identify a group of models which serve a particular function and determine the criteria which would qualify them as acceptable for use. This report provides a review of the OSWER draft report and the proposed pilot project by the EEC Modeling Project Subcommittee (MPS).

The EEC received a preliminary briefing on the OSWER project from Mr. Asa R. (Jack) Frost and OSWER staff at its regular meeting on October 26, 1990. The MPS was formed (see the MPS listing in the front of this report), and held a teleconference meeting on December 7, 1990. The Subcommittee was given the charge to evaluate the quality and utility of the draft report, and the appropriateness and scope of the proposed pilot project (See Appendix A for the charge, including a description of the concept of the proposed modeling project, as well as a listing of specific questions for the SAB to consider concerning the proposed modeling project.)

The teleconference began with a short briefing on the project by OSWER staff. The Subcommittee then discussed the study with OSWER staff, contractors, and personnel from the EPA Office of Research and Development (ORD). The following presents the Subcommittee findings on the draft report and the proposed pilot project.

3. REVIEW OF DRAFT REPORT

The Subcommittee finds that the study presented in the draft "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs" was well planned and executed, and was very responsive to the issues raised in the SAB EEC Modeling Resolution. Issues raised in the Modeling Resolution include the need for better management of model selection and use at the Agency, and the need to hire

and support engineers and scientists with modeling development and applications skills. The Subcommittee commends this systematic effort to gather and report information on the use of models by the OSWER program, and finds that the conclusions drawn in the report are consistent with the data and information presented. The Subcommittee recommends some specific ways in which the report can be improved, including:

- a. A brief summary of the Phase I report should be included in the Phase II report.
- b. OSWER and its contractors should review the list of models for accuracy of classifications and names. In particular, some models which are known by multiple names or acronyms appear to have separate listings for each of the names. This should be corrected.
- c. The draft report indicates that "...there have been relatively few incidents of model abuse or mismanagement in the hazardous waste and Superfund program..." Further discussion of what constitutes model abuse or mismanagement is needed, as well as discussion of the factual basis for concluding that some, though little, of this has occurred.

It is also recommended that follow-up work be conducted to improve the overall value of the study for characterizing model use in hazardous waste/Superfund programs. The recommended activities and rationale include:

- a. Conducting several case studies illustrating how models were used and applied by EPA personnel. How were particular models selected and justified for a given application? What difficulties were encountered in trying to use the models? What protocol was followed in the application of the models, particularly regarding peer review of the model formulation, code validation, site-specific validation of the model application and input parameters and model sensitivity and uncertainty analysis? Finally, did the program office get the results and information they were seeking from the model application; did the model results contribute to the ultimate regulatory decision in an effective and timely manner? The case studies could be developed by reviewing the regional office interviews and conducting follow-up interviews to supplement the information. The insights gained from the case studies should be very useful to the Agency for identifying common trends and concerns.

- b. The models listed in the report should be identified and categorized according to their primary function (e.g., ground water flow model, surface water quality model, aqueous chemical speciation model, air quality plume model, etc.), and information provided on the scientific basis for the models and their major assumptions (e.g., conservation of mass vs. empirical statistical relationships, steady-state vs. dynamic). This would complement the information provided in the report on the use of the various models in different phases of the RCRA and Superfund activities. It would also be useful to know if models developed for different media have been used conjunctively; for example, ground water models used to develop a source term for aqueous discharges to surface waters or gaseous emissions to the atmosphere.
- c. Further consideration should be given to the different levels of education and training needed for performing different activities and model tasks. For example, do Agency personnel desire or need: 1) more training in fundamental physical and mathematical concepts underlying models; 2) hands-on experience in the use of models; or 3) skills needed to review model applications by others critically? The study should also consider whether objective measures of modeling skill could be obtained to complement the self-evaluation categories (i.e., expert, knowledgeable, novice) provided in the report. Also, more consideration is needed on the role and use of outside contractors for modeling studies, and how Agency personnel assess their qualifications and review their results.

4. PROPOSED MODEL PILOT STUDY

The pilot study originally was designed as a collaborative study between OSWER and ORD to identify and develop a set of acceptable models for soil contamination in the unsaturated zone. It was noted that the problem of soil pollution is frequently encountered in Superfund site remediation efforts, and regional personnel often inquire as to which models can be used for this purpose. At many sites, the requirement to make timely decisions on soil cleanup plans and cleanup target levels has led personnel to use whatever tools were available, though the models used may not have been appropriate for the particular application. OSWER thus proposed a project on soil contamination models to study how best to manage model selection and use by the Agency, while also meeting the needs of the Superfund program to provide improved tools and guidance for soil cleanup efforts.

The difficulty with the proposed project arises from the limited and preliminary nature of mathematical models for the soil contamination problem. This is due to limited scientific understanding of the physical, chemical and biological processes which influence the level of soil contamination in the unsaturated zone. Considerable research on the soil pollution problem is currently taking place and involves studies of multiphase interactions, vapor phase transport, surface wetting phenomena, complex surface chemistry, and biological growth and uptake in alternatively oxidative and reductive environments. As such, models which can reliably predict levels of soil contamination are still very much in the research phase. As an example, Pennell et al. (1990) found that even for the relatively simple, well-studied case of aldicarb and bromide transport from the top layer of an agricultural field site, "None of the models (CMLS, MOUSE, PRZM, GLEAMS or LEACHMP) accurately described measured solute concentration distributions." Soil contamination problems at Superfund sites are often much more complex than the pesticide application problem examined in the above referenced study of Pennell et al. (1990). Hence, it will be difficult to obtain a broad consensus as to what constitutes an acceptable model or set of models for a soil pollution problem. This does not imply that the study and field validation of soil contamination models is not of vital importance to EPA, but rather that this application area may not be appropriate for a pilot project on model administration.

As an alternative to a pilot project on soil contamination models, the Subcommittee suggested that OSWER consider a study on the use of ground water flow models, with possible extension to solute transport models applied to the saturated zone. Ground water flow models have been used in a wide range of applications for a number of years, and several good models are widely accepted as standard tools (NRC, 1990). Problems occur in identifying appropriate dimensionality and estimating parameter values for a particular site application, especially when there is a high degree of heterogeneity in the aquifer (now recognized to be the rule, rather than the exception), and when fractured media are present. As such, there is a fair degree of uncertainty present as to which model to choose and how to parameterize it in a given application, but it is far less than the fundamental uncertainty in physical principles and basic processes which surround the formulation of unsaturated zone soil pollution models.

The Subcommittee discussed at length the benefits and tradeoffs involved in conducting 1) a pilot study in the newly developing area of soil contamination vs. 2) a study of models in a more mature area with a longer history of model development and testing, such as ground water flow models. The former alternative would require extensive scientific research to investigate processes and test the basic assumptions of models. It would also test the ability to guide model use in a domain with rapidly evolving knowledge, and this often occurs in regulatory problems. The latter alternative would allow a greater focus on administrative issues, including:

- a. evaluating whether models for a given application should be identified as part of an "EPA-approved" list, or rather that only the qualifications of an acceptably validated model should be given, without restricting the selection to particular models;
- b. determining criteria for approval or acceptable validation, such as degree of documentation, ease of application, prior peer-review, and availability of case application-validation studies;
- c. guidance for selecting a particular model from a set which meets acceptable validation criteria, such as availability of options necessary for particular applications and previous experience with the model;
- d. establishing a protocol for proper model application, including adequate documentation of assumptions and results, site-specific validation where appropriate, and model sensitivity or uncertainty analysis;
- e. encouragement of new model development and innovations; and
- f. mechanisms for education, information dissemination and model user support.

Both types of projects would be beneficial to EPA. The former, more scientific study would encourage progress in a particular problem area of great importance to the Agency. The latter study would allow focus on the broader issues of concern relative to model selection and use by the Agency, and may thus be more appropriate as a pilot study of model management. The latter study could also provide an opportunity to explore model selection in highly uncertain and rapidly evolving domains by including applications of ground water flow models in cases with karst or highly fractured aquifer media. A comparative assessment of model management could then be made along a continuum from more established to less established modeling applications. The Subcommittee noted that in order to decide which type of project to choose, OSWER must first establish its study goals and priorities, but that a study of a more established model application area, such as ground water flow models, would be preferred on the basis of what the Subcommittee perceived to be the primary goal of improving model management.

The MPS and EEC recommend that a pilot project be selected that will allow the study emphasis to be placed on the administrative issues of model selection and use. With this recommendation, we endorse the overall concept of the pilot project study and its eventual extension to consider model use throughout EPA. The EEC would be pleased to have the opportunity to review the results of the study as it progresses.

CONCEPT OF THE PROPOSED PILOT MODELLING PROJECT

Background

The Office of Solid Waste and Emergency Response (OSWER) management has been concerned with the growing use of computerized environmental models to support decision-making in the hazardous waste and Superfund programs. Echoing a finding in the Science Advisory Board's Modeling Resolution, OSWER is addressing the need for systematic management of model review, selection and application.

The OSWER Information Management Staff has documented the modeling activities within the Agency, particularly within the Office of Research and Development, and documented model use with the regional hazardous waste and Superfund programs. Its draft "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs" contains recommendations for action in five areas. Those conclusions and their sections in the Report are:

1. training in general modelling concepts (section 4.2);
2. policy statement regarding the use of models (4.5);
3. dissemination of information on acceptable models (4.3);
4. technical support (4.4);
5. Agencywide authority for determining standards for model development, verification, validation, and review/approval procedures. (4.5)

Purpose

The following proposed pilot project addresses two of the recommendations above. There is a need for some initial experience in identifying a number of models which are "acceptable" for use, in order to disseminate that information to the potential users (3. above). There is also a need for some initial experience in determining the criteria for reviewing models for "acceptability" as a prototype for the eventual Agencywide standards (5. above).

Description of Pilot Project

The major activity of the pilot will be to review computerized models for only one area of concern to OSWER (e.g. soil transport and fate). It will be useful to limit the review to an area of modelling where acceptable models are believed to exist and for which the number of existing models is a manageable number for review purposes.

An ad hoc advisory committee will be established to provide guidance to and oversight of the project. If soil transport and

fate modelling is the category selected for review, a high level representative from each of the ORD labs doing research on this topic will be invited to participate. Participants will also include members from: the Office of Environmental Engineering and Technology Demonstration, the Office of Environmental Processes and Effects Research, technical staff from two to three regional waste management programs, staff from each of the Offices within OSWER, Dorothy Canter (science advisor for OSWER), a member from the Office of Water and from the Office of Information Resources Management. The OSWER Information Management Staff will lead the pilot project.

The charge of the Committee will be to define the exact type of modelling to be reviewed and establish a core group of acceptable models of that type. Based upon the characteristics of these models and the expertise of the Committee members, the Committee will then establish criteria for reviewing additional models of this type, to determine their level of acceptability. The Committee will determine whether to list all the identified soil transport and fate models in a data base or to limit the listing to those judged to be acceptable. The Committee will identify the strong points and limitations of each of the models. It will also identify the nature and extent of information to be included in a data base on the models. It will develop a mechanism for the ongoing review of new models and for regular re-review of existing models.

The data retrieval, data development, establishment of and data entry into the data base, and general support functions for the OSWER pilot project will be performed by a support contractor.

The products of the pilot project will include: criteria for evaluating models; comprehensive information about each of the models, including the contact for technical support and previous users of the models; proposed mechanism for ongoing review and approval; and dissemination of information on the models in hardcopy and by electronic bulletin board.

This pilot project will aid the Agencywide modeling authority recommendation (see 5. above) by providing the results of the Committee's determinations regarding model evaluation criteria and procedures. (Note: the SAB has been requested to consult on the initial definition of the charter and action plan of the Agencywide modeling authority, in February 1990.)

QUESTIONS FOR MEMBERS OF THE SCIENCE ADVISORY BOARD
ON THE CONCEPT OF THE PROPOSED PILOT MODELLING PROJECT

The Office of Solid Waste and Emergency Response (OSWER) has written the draft "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs". It documents the results of information gathering regarding the selection and use of models. It also includes conclusions based on the findings.

Questions on the Report

1. Based on the findings in Chapters 2 and 3, do you agree that the conclusions in Chapter 4 are basically correct?
2. Do you believe the issues regarding model selection and use are important enough to warrant the implementation of a number of recommendations ?

One such recommendation has led to this proposal for a pilot project which would be directed by OSWER and would have participants from the hazardous waste and Superfund programs at headquarters and in the regions. ORD laboratories and other media offices, as well as the Office of Information Resources Management, would also participate. The purpose of the pilot project is to identify a group of models which serve a particular function and to determine the criteria which would qualify them as acceptable for use. Information concerning the models, as well as technical contacts, would be disseminated to staff in OSWER programs in the regions and at headquarters.

Questions on the Concept of the Proposed Pilot Modelling Project

1. Is the scope (a core set of models) reasonable?
2. Are the products of the pilot project (core set of models, criteria, procedures, and model information) feasible?
3. Would the products be useful for defining the mission, charter and action plan for the Agencywide modeling group? (See Report, Section 4.5.)
4. Would the products have a beneficial effect on the selection and use of models for the application area (soil transport) by regional and headquarters waste management programs?
5. What suggestions do you have regarding: selection of an initial set of models; participants in the ad hoc advisory Committee; information gathering to support the development of the criteria; other?
6. Would you be willing to consult with OSWER on the results (products) of the pilot project?

APPENDIX B - GLOSSARY OF TERMS AND ACRONYMS

CMLS	CHEMICAL MOVEMENT IN LAYERED SOILS (MODEL)
EEC	ENVIRONMENTAL ENGINEERING COMMITTEE
GLEAMS	GROUND WATER LOADING EFFECTS OF AGRICULTURAL MANAGEMENT SYSTEMS (MODEL)
LEACHMP	LEACHING ESTIMATION AND CHEMISTRY MODEL- PESTICIDES
MOUSE	METHOD OF UNDERGROUND SOLUTE EVALUATION (MODEL)
MPS	MODELING PROJECT SUBCOMMITTEE OF THE ENVIRONMENTAL ENGINEERING COMMITTEE
NRC	NATIONAL RESEARCH COUNCIL
ORD	OFFICE OF RESEARCH AND DEVELOPMENT, US EPA
OSWER	OFFICE OF SOLID WASTE AND EMERGENCY RESPONSE
PRZM	PESTICIDE ROOT ZONE MODEL
SAB	SCIENCE ADVISORY BOARD OF THE ENVIRONMENTAL PROTECTION AGENCY
US EPA	UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

APPENDIX C - REFERENCES CITED

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- 4) U.S. EPA, 1990. Office of Solid Waste and Emergency Response (OSWER), Information Management Staff, "Report on the Usage of Computer Models in Hazardous Waste/Superfund Programs," OSWER Models Management Initiative, Phase II, draft, November 1990.

