VOLUME I

PROCEEDINGS
OF THE
MODSIM'97 USA WORKSHOP

September 22-24, 1997

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Acknowledgments

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We also would like to thank the plenary speakers and the plenary panel speakers: Gerald Boyd, the Deputy Assistant Secretary for the Department of Energy's Office of Science and Technology (DOE/OST); Tom Baca, Program Director, Environmental Management Division, Los Alamos National Laboratory; David McWhorter, Professor of Chemical and Bioresource Engineering, Colorado State University; David Bluck, Simulation Sciences Inc.; Caroline Purdy (DOE/OST); Subhas Sikdar (EPA); Lester Lave (Carnegie Mellon University); Alan Pritsker (Pritsker Corporation); and Jeffrey Holland (DoD).

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EXECUTIVE SUMMARY

Although application modeling and simulation methodologies are widely recognized to be an essential component of a successful endeavor, this is not generally the case in the area of environmental restoration and waste management. Such methods are used, particularly for risk assessment, but their application to decision making for environmental cleanup and waste management is much less recognized and accepted.

In late 1996, the Department of Energy’s Office of Science and Technology (DOE/OST) asked the Environmental Management Program Office (Integrated Science and Technology Program) at Los Alamos National Laboratory to host a workshop that would define the future role of modeling and simulation in addressing global and national environmental problems. This workshop would be designed to answer the question of whether modeling and simulation is important to environmental remediation, waste management, and other environmentally-related activities and to make recommendations accordingly.

Workshop Goals

The four basic goals of the Environmental Management Modeling and Simulation Workshop (the ModSim’97 USA Workshop) were to:

1. Establish the role of modeling and simulation activities in successful environmental cleanup and treatment activities.

2. Establish why the modeling and simulation activities were successful (or failed).

3. Prove the value of further development of modeling and simulation activities.

4. Prepare a report documenting the conclusions and recommendations generated by the workshop participants.

Participants were selected from a large applicant listing that included technical experts from government agencies, academia, industry, and the national laboratories. Scientists from the former Soviet Union, the Republic of China, Poland, the Czech Republic, and Denmark also attended.

Workshop participants could join eight different interest areas: Actinides, Decontamination and Decommissioning, Environmental Security, Health and Ecological Effects, Infrastructure, Manufacturing and Pollution Prevention, Subsurface Contamination, and Waste Treatment. Recommendations from each interest area are discussed in Volume I of these Proceedings, and detailed discussions from each interest area are compiled in Volume II.

Overall Needs/Recommendations

Workshop participants identified four basic needs that have not been addressed sufficiently or successfully by modeling and simulation and offered recommendations for meeting these needs.

1. Incorporation of Modeling/Simulation into Project Planning

Need: Modeling and simulation needs to be an integral part of environmental management projects.

Recommendation: Provide guidelines for management that indicate how modeling should be used during each stage of project planning and execution. Involve both modeling/simulation and field site experts in initial planning. Ensure that risk assessment is a key goal in all modeling. Clearly define goals at the start.

2. A Systems Approach to Modeling/Simulation

Need: The complex relationships among systems (e.g., groundwater, atmosphere, biosphere, manufacturing) generally are not captured in modeling/simulation activities. In general, specific aspects are oftentimes modeled without consideration of the whole.

Recommendation: Promote coupling among systems. In specific site-related planning, promote an integrated risk assessment approach that relies on coupled models. Couple social and economic models to environmental systems.

3. Communication

Need: There needs to be much more effort put into improving communication, and therefore mutual understanding, between decision makers and modelers. Each group needs to communicate its perspective to the other.

Recommendation: Form an interagency working group consisting of decision makers, project leaders, field scientists and engineers, and modelers, with the goal of advising how models can be used in various classes of environmental problems. This working group would be open to international participation so that nations can leverage each other's experience.

4. Limitations and Strengths of Modeling/Simulation

Need: Modeling needs to be represented honestly and fairly in the environmental community.

Recommendation: Increase awareness that modeling and simulation go hand in hand with field data and experiments in solving environmental problems. While being based on some level of observational/experimental understanding of a system, modeling can also further guide and help such work; however, modeling does not replace data. Modeling and simulation always involves some uncertainty, and this needs to be considered in planning. It is important to perform cost/benefit analysis on the use of modeling versus its absence.

Specific Needs/Recommendations by Interest Area

The paragraphs below give one additional specific recommendation from each interest area.

Actinides

- Collect all existing and future site-specific and basic actinide data into one useable and accessible database.

Decontamination and Decommissioning

- Use modeling and simulation to improve business processes by enhancing the flow of information between senior management and individual project management.

Environmental Security

- Establish a set of reference models, validated databases, and performance metrics for use in validating environmental security modeling codes.

Health and Ecological Effects I

- Develop consensus of the public, regulators, and decision makers on risk-based endpoints.

Health and Ecological Effects II

- Gather data for models in a manner that leads to credible input parameters (including uncertainty).

Infrastructure

- Take advantage of new simulation techniques that are well suited to model the behavior of large-scale, nonlinear, complex socioeconomic environmental systems.

Manufacturing/Pollution Prevention

- Adopt an environmental decision support framework that includes objective functions for environmental options, addresses environmental impacts and other regulatory concerns, and incorporates uncertainty and sensitivity into models more effectively.

Subsurface Contamination I

- Improve communication among modelers, stakeholders, management, and regulators by establishing clear and realistic goals and objectives and communicating modeling results, assumptions, limitations, and uncertainties.

Subsurface Contamination II

- Provide incentives for using the best available remediation/modeling technology.

Waste Treatment

- Use modeling to improve the institutional memory of treatment methods and systems.

Section 1. Introduction and Background

The Environmental Management office of the Department of Energy (DOE/EM) is responsible for cleaning up the environmental legacy of the Cold War at DOE sites and formulating and managing strategies that will minimize the impact of ongoing operations. Much of DOE/EM's effort to date has focused on characterizing and remediating existing environmental problems. The question has arisen as to whether increased use of modeling and simulation techniques could play a larger and more effective role in DOE/EM's mission. Could modeling and simulation contribute to making DOE/EM's mission more cost effective, while minimizing risk to workers, the public, and ecosystems?

In order to address these issues, modeling and simulation researchers, users, and decision makers were brought together in a workshop held at the Crowne Plaza Pyramid in Albuquerque, New Mexico, on September 22-24, 1997. This workshop was called ModSim'97 USA. Approximately 200 participants from academia, the government, the national laboratories, and industry attended the workshop. Scientists from the former Soviet Union, the Republic of China, Poland, the Czech Republic, and Denmark were also in attendance. The main sponsor of the workshop was DOE/EM/OST (Office of Science and Technology). Co-sponsors included other agencies with environmental interests: the Department of Defense (DoD), and the Environmental Protection Agency (EPA).

An Executive Committee structured the workshop so that the participants would all be working toward a common goal and yet be able to bring their own ideas to the table. The Executive Committee representatives were from the sponsoring agencies and technical communities, and included a range of skills from managers to researchers. This broad representation allowed workshop participants to look for areas of overlap among the sponsoring agencies. Such overlaps are opportunities for increased efficiency if the agencies can work together to leverage each other's efforts. The Executive Committee members were:

- *Gerald G. Boyd*, Deputy Assistant Secretary (Acting), DOE/EM OST
- *Caroline B. Purdy*, DOE/EM OST (EM-53)
- *Mathew J. Zenkowich*, DOE/EM Office of Waste Management (EM-35)
- *Harry M. Thron Jr*., DOE/EM Office of Environmental Restoration (EM-42)
- *John A. Marchetti*, DOE/Defense Programs (DP-45)
- *Steven V. Cary*, Department of Defense/ODUSD(ES)
- *Heriberto Cabezas*, EPA National Risk Management Research Laboratory
- *W. Lamar Miller*, University of Florida
- *David B. McWhorter*, Colorado State University
- *Alan Pritsker*, Pritsker Corporation
- *Bruce Erdal, Marja Shaner, Greg Valentine, and Ed Van Eeckhout*, Los Alamos National Laboratory

What is Modeling and Simulation?

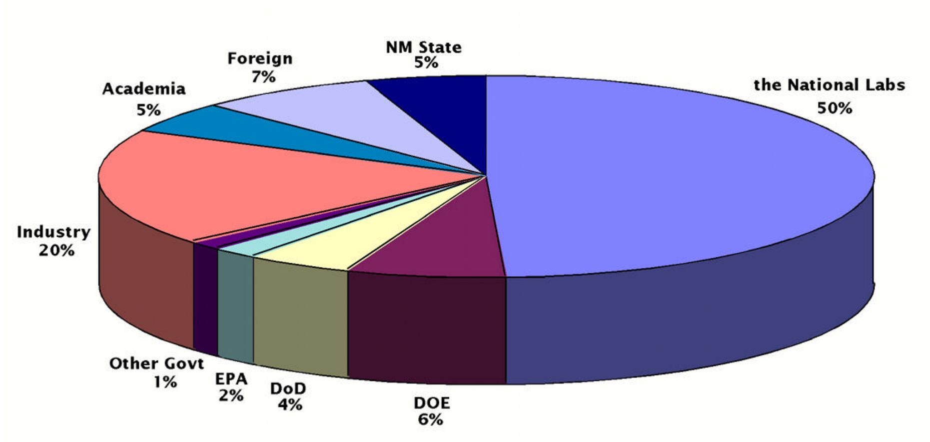
A common theme expressed by workshop participants from all backgrounds and institutions was the need to explain the underlying concepts and uses of modeling and simulation for a broad audience. Communication on modeling and simulation issues too often gets bogged down with technical jargon that decision makers and the public cannot relate to. The general definitions below are based on discussions and plenary talks during the workshop.

· A *model* is a mental, physical, or mathematical construct intended to capture some aspect (or set of aspects) of nature or a process. Models can range from conceptual to quantitative. Conceptual models tend to be based on observations and experiments; they are basically an organized framework of facts and a generalization of knowledge about a process or site. Numerical models, which are quantitative models that solve physical or process equations, work both ways—a conceptual model forms the basis for setting up a numerical model. The results of the model may show areas where uncertainties are high, so that the modelers can in turn refine the conceptual model.

· *Simulation* refers to (1) executing a numerical model (which hopefully produces results that appear to "simulate" nature or the process being modeled), and (2) conducting an ensemble of calculations that are individually quite simple, but when combined capture some aspect of nature or the process (for example, a Monte Carlo simulation). Modeling and simulation aids in the discovery of new knowledge and helps instill a certain level of discipline into field observations and experiments. The latter occurs when results show areas where more knowledge would be most useful, thus minimizing what might otherwise be a "shotgun" (and unnecessarily expensive) project. Modeling and simulation approaches of principal concern to workshop participants are quantitative, mathematical solutions to equations that are implemented on computers.

Structure of the Workshop

The list of workshop attendees is provided in Appendix A. The final breakdown of attendees (201 total) by general category is shown in the figure below:



The workshop spanned three days, beginning with a plenary session on Day 1 that set the stage for further discussions during the rest of the workshop. A summary of the plenary session is presented in Appendix B.

The workshop's Organizing Committee identified eight interest areas of particular interest: Actinides, Decontamination and Decommissioning, Environmental Security, Health and Ecological Effects, Infrastructure, Manufacturing and Pollution Prevention, Subsurface Contamination, and Waste Treatment. These eight areas were designed to cover all the major environmental concerns of DOE, DoD, and EPA. Workshop attendees would center their discussions of these interest areas around business systems, decision support, economics, enabling science, fate and transport, process modeling, analysis and simulation, regulatory and public involvement, risk analysis, and uncertainty.

Following the plenary session, participants were divided into 10 interest area teams to discuss the eight different interest areas. Two interest areas were discussed by two separate groups: Health and Ecological Effects and Subsurface Contamination. In general, the number of participants in each group was kept to a maximum of 25; some teams were a bit larger and some were much smaller. The team discussions began the afternoon of Day 1 and ran through Day 2 of the workshop.

The interest area teams were given a set of 12 questions developed by the Executive Committee members for consideration. Although teams were not required to focus on these particular questions, most teams did direct their attention to them. The questions were:

1. What are the important problems to be addressed by modeling and simulation? Political? Societal? Economic? Environmental?
2. Which questions in this area can be answered with models?
3. What is the size/imminence of this problem?
4. What is the current level of effort toward solving the problem(s)? When is enough enough?
5. Have modeling, simulation, and analysis been used to address problems in this interest area, and if so, which ones and how effectively?
6. What can be done with modeling, simulation, and analysis in this area? (Examples, success or non-success stories)
7. If modeling and simulation techniques are not being used, or not being used successfully, why not?
8. Is there a gap between the development of models and simulation tools and methodologies and their application? Are new models, tools, and/or methodologies needed?
9. Have there been cost/benefit studies for various models and simulation, and analysis tools and methodologies? Do we expect a good payoff if efforts are expanded into modeling and simulation?
10. What modeling and simulation techniques are shared with other interest groups?

11. What are the other benefits that can be obtained from modeling and simulation?
12. What measures can be used for assessing how well modeling, simulation, and analysis are being applied?

On Day 3, the last morning of the workshop, all the interest area teams presented their results in a general forum. In the afternoon, the Organizing Committee met and further discussed gathering the information into a final document.

Structure of the Proceedings

This report consists of two volumes. Volume I synthesizes the major conclusions and recommendations from the 10 interest area groups and includes recommendations, potential interdisciplinary approaches, and problems that can be leveraged across sponsoring agencies. Volume II of the Proceedings provides the list of attendees and interest area team members (Appendix A), a summary of the plenary session (Appendix B), and the detailed proceedings of each interest area (Appendices C-L). These summaries of the team discussions will aid readers who are interested in learning how conclusions were reached.

Section 2. Interest Area Team Summaries of Issues and Recommendations

Paragraphs 2.1 through 2.10 summarize the issues and recommendations presented by each of the interest area teams. Refer to the Appendices indicated for details of each workshop discussion.

2.1 Actinides (see Appendix C)

The area of actinides poses several unique and very difficult problems with respect to modeling and simulation. Actinides, especially the transuranic elements, are characterized by radioactivity which may take the form of several decay mechanisms. These may include alpha, beta, gamma, and neutron decay to daughter products. This characteristic of changing elemental form, and the subsequent potential changes in chemical behavior, pose significant challenges to models that simulate processes, wastes, and storage. In addition, actinides typically require very long time frames, sometimes more than hundreds of thousands of years, to follow the decay chain to final, stable products. In some instances, such as in the case of the Waste Isolation Pilot Plant and other repositories, the time scales are far longer than human experience so their is a heavy reliance on modeling to simulate events that may occur thousands of years hence.

Other issues that contribute to the difficulty in dealing with actinides in the environment are the highly charged political debates typically surrounding nuclear issues and the public perception of risks, which may be totally inconsistent with actual risk.

Recommendations

The Actinide interest area team summed up their discussions and concerns with the following three recommendations:

(1) Collect existing site-specific and basic actinide data and collate the data into an accessible/usable form. Integrate the extensive, but dispersed, DOE and other U.S. activities with international activities. Identify gaps in data, provide database maintenance, and develop coherent funding for these activities.

(2) Form a DOE or interagency modeling/simulation working group that is knowledgeable about existing tools and their applications (existing and potential). This group would serve as a focal point for the collection of documentation on applications and limitations, as well as the development of enhancements and new approaches.

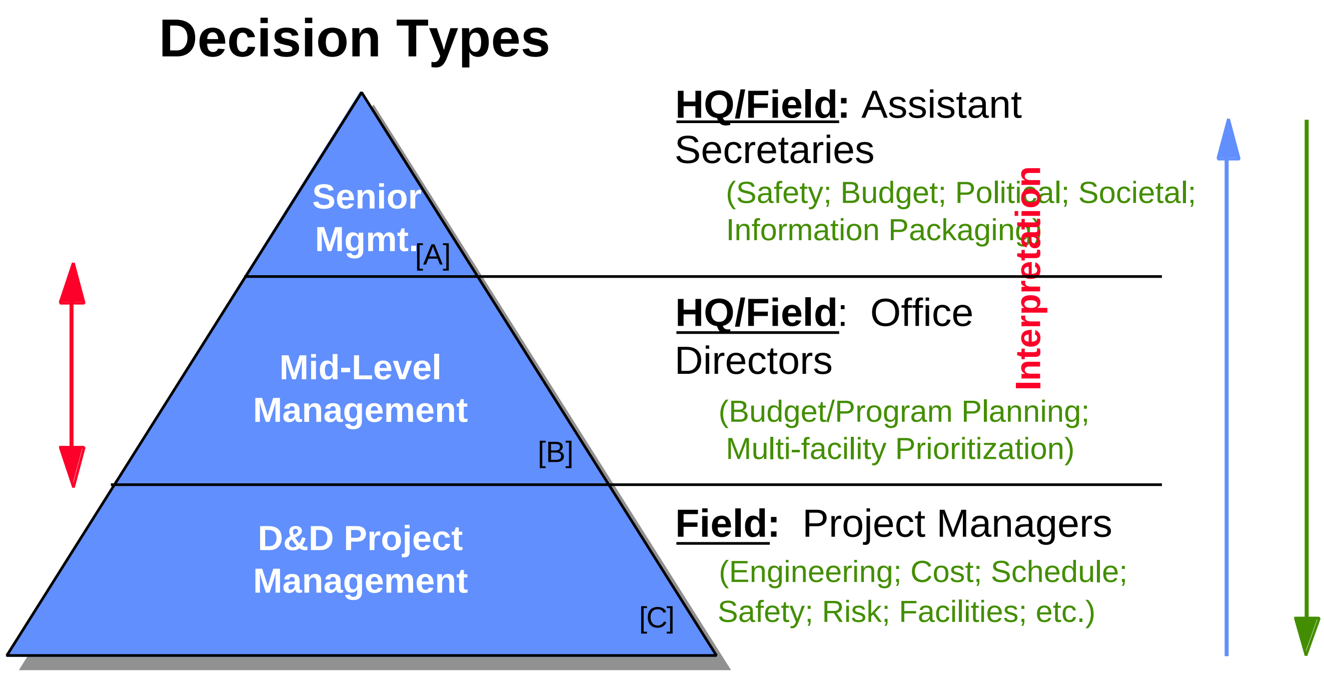
(3) Develop modeling and simulation methods that enhance the flow of information and the development of structured conceptual and decision activities. The development of such methods would enhance communication among user groups (operations, scientists, managers, oversight, and public realms) and among models (from a high level conceptual/decision to detailed processes/unit levels).

The interest area team believed that these three recommendations could be effectively focused through an ASCI (Advanced Strategic Computational Initiative) type activity for environmental modeling and simulation.

2.2 *Decontamination and Decommissioning (see Appendix D)*

The decontamination and decommissioning (D&D) activities are cross-cutting in nature and integrate many of the workshop interest areas, including subsurface contamination, health and ecological effects, infrastructure, waste treatment, actinides, and manufacturing and pollution (e.g., waste minimization, pollution prevention, recycling). Modeling and simulation for D&D must consider economics (life cycle cost and mortgage reduction), safety, environmental impacts, political and stakeholder concerns, risk, regulatory compliance, and a holistic view point (an integration of multiple disciplines). The interest area team determined what decisions modeling and simulation could address within the DOE-EM 2006 planning process and within the planning processes at headquarters, field offices, and facilities undergoing a D&D activity.

The team designed a decision-maker pyramid to define and describe the decisions/planning and communication flows. In this pyramid, shown below, the business or senior managerial level is Level A, mid-level management is Level B, and project management is Level C .



Recommendations

The team made three main recommendations :

(1) Modeling and simulation could be used effectively in the D&D arena to improve the business processes to provide a better interface between Levels A and C of the pyramid (between the business or senior managerial level and the project management level), which could result in a possible savings of $8M in efficiency improvements in the DOE-EM 2006 plan. An assessment of available business processes used in private industry (Fortune 500 companies), such as Enterprise Resource Planning, may provide the integration needed.

(2) Modeling and simulation could be used to standardize the dose and risk based criteria for the release of facilities and equipment in order to streamline the process for release of sites or equipment. The available models should be assessed to determine how are they being applied (and how they interface), how the job can be done better, and how the integration can be improved.

(3) Modeling and simulation could be used to increase the opportunities for interagency collaboration in order to optimize cost, schedule and engineering. Interagency modeling and simulation at the beginning of the process will aid in the reduction of the mortgage, capture and integrate existing efforts and capabilities, and evaluate lessons learned.

2.3 Environmental Security (see Appendix E)

The Environmental Security interest area team was composed of a diverse group of individuals from different countries and disciplines. Environmental security has many facets; individuals, and even agencies, address these facets with varying degrees of emphasis. Given its diverse background, the team chose not to develop a single definition for “environmental security.” Instead, the participants described the activities they felt should be included under that name. These activities ranged from environmental issues affecting regional stability to maintaining a secure environment for operating facilities. At one end of the spectrum, the view encompassed large-scale phenomena with closely coupled social and political implications. At the other end of the spectrum, it included management and operational procedures that make a facility safe in normal times and emergency situations, and identified conditions where a release of radioactive material would cause health and ecological problems.

One common theme that emerged from the discussions is that environmental security requires a coupling of models of natural and social systems. Environmental impacts from a contaminant release or resource use can result from, or lead to, social and/or political instability. Scenarios for environmental security must consider these elements in addition to biological and ecological ramifications. Another key feature of environmental security that emerged is the multiplicity of spatial and temporal scales inherent in this interest area—local, regional, and global spatial scales are included as part of environmental security. Local scales are pertinent for plant operations or for remediation at foreign site. Examples of the regional scale include airsheds, river basins, and perhaps even political units. The global scale includes the effects of changes in the atmosphere, particularly those closely associated with climate variability. Temporal scales are likewise quite variable, ranging from minutes (e.g., accidents) to years to decades (e.g., global climate effects).

The team knew of no models that coupled detailed phenomenological models with models of systems to address environmental security issues. The team identified a number of elements as being necessary in order to achieve internationally acceptable modeling of environmental security problems. Without international agreement on all of these elements, environmental security problems will not be resolved to the satisfaction of the parties involved. These elements were to:

- Establish a set of accepted references models.
- Agree upon validated databases for a range of environmental security problems, and make the databases readily available to the international community.
- Establish metrics for performance/quality.
- Validate codes. All codes used for environmental security should be validated against the above (models, databases, and metrics).
- Agree upon a “common currency” (an agreed-upon metric for use by entities such as governments so that results are viewed from a common reference point. An example of a “common currency” is casting all results in terms of risks to human health and the environment).
- Conduct cost/benefit systems for environmental security problems across the international community.

2.4 Health and Ecological Effects I (see Appendix F)

The theme that pervaded the discussions on the role of modeling and simulations in human health and ecological effects was that risk management is the new paradigm for federal facility operations. Risk is an appropriate measure for evaluating both human health and ecological impacts. Because human health and ecological impacts are endpoints for decisionmaking procedures, models of source term and physical transport must be designed to provide inputs to the human health and ecological models at the appropriate scales in time and space.

There are similarities between human health and ecological risk assessment, for example in terms of pathway analysis. However, there are differences in terms of endpoints, such as toxicology. Human health risk is considered "old," whereas ecological risk is "new." Both can be addressed together, but the differences need to be identified. The issues should not be restricted to a radiological focus, even though previous risk assessment work has had a tendency to focus in this area.

Models are the only practical tools for analyzing these systems and supporting risk management decision making, on the basis of both cost and technology.

Modeling and Simulation Limitations

- *Data availability.* The need for new data to provide a foundation for improving models and model predictions cannot be overstated.
- *Credibility*. There are many critics of modeling. Ways must be found to improve the acceptance of modeling as a credible tool for performing analysis of risks.
- *Goals.* Good modeling practice requires a clear statement of goals, yet a clear consensus on endpoints for human health, and especially for ecological systems analysis, is currently lacking.
- *Planning*. Modeling should be an integral part of the planning process. Many planners have an inadequate understanding of the appropriate scheduling of modeling activities and the improvement of results that come from adopting an adaptive management strategy for program management.

Modeling and Simulation Benefits

- Quantifying uncertainties and allowing them to be decomposed so that we know where to focus our data collection activities.
- Testing assumptions and theories so that we know where better understanding of fundamental processes is required.
- Formalizing conceptual models to reduce ambiguities that can cloud understanding and acceptance of our method.

- Facilitating reductions in cost to ensure that we achieve maximum effect for the dollars spent.
- Improving public acceptance of activities through the use of models as communication tools to foster confidence and credibility.
- Engendering a more businesslike approach to environmental management by providing forecasts for use in planning, cost/benefit analyses, etc.
- Identifying where research can lead to further efficiencies and better targeting of scarce resources.

Recommendations

The team made six basic recommendations:

(1) Modeling and simulation should be integrated into project planning.

(2) Integration across media (e.g., atmosphere, groundwater, biosphere) is a necessity, especially for ensuring that models are consistent in scale and that interfaces between various models or components are appropriately implemented.

(3) The involvement and education of the public, regulators, and decision makers is an essential strategy for ensuring success, but it is a process that requires development.

(4) There is a need to develop a consensus on risk-based endpoints.

(5) There is a need to develop more knowledge about ecological systems that are subjected to impacts. (Most current efforts are directed toward the understanding of natural ecosystems.)

(6) More resources should be devoted to model development on two levels: (1) improving existing models, and (2) developing the tools necessary to facilitate the building of new state-of-the-art models from reusable components, including components based on advanced visualization technologies.

2.5 Health and Ecological Effects II (see Appendix G)

The thrust of this interest area team was on problem-driven models in a variety of applications settings. The team focused on science-based models developed or used for the conceptualization of integrated processes. These processes are generally defined by a user or group of users who require solutions to problems ranging from (but not limited to) contaminants in the environment, to economic impacts of remediation efforts, to non-contaminant effects on humans and ecological receptors.

Needs

The team identified several needs or issues related to modeling and simulation in this interest area:

- Constraints and variables that control modeling efforts. Constraints on models include the limits within which a model can be used and the data available to use in the model.
- Availability and adequacy of models.
- Existence and actual use of the models.
- Types of models considered. Models available and applicable to different problems include cost/benefit and risk/benefit models; fate and transport models used to simulate the transformation of contaminants, and the means by which contaminants move from source areas to areas where exposure to various receptors occurs; and exposure models.

Recommendations

· *Credible data for input parameters.* One of the main needs of modelers is a source of credible data for input parameters, including uncertainty. One of the largest sources of uncertainties in modeling environmental processes is the variation in input parameters.

· *Interaction of different agents*. This issue has not been addressed adequately within the human health or ecological risk assessment frameworks, partly because of the lack of data on synergistic or antagonistic effects of different chemicals and receptors.

· *Bioavailability of chemicals*. Currently, the bioavailability of different chemicals is not adequately factored into different modeling scenarios.

Contaminants and non-contaminant stressors. Contaminants are frequently the only stressors to which human and ecological receptors are exposed. While difficult at present to quantify, non-contaminant effects should be factored into models of human health and ecosystem behavior. Competing risks, or the effects of different risks on receptors, have not been used in many risk assessments. Because of the risk inequality, more attention can be paid to the contaminants responsible for the most risk to a target receptor. This approach could be used to target remediation efforts or guide the immediate actions that are required.

Transformation of chemicals after deposition in the environment is a problem that is addressed in some models and ignored in others. Transformation often renders a chemical less harmful to receptors, but there is evidence that transformations of some substances produce products of higher risk if ingested, inhaled, or contacted dermally.

Modeling applications also can be better used to direct or guide data gathering with regard to effects to humans and ecological receptors exposed to various contaminants. Conceptual models or screening-level models can be valuable tools to differentiate those areas where potential adverse effects would be highest at a site of interest, and these estimates can be made using minimal environmental data. The selective use of the information can be used to focus resources on sampling the areas of most concern while minimizing sampling in those areas that are not of the most concern.

· *Uncertainty and statistical analysis.* Analysis of uncertainty in any model continues to be an area of needed improvement. While predictions of risks and exposures are useful tools for decision making, the expected variation within the predictions is also a needed piece of information. Use of current uncertainty analysis tools and techniques needs to continue, as does model development with uncertainty analysis as a built in. Both temporal and spatial variation need to be included explicitly in the models so that the effects of the variation can be factored into the risk assessments.

2.6 Infrastructure (see Appendix H)

The Infrastructure interest area team formulated a vision and goal for its discussions:

Vision: *Better Decisions through Better Analysis through Better Modeling and Simulations.*

Goal: *Provide better support for Environmental Management (EM) policy decisions that lead to resource allocations.*

To accomplish the team's vision, participants identified a special need for overall system models that address broad policy issues involving resource allocations by integrating various existing environmental models, tools, and methodologies, including those that specifically address infrastructure issues. The team concluded that the development of the suggested integrated systems models should be addressed using a "system of systems approach." This approach would be used to treat all important aspects, such as complete life cycles and human behavior where necessary, in examining significant interactions and interdependencies and potential emergent behavior of the complex natural and artificial systems to be modeled.

Team members saw a potentially great benefit in increased application of systems engineering principles in general to the design of complex infrastructure physical systems and societal processes, including governmental, and in particular to the design of infrastructure, processes, and products. The team members further concluded that various new techniques are well-suited for developing models and performing simulations and analyses that address various EM issues, including human behavior, in an integrated manner.

The team identified a pressing need to do a better job of communicating model capabilities and results to EM decision makers. Because the principal objectives of much modeling, simulation, and analysis are effective management and, where feasible, reduction of risk, it is important to address the risk perceptions and preferences of decision makers. The team suggested the following infrastructure options for improving communications among decision makers and the modeling and simulation community:

· Assisting decision makers in acquiring hands-on experience in running calculations and simulations and interpreting results. This assistance could be provided, for example, through one-on-one interactions and/or workshops. It would help decision makers understand what is required to obtain meaningful results, how to use these results, and/or how to obtain their own results on a more or less routine basis.

· Establishing an interagency modeling and simulation working group. Examples of tasks performed by this group would include coordinating activities and interactions with decision makers; establishing and maintaining critical databases; ensuring the establishment and maintenance of other importance resources; making sure that infrastructure once developed does not disappear without a trace; promoting, where feasible, the transfer of government-funded products to the private sector; translating results for decision makers; and generally championing modeling and simulation within and across agency and department boundaries.

· Forming separate working groups within intra-agency and/or inter-departmental organizations. These groups or individuals would accomplish the same objectives as described above for the interagency modeling and simulation working group, but within the various agencies or departments and/or across department and agency boundaries.

The group identified four broad categories of infrastructure as being particularly important. The criteria used by the team to assess importance included such factors as complexity with respect to the decisions to be made as well as economic, health, safety, societal, and environmental impacts. The four categories included:

(1) The processing of radioactive, chemical, and biological wastes to render them innocuous or to convert them to forms suitable for interim storage or ultimate disposal, and the cleanup of sites contaminated with such wastes.

(2) Transportation. Transportation is a key issue because of the transportation of radioactive, chemical, and biological wastes, including packaging and handling.

(3) The interim storage and final disposition of radioactive, chemical, and biological wastes.

(4) Electric power production fueled by fossil energy. This is a key category because of emissions from generating units, including toxic wastes and greenhouse gases.

2.7 Manufacturing/Pollution Prevention (see Appendix I)

The focus of the Manufacturing/Pollution Prevention area team was the application of modeling and simulation to the improvement of manufacturing and other industrial processes, especially for the purpose of reducing the toxicity and volume of releases of waste materials to the environment. The interest area team examined improvements at all stages of the life cycle of production facilities—permitting, design, construction, operations, decontamination and decommissioning, and remediation of past facilities. Less emphasis was placed on decommissioning and restoration because these areas were incorporated in part in other interest areas.

The team reviewed efforts in modeling and simulation of detailed industrial processes, such as chemical process models, as well as decision-aiding tools that may not model processes explicitly. Cost/benefit models, value of information models, and risk-based prioritization models were included. Also examined were analytical tools for evaluation of parameter uncertainty and sensitivity, and for sophisticated data visualization.

The team defined five problem areas for manufacturing and pollution prevention that constituted progressively more inclusive domains of modeling and simulation of environmental and economic impacts of operations. These problem areas were Resource Conservation, Pollution Prevention, Design for Environment and Life-Cycle Analysis, Industrial Ecology, and Sustainable Development. As discussed in the plenary session (see Appendix B), well-defined objectives are needed when attempting to design, develop, or use models and modeling tools. The team therefore developed a set of nine questions that need to be addressed when developing models for each of the defined problem areas.

Modeling Question	Task Title for Problem Area
What is the problem area?	Problem Definition
What do we want?	Goal Definition
What do we know?	History Matching
What else do we need to know?	Uncertainty Analysis
What can happen?	Prediction
How can we choose?	Prioritization
How can we show what we know?	Visualization/Communication
How can we test what we know?	Validation
How much is enough?	Performance Measurement

Models have been developed for some of the defined problem areas to address some or all of the questions listed above. For example, models for Industrial Ecology and Sustainable Development are quite primitive, and have been developed primarily to focus discussion on defining what must be included in an ecological model for industry, or what constitutes sustainable development. At progressively deeper levels, models have been developed that address, or could address, nearly all of these questions.

Recommendations

The interest area team examined the current level of modeling capability and listed examples of applications for each problem area, with the strengths and weaknesses of models applied. The team then consolidated the weaknesses of models for each problem area into six areas, and made the following recommendations for further development:

(1) ***Environmental Decision Support Framework.*** DOE and other governmental organizations could improve in the area of early problem definition and the setting of goals with respect to those problems. Failure to do so supports suboptimal solutions that fail either at the deployment stage or later. The team recommended that an environmental decision support framework be adopted or developed for pollution prevention that:

- includes defining, and documenting the basis for, objective functions for environmental options
- addresses environmental impacts and other regulatory concerns
- incorporates uncertainty and sensitivity into models more effectively.

(2) ***Improvements in Process Models.*** Many existing manufacturing or chemical process models are limited in their ability to model a variety of types of processes for environmental concerns; therefore, significant environmental impacts are not effectively evaluated. The team recommended supporting a better adaptation of chemical process modeling techniques to environmental problems, including dynamic, non-equilibrium, and rate-limited processes as well as dilute thermodynamic calculations.

(3) ***Closing the Loop.*** Models for the problem areas of Life-Cycle Analysis, Industrial Ecology, and Sustainable Development do not capture sufficient reality to provide meaningful support to decisions. To avoid continued suboptimization, these integrated models are essential. The team recommended that before Congressional action defines the field, models should be developed that link physical-chemical models of industrial processes (especially those operated by DOE), economic and environmental impacts, and sociological constraints and responses. This linkage is necessary so that Environmental Managers (which increasingly means all managers) can begin to understand their options with respect to reasonably closed processes.

(4) ***Support for Externally Developed Modeling Tools.*** DOE and other agencies have participated in only limited interagency interaction as well as limited industry interaction in sharing knowledge and modeling and simulation efforts in the environmental arena. The team recommended that efforts be expanded to evaluate, use, and support, where appropriate, existing environmental modeling and simulation efforts outside individual agencies or organizations.

(5) ***Behavioral Modeling.*** Although DOE and other agencies have recognized that models and technology have repeatedly failed to be adopted, they have not been inclined to invest in research to understand what it takes to implement change. The team recommended an investigation, as part of the development of an environmental decision support framework, of the literature of innovation and a study of significant successes and failures. Guidance should be provided to both modelers and decision makers on how to ensure that technical solutions are implemented.

(6) ***Prescriptive Modeling.*** Current models are largely descriptive, resulting in identification of the nature and magnitude of significant issues. For the most part, these models lack the capability to translate issues into prescriptive solutions, in the manner of expert systems. The team recommended support of the development of techniques and tools to link identified problems to desired outcomes by matching problems with available solutions.

2.8 Subsurface Contamination I (see Appendix J)

Subsurface contamination is an area of extensive model development and application. A strong technical community exists that has sophisticated physical/chemical/biological-based process models at its fingertips. Modeling is used extensively to assess fate and transport, guide site characterization, and assist in the selection and design of remediation and monitoring systems.

Successes and accomplishments of modeling efforts in the area of subsurface contamination are numerous. Very few large-scale problems of subsurface contamination have been attacked in the U.S. without the aid of models at some stage. However, not all model applications have been successful. In some cases, unclear objectives and unrealistic expectations have contributed to the lack of success. A clear understanding must be achieved among the modelers and decision makers as to the specific needs and requirements of the project, the form in which those needs can best be satisfied, the ability of the models to meet such requirements, and the data and finances required to support the modeling effort. It is from such communication and two-way education that clear, specific objectives and expectations will emerge.

While modeling is highly developed in the area of subsurface contamination, further research and development is needed in some areas. In addition, state-of-the-practice models generally do not include the complex processes that are available in state-of-the-art models. Using models with enhanced processes should lead to better predictions of site behavior.

The numerous successes of modeling efforts notwithstanding, the analysis of the costs and benefits of modeling in subsurface contamination problems has been spotty. There is a need for documentation of the costs and benefits of modeling. Documentation of the costs and benefits of modeling based on case histories of actual projects will confirm their usefulness, help educate decision makers about what models can do for them, and promote even more effective and extensive use of models. The team believed a primary benefit of modeling is the elimination of unnecessary effort and expenditures. Among the factors contributing to this overarching benefit are:

- Design and optimization of site characterization
- Optimize remediation-system design
- Evaluate systems that are inaccessible or dangerous
- Estimate long-term behavior that is inaccessible to experiment
- Demonstrate understanding, build confidence, and alleviate public fears
- Know when “enough is enough”

Recommendations

The Subsurface Contamination I interest area team proposed the following recommendations and conclusions:

(1) Improved Communication

· All parties involved in the effort (modelers, stakeholders, management, and regulators) should strive for improved communication. Clear, specific, and realistic goals and objectives should be established at the onset and throughout the life of the project. Modeling results, assumptions, limitations, and uncertainties should be clearly communicated in a way that is meaningful and commensurate with the decision makers' context and background. Provisions for such efforts should be set out in the project scope and budget.

· The mutual education of modelers and decision makers is critical. This will promote clear objectives and expectations on specific projects and foster more extensive and appropriate use of models across the board. Workshop(s) are recommended to promote mutual understanding of needs, capabilities, constraints, and points-of-view.

(2) Continued Research and Development

· Continued research and development is needed to improve modeling capabilities for complex processes. Those processes believed of high priority in this regard are reactive chemical transport, immiscible fluid flow, multi-scale heterogeneity, bioremediation, integration of fate and transport models with biosphere and exposure pathway models, colloid transport, and uncertainty analysis.

· The importance of continued feedback between the modeling and data gathering efforts to update the site conceptual model needs to be recognized and provided for. Modeling and simulation should become an integral part of site characterization, testing, and monitoring.

· Deployment of models should be improved through additional efforts of technology transfer. This would decrease the lag time between state-of-the-art models becoming the state-of-the-practice.

· Continued international cooperations (e.g. benchmarking, code comparisons, and comparisons with field data) will enhance modeling and simulation.

(3) Case Studies

· Case studies should be used to establish the benefits and costs of modeling and simulation. Objective documentation of the benefits of costs will promote the effective use of models and help ensure their application in appropriate circumstances.

2.9 Subsurface Contamination II (see Appendix K)

The Subsurface Contamination II interest area team discussed the benefits of modeling and simulation in this area, and concluded that the full benefits of modeling and simulation (i.e., cost-effective cleanup) can be realized only in a systematic framework that relates site activities to clearly defined objectives. These objectives should be developed with the early and continuous involvement of a management team made up of decision makers, site managers, regulators, stakeholders, and modelers (scientists/engineers). In the context of this holistic framework, modeling provides the organizing infrastructure to guide site activities that are responsive to decision making needs. Our models must necessarily adapt to new and better information that can alter management strategy given our limited and evolving understanding of contaminant behavior at a given hazardous waste site. Therefore, an explicit and dynamic linkage exists between data collection, assessment of remediation options, optimization of remedial design, the management team, and the decisions that need to be made.

Recommendations

The Subsurface Contamination II interest area team made the following recommendations:

(1) Improve communication between modelers, regulators, decisionmakers, and stakeholders.

- Establish clear objectives and expectations.
- Communicate the objectives and expectations early and often.
- Communicate technical information in a form suitable to decision makers.

(2) Improve the integration of cleanup activities.

- Establish a clear link between each activity and its correlated decision making process.
- Establish a mechanism, such as a database, to adapt to new information.
- Use the best available technology.

(3) Adopt an holistic approach to remediation projects by focusing on integration, not just organization.

- Establish a systematic framework that truly integrates the project activities in support of the decision making process.
- Formulate work teams that include at least one modeler, one field scientist, one manager, one regulator, and one stakeholder.
- Ensure that management teams communicate (not just inform) early and often.
- Implement modeling tools that link project activities by using a mechanistic understanding of contaminant behavior in environmental systems.
- Implement an adaptive management infrastructure.

(4) Provide incentives for using the best available remediation/modeling technology.

- Insist on realistic lifecycle costs when assessing technologies.
- Reward the deployment of demonstrated innovative technologies.
- Provide opportunities to demonstrate the benefits of an integrated project framework.
- Reward the use of advanced simulation capabilities that improve the resolution of process mechanisms important to the remediation.
- Provide opportunities to demonstrate the benefits of advanced computational and mathematical approaches that improve decisionmaking and project management/ business practices.
- Reward partnering between government agencies.

2.10 Waste Treatment (see Appendix L)

The Waste Treatment interest area team first considered the major problems in process modeling and simulation and then re-evaluated these generic problems in order to develop more specific suggestions of needs.

Problems

(1) Most efforts and modeling/simulation problems are site-specific with little effort and incentive to make them more generic in nature.

(2) Little effort is made to evaluate when data gathering becomes excessive or of diminishing value.

(3) Too little effort is made to model treatment processes when the available database has a wide variety of parameters.

(4) Not enough effort is made to improve data management and reliability.

Important Needs

(1) A fully integrated system for waste treatment is needed that includes, at the very least, a consideration of life-cycle effects, waste quantity, the risks presented by the wastes, and waste transport.

(2) DOE Complex-wide generic models need to be developed and applied at each site. New technologies or competing technologies should be evaluated as modeled systems. The models should include costs, waste forms, classification of waste (e.g., TRU-waste, low level), environmental impacts, risks, and safety measures. Other potential areas that need to be modeled include the use of uncertain data; projected waste loads; project schedules; treatment optimization; long term storage models; safety rules and guidelines; availability of technology; technology reliability; no-action scenarios; socio-economic issues; air pollution control on treatment processes; and optimization of business practices.

Recommendations

The four basic recommendations of the team were to:

(1) Integrate and expand site-specific models to DOE Complex-wide application models.

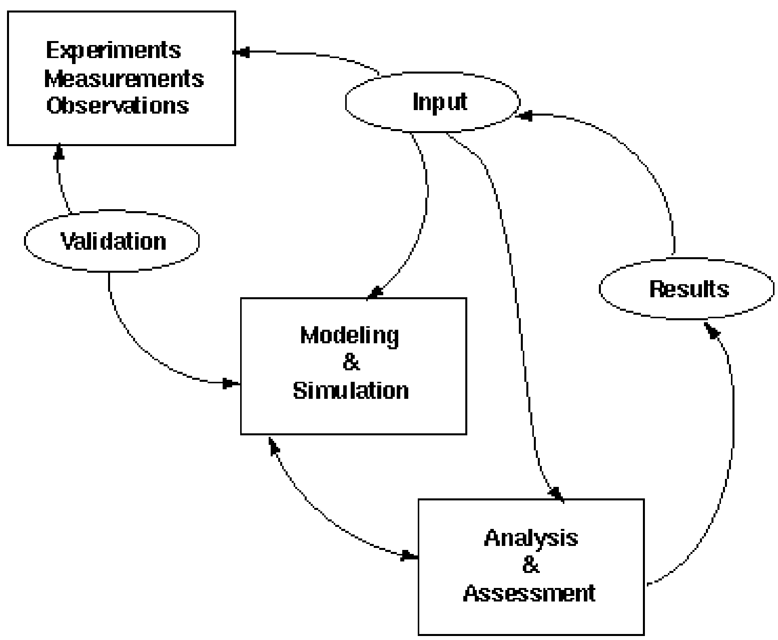
(2) Create a DOE Complex-wide Council on Modeling and Simulation. This Council could be patterned on the Strategic Laboratory Council, with a representative from each laboratory, a representative from each major site, and representatives from major contractors.

(3) Use modeling and simulation in waste treatment systems to improve the institutional memory of treatment methods and systems. Models can identify, through sensitivity analysis, what is more important and where the critical paths are, and aid in the communication of these findings. Models should aid decision makers in understanding where the particular problems are, and greatly enhance their knowledge and understanding of waste treatment problems in general. Other important advantages of online models are that they save money, reduce risk, reduce waste, and point the way to improved design changes.

(4) Use metrics (e.g., frequency of use, costs of the model, adaptability to new problems, diversity of use, and supportiveness) to estimate the effectiveness of modeling efforts. A model should be user friendly, well documented, reliable, portable, well defined, and low maintenance. Training in its use must be available.

Section 3. Summary and Conclusions

Many examples exist of areas in which modeling has been absolutely indispensable: reactor safety, nuclear weapons stockpile stewardship, chemical plants, air transportation, and others. Why then has it been so difficult to point out where modeling is useful in environmental technologies? From the discussions in the ModSim'97 USA workshop, it appears that modeling/simulation has often been *oversold* and that models have not delivered. It also seems that *communication* among researchers, practitioners, funders, and users has been lacking: researchers often have kept results to themselves rather than applying them to reality, and explanations of modeling/simulation work have been overly complicated instead of clear and simple. The diagram below, developed by the Executive and Organizing Committees at a working session following the workshop, shows how modeling and simulation should be used. Input from decision makers, project managers, scientists, field engineers, and modelers feeds into experiments, measurements, and observations; modeling and simulation; and analysis and assessment. The results go to decision makers, who then provide additional feedback as input.



The discussions within each of the interest areas were quite interesting. The Infrastructure interest area team went from talking about modeling of infrastructure to the infrastructure of modeling. They settled on the latter, which is, in fact, precisely what modeling/simulation needs to develop. The Environmental Security interest area team was the most international in terms of the participants themselves and the interesting global issues that were considered. While the two Health and Ecological Effects teams took two different approaches in their discussions, the two Subsurface Contamination teams took similar approaches. All of the teams developed some common themes and agreed on some basic concepts. For example, consensus was reached on what modeling is *not*:

- Modeling is not a substitute for data.

- Modeling is not exact reality.
- Modeling does have uncertainty but this uncertainty is useful.
- A gap exists between what decision makers want and what models provide.
- Dose models are a problem.

The common themes developed by the teams address large problems and broad issues rather than single, specific problems:

- An infrastructure of modeling—a systems approach—is needed.
- Models need to be integrated.
- Further communication among researchers, users, and decision makers across agencies is needed. An interagency group may already exist that could broaden and strengthen its charter to fulfill this need.
- Efforts to strengthen the Environmental Security aspect of modeling is extremely important. Environmental and energy issues transcend national boundaries, incorporate nearly all of the interest areas, and affect us all.