ERDC/EL TR-00-6

Environmental Laboratory

US Army Corps of Engineers®
Engineer Research and Development Center

Summary Report, Risk Assessment Modeling Workshop

14-15 May 1998, New Orleans, Louisiana

Patrick N. Deliman, Carlos E. Ruiz, and Jeffrey A. Gerald

July 2000

ERDC/EL TR-00-6
July 2000

Summary Report, Risk Assessment Modeling Workshop

14-15 May 1998, New Orleans, Louisiana

by Patrick N. Deliman and Carlos E. Ruiz

Environmental Laboratory
U.S. Army Engineer Research and Development Center
3909 Halls Ferry Road
Vicksburg, MS 39180-6199

Jeffrey A. Gerald

AScI Corporation
1365 Beverly Road
McLean, VA 22101

Final report

Prepared for U.S. Army Corps of Engineers
Washington, DC 20314-1000

Engineer Research and Development Center Cataloging-in-Publication Data

Risk Assessment Modeling Workshop (1998 : New Orleans, Louisiana)
Summary report, Risk Assessment Modeling Workshop, 14-15 May 1998, New Orleans, Louisiana / by Patrick N. Deliman and Carlos E. Ruiz, Jeffrey A. Gerald ; prepared for U.S. Army Corps of Engineers.
273 p. : ill. ; 28 cm. — (ERDC/EL ; TR-00-6)
Includes bibliographic references.
1. Ecological risk assessment — Congresses. 2. Environmental risk assessment —Congresses. 3. Health risk assessment — Congresses. 4. Environmental impact analysis —Congresses. I. Deliman, Patrick N. II. Ruiz, Carlos E. III. Gerald, Jeffrey A. IV. United States. Army. Corps of Engineers. V. Engineer Research and Development Center (U.S.) VI. Environmental Laboratory (U.S.) VII. Title. VIII. Series: ERDC/EL TR ; 00-6.
TA7 E8 no.ERDC/EL TR-00-6

Contents

Preface

The work reported herein was conducted by the U.S. Army Engineer Research and Development Center (ERDC), Environmental Laboratory (EL), Vicksburg, MS, for Headquarters, U.S. Army Corps of Engineers (HQUSACE). Funding was provided by the HQUSACE Installation Restoration Research program (IRRP), Fate & Effects Thrust Area, Work Unit entitled Risked-Based Cleanup Decision Support/Assessment System-Remediation Assessment Modeling System (RAMS). Dr. Clem Myer was the IRRP Coordinator at the Directorate of Research and Development, HQUSACE. The IRRP Program Manager was Dr. M. John Cullinane, EL.

This report was prepared by Drs. Patrick N. Deliman and Carlos E. Ruiz, Water Quality and Contaminant Modeling Branch (WQCMB), Environmental Processes and Effects Division (EPED), EL, and Mr. Jeffrey A. Gerald, AScI Corporation, McLean, VA. Ms. Lillian Schneider and Dr. Christian J. McGrath, WQCMB, EL, were technical reviewers for this report.

The work was conducted under the general supervision of Dr. Mark S. Dortch, Chief, WQCMB, Dr. Richard E. Price, Chief, EPED, and Dr. John W. Keeley, Acting Director, EL.

At the time of the publication of this report, Director of ERDC was Dr. James R. Houston. Commander was COL Robin R. Cababa, EN.

This report should be cited as follows:

> Deliman, P. N., Ruiz, C. E., and Gerald, J. A. (2000). "Summary Report, Risk Assessment Modeling Workshop," ERDC/EL TR-00-6, U.S. Army Engineer Research and Development Center, Vicksburg, MS.

1 Introduction

Background

The Fate & Effects Advisory Committee (FEAC) identified the need for the development of models capable of providing information relating to the fate and effects of Military Relevant Compounds (MRCs) on both ecological and human resources. Stated was the requirement for better modeling capabilities of contaminant concentration over time for risk assessment. In an effort to address the requirement, a work unit was initiated for the development of an Army Risk Assessment Modeling System (ARAMS). This system will incorporate other research efforts conducted in the Fate & Effects research program and will enable thorough evaluation of ecological and human risk assessments.

The ARAMS will be developed for the purpose of conducting ecological and human risk assessments. Development of this system will incorporate current state-of-the-art modeling technologies and will further utilize concurrent research efforts in the Fate and Effects Research Program. The ARAMS is a tool to characterize, integrate, and estimate ecological risk. The system will provide several tiers of complexity such that screening level and complex models issues can be addressed. The system will include: (a) screening level assessments based on simple exposure-response relationships and limited spatial and temporal scales, (b) an expanded assessment capability based on linkage of more rigorous exposure and ecological assessment techniques and (c) linkage of ecological risk, comprehensive exposure models, and integrated temporal-spatial exposure,..i.e., probabilistic estimate of exposure for individuals/population in time and space.

Objective

The objective of this workshop was to ascertain the current state-of-the-art in risk assessment modeling and to facilitate discussion of the components required for an ARAMS.

Presentations

The presentation topics at the workshop were selected to provide a foundation for the discussion of the development of ARAMS. Each topic was considered to be a potential building block for the conceptualization of the system. The topics presented were: Ecological Risk Assessment Concepts; A WEB-Based Approach for Developing Risk Assessment Modeling System; The Groundwater Modeling System; The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES); Dredged Material Modeling—Risk-Based Concepts, Bioaccumulation Modeling Concepts, and Principles/Contemporary Issues; Ecosystem Models for Ecological Risk Analysis: Single Species to Communities; You Don't Need to Know a Lot of Ecology to Make a Comprehensive Ecological Risk Assessment; Risk Analysis of Potentially Contaminated Sites Using the U.S. Environmental Protection Agency (EPA) MMSOILS Multimedia Model; Metapopulation Models and Ecological Risk Analysis: A Habitat-Based Approach to Biodiversity; Ecological Risk in an Integrated Intermedia System, and Exposure Assessment - Trophic Transfer to Birds. A brief description of the topics presented at the workshop follow. Appendix A presents the "Conference Agenda and List of Participants." Copies of the actual presentation documents from each speaker at the workshop are shown in Appendixes B through K with the exception of "A WEB-Based Approach for Developing Risk Assessment Modeling System" and "The Groundwater Modeling System." Hard copy versions of these two presentations were not available.

Ecological risk assessment concepts

Ecological risk assessment modeling may be broken down into four areas of interest: (1) problem formulation, (2) exposure assessment, (3) effects assessment, and (4) risk characterization. The Department of Defense (DoD) has historically emphasized human health protection, but ecological concerns are becoming more prominent.

An ecological risk assessment survey of 190 Army facilities indicated that more than 50 percent were/anticipated conducting ecological risk assessments. DoD risk assessment needs include (a) modeling/software tools for risk characterization, (b) modeling/software tools for projecting effects beyond individual organisms, (c) modeling/software tools for incorporating spatial and temporal issues when assessing risk, and (d) modeling/software tools for quantifying uncertainties.

WEB-based approach for developing risk assessment modeling system

A web-based approach was presented to demonstrate the utility of updating and maintaining databases via the Internet. The newly developed Land

Management System (LMS) was given as an example. This system contains components of the Watershed Modeling System (WMS), and a demonstration of was presented showing how the CASC2D hydrologic model within the WMS could be initialized and run across the Internet. The United States Geological Survey's (USGS) topographical databases were accessed and dowloaded incorporating the WEB-based approach. This downloaded information could then be used to setup the grid structure for the CASC2D model. A previously developed CASC2D model application was then run (in an effort to save time) from a remote access site to display the features of incorporating offsite computing resources for conducting modeling runs or scenarios.

Groundwater modeling system

The Groundwater Modeling System (GMS) was developed by the DoD in partnership with the Department of Energy, the U.S. Environmental Protection Agency, Cray Research, and 20 academic partners. The GMS provides an integrated and comprehensive computational environment for simulating subsurface flow, contaminant fate/transport, and the effectiveness of remediation design alternatives.

GMS integrates and simplifies the process of groundwater flow and transport modeling by bringing together all of the tools needed to complete a successful study including both pre- and postprocessing tools. GMS provides a comprehensive graphical environment for numerical modeling, tools for characterization, model conceptualization, mesh and grid generation, geostatistics, and sophisticated tools for graphical visualization. The system is also currently available for both PC- and UNIX-based operating systems. Several types of models are supported by GMS. The current version of GMS provides a complete interface for the codes FEMWATER/LEWASTE, MODFLOW, MODPATH, MT3D, RT3D, and SEEP2D . Anticipated model additions in the future include UTCHEM, NUFT3D, ParFlow, and ADH.

The framework for risk analysis in multimedia environmental systems (FRAMES)

FRAMES is a software platform that allows models, developed by different people, to link and communicate with each other, while maintaining the legacy of the original models. FRAMES provides several functions: (a) it allows users to implement preferred models, (b) it allows users to link preferred models to and communicate with other models, (c) it allows for a standard, base set of models (regulatory review), (d) it maintains the legacy of models, (e) it provides a "plug-and-play" environment, and (f) it helps the user with the conceptual site model. The traditional multimedia modeling approach involves thinking in the abstract with complex flow charts for inputs, transport pathways, exposure routes and outputs, but FRAMES offers a nontraditional approach which offers the multimedia modeler the capability to conceptually build the system to be modeled through a graphical user interface (GUI) and drag and drop modules.

The modules communicate to other modules through the use of data processors and a data standard specification which is built into the FRAMES user interface.

Dredged material modeling—Risk-based concepts

Technical evaluation of the environmental acceptability of dredged material disposal is an effects-based process compatible with risk assessment. Computer programs and databases have been developed to aid in the evaluation and include the Automated Dredging and Disposal Alternatives Modeling System (ADDAMS) and the Environmental Effects Determination Database (E2D2). ADDAMS) is a PC-based system for DOS and Windows 95. It is a collection of 16 modules which are simple, nonintegrated, computerized tools and models for dredged material management and environmental effects evaluation. The modules in ADDAMS are predominantly stand-alone screening-level models linked under a common shell or menu. E2D2 is a web-based database of literature on environmental effects of contaminant residue in tissue of aquatic organisms. It provides for the interpretation of bioaccumulation data to determine environmental significance in absence of criteria.

Bioaccumulation modeling concepts and principles/contemporary issues

The allowable dose for any animal anywhere in an aquatic system is the intake from water ingested plus the intake from food/prey ingestion. We can define the bioconcentration factor (BCF) as the ratio of chemical contaminant in food-to-water concentration for exposure to water only. The major advantages of this are (a) that the BCF is easily determined in the laboratory under controlled conditions with "standard" (small) fish and (b) it is not dependent on site characteristics. This method allows for a neat and clean, site-independent national water quality criterion (WQC). If a WQC is used that is based on a bioaccumulation factor (BAF) which is dependent on the food web, a not-so-neat-and-clean method results. This method is site dependent and makes a national WQC possible only for a generic food web.

How do you determine the allowable waste load allocation of chemicals that may bioaccumulate? The proposed approach is to regulate on allowable tissue concentration at assigned frequency of exceedance percentile and to determine the allowable frequency distribution of chemical input load.

Ecosystem models for ecological risk analysis: Single species to communities

To justify regulatory and mitigation decisions, toxicologists are often asked the "so what?" questions that demand predictions about the population or even ecosystem response to contamination. Ecotoxicology is microcomputer software specifically created to help toxicologists answer such questions by extrapolating effects on organisms observed in bioassays to their eventual population-level consequences. It provides a software shell from which users can construct their own models for projecting toxicity effects through the complex filters of demography, density dependence, and ecological interactions in food chains. It allows various standard choices about low-dose response models, which vital parameters are affected by the toxicant, the magnitudes and variabilities of these impacts, and species-specific life history descriptions. During the calculations, the software distinguishes between measurement error and stochastic variability. It forecasts the expected risks of population declines resulting from toxicity of the contaminant and provides estimates of the reliability of these expectations in the face of empirical uncertainty. This risk-analytic endpoint is a natural summary that integrates disparate impacts on biological functions over many organizational levels.

You don't need to know a lot of ecology to make a comprehensive ecological risk assessment

There are five problems which lead to lack of trust in the risk analysis: (1) tool for obstructionists, (2) help for the other side, (3) need for too much data, (4) too expensive (requires consultants), and (5) too complicated. A good uncertainty analysis can alleviate the last three problems, and even though uncertainty is often large, it may still permit clear decisions.

There are three major problems with risk analysis: (1) correlation and dependency are ignored, (2) input distributions are unknown, and (3) mathematical structure is questionable.

Correlations and dependencies in uncertainty analysis are typically based on one of the following independence assumptions: dispersive Monte Carlo sampling, or dependency bounds analysis. Dispersive Monte Carlo sampling assumes extreme correlations so the result is as broad as possible. It is also computationally cheaper than ordinary Monte Carlo methods.

The default distributions for unknown input distributions are typically maximum entropy or probability bounds (P-bounds). Maximum entropy generalizes Laplace's Principle of Insufficient Reason and yields a distribution with minimum bias and maximum uncertainty under the constraints. Probability bounds (min, max, mean, median, shape, etc.) and P-bound arithmetic are quicker than Monte Carlo and are guaranteed to bound answer and provide the optimal solutions in most cases.

A questionable mathematical structure can be made more sound by incorporating a comprehensive battery of checks and incorporating model uncertainty into the analysis. The battery checks should provide general checks (e.g., dimensional and unit concordance) and checks against domain knowledge (e.g., population size nonnegative). The advantages of P-bounds as the uncertainty tool are: (a) much faster than second-order Monte Carlo, (b) easy (graphical) parameterization, (c) handles uncertainty about parameter values, distribution shapes, dependence and correlation among variables, even the form of the model itself, and (d) faithful to most frequent interpretation.

Risk analysis of potentially contaminated sites using EPA's MMSOILS multimedia model

The purpose of this presentation is to provide an introduction to the MMSOILS model, its uses and limitations, and to demonstrate how MMSOILS was used in one EPA program, Hazardous Waste Identification Rule (HWIR), to provide an initial assessment of many sites. Some selected features of MMSOILS multimedia model are

a. Contaminant transformation and fate processes

b. Intermedia contaminant fluxes

c. Exposure pathways

d. Human health risk measures

e. Media-specific transport.

The purpose of EPA's HWIR is to evaluate if certain low-risk wastes can be disposed of as nonhazardous. The EPA "Exit" Rule is the question : at what concentrations can specific chemicals "exit" hazardous waste disposal requirements and be protective of human health and environment? The scope of HWIR is nationwide and is specific to chemicals and waste management unit (WMU) types. HWIR specifies approximately 400 chemicals and WMU types of landfill, impoundments, and waste piles. EPA's approach to implementing HWIR is through a multimedia/multipathway, risk-based(human health and ecological), and site-based (create plausible sites and assume each chemical could be disposed at each site) methodology.

Factors that influence computational effort to implement HWIR are: (a) there can be hundreds of sites, (b) five to six source types, (c) 400 plus chemicals, (d) the range of source concentrations, and (e) Monte Carlo loops. The computational burden on a computer processing unit (CPU) to implement a modeling scenario can easily approach centuries when Monte Carlo uncertainty is used. Means to reduce computational burdens, such as making use of linearity, grouping of chemicals, risky versus nonrisky sites, and minimizing the number of random variables are required.

Metapopulation models and ecological risk analysis: A habitat-based approach to biodiversity

Metapopulation dynamics are important in ecological risk analysis, and modelers ignore spatial structure at their own risk. Spatially explicit metapopulation models provide practical compromise between complexity and applicability. Future directions for ecological risk analysis modeling will be to incorporate habitat relationships, involve multispecies approaches, and allow metapopulations in trophic chains. Metapopulation models are important because they allow assessment of impacts, evaluate management options at the metapopulation level, and also allow complicated population dynamics to be simulated.

Factors that affect population dynamics are:

a . Demography: survival, fecundity, and growth.

b. Age or stage of structure.

c. Density dependence.

d. Environmental fluctuations, catastrophes.

e. Demographic stochasticity.

Factors that affect metapopulation dynamics include all of the ones for population dynamics, but additionally include:

a. Number of populations.

b. Geographic configuration.

c. Spatial correlation.

d. Migration patterns.

The occupancy metapopulation model has the advantages of analytical solution and generalizations. It has disadvantages of unrealistic assumptions, difficult parameters, and few or infinitely many patches. The spatially explicit metapopulation model has the advantages of being flexibile and realistic with few implicit assumptions. Its disadvantages are that it is data intensive, difficult to add genetics, and numerical errors may occur. The individual-based metapopulation model has the advantage of being very flexible and realistic. Its disadvantages are that it is easy to make numerical and/or logical errors, is very data intensive, and is sensitive to behavioral assumptions.

Future directions in metapopulation modeling will be in multispecies assessments and in developing community-metapopulation models. In community-metapopulation models, each trophic level would be represented as a metapopulation, each metapopulation would have a different spatial scale, and connections between metapopulations would be based on energy flow.

Ecological risk in an integrated intermedia system

Models and tools are needed to bridge the gap between source, fate, transport, and the resulting ecological impacts. A phased approach is presented for varying levels of detail to match tools to assessment needs. This approach provides for a preliminary as well as a detailed assessment.

The ecological models discussed include the Wildlife Ecological Assessment Program (WEAP), the Ecological Contaminant Exposure Model (ECEM), the Health and Ecological Risk Management and Evaluation System (HERMES), and the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES).

The WEAP model represents a preliminary assessment to ecological risk analysis. It correlates exposure and effect using laboratory data. It analyzes and correlates concentration and duration of exposure. The model also accounts for frequency of occurrence.

The ECEM model is an ecological risk assessment modeling tool. It estimates exposures from metals, organics, and/or radionuclides in terrestrial and/or aquatic environments. The model is based on a food-web architecture and helps environmental managers assess impacts as part of a regulatory or decision-making process. User inputs for the model are:

a. Contaminants of interest.

b. Species of interest and species in the food web.

c. Environmental data.

Results of the model are:

a. Body burden or dose rate.

b. Compared to environmental benchmarks to calculate the environmental hazard quotient.

c. Can be used as input into human health assessments.

The HERMES model is a flexible visualization and analysis program which helps environmental restoration, land use, and resource managers make decisions. It allows interactive evaluation of impacts with user-selected restoration costs and species values. Other decision dimensions, such as human health, ecological risk, and ecosystem function, can be included as extensions to the model. The advantages of the HERMES model are:

a. Usable - links with user's existing databases.

b. Portable - can be run on a laptop computer, which facilitates public involvement.

c. Easily manipulated - user can control data input values

d. Expandable - modular design allows inclusion of additional decision dimensions.

The FRAMES user interface serves as the integrating platform for all the models discussed. It provides linkages between fate and transport, ecological, and human-health models.

Exposure assessment—Trophic transfer to birds

Why quantify trophic transfer to birds? There are four main reasons which include (1) to computing contaminant levels in species of interest (contaminant levels can be used to assess the potential for toxicity), (2) establishing pathways of contamination, (3) projecting future concentrations, and (4) establishing the potential for effects on population dynamics.

Bioaccumulation can be computed in several ways:

a. Trophic transfer ratios, bioaccumulation factors.

b. Steady-state model.

c. Time-variable simulation model.

BAFs are the simplest, but have the highest degree of uncertainty. The steady-state model is one step above the BAF with the strength of species-specific parameterization, but with the limitation of life-cycle accumulation and temporal changes in exposure sources and levels. Time-variable models have the strength that changes in relative importance of sources can be evaluated and have the limitation that it requires modeling capability and information on parameters. A calibrated model has the strength of reduced uncertainty, but the limitation of requiring site-specific data. Uncertainty analysis for calibrated and uncalibrated models differ. The calibration of a model reduces uncertainty by restricting the parameter sets that are consistent with field measurements.

Technical Issues

Prior to the workshop, a list of questions was generated to aid in focusing the discussions at the workshop. These questions along with the oral presentations provided the background for the Risk Assessment Modeling Workshop. The following questions were used to stimulate discussion at the workshop:

a. What is the state of the art in risk modeling?

b. What are the requirements for a simple- or screening-level risk assessment?

c. What are the requirements for a comprehensive risk assessment?

d. What tools are required for a risk assessment ?

(1) Exposure component.

(2) Effects component.

(3) Other potential components.

(4) Are these tools applicable for a comprehensive risk assessment, and can the tools be integrated in a common (object oriented) environment?

e. What tools are currently available?

(1) Exposure component.

(2) Effects component.

f. Should we develop tools (state-of-the-art) or incorporate existing ones?

g. Is there a need for a risk assessment modeling system/environment? This system would include gains, losses, and advancement of the current state-of-the-art.

h. What is the feasibility of developing a risk assessment modeling system (beyond the current capabilities/state of the art)? Such a system must include structure/platform and output.

i. Can/should the screening-level and comprehensive exposure models coexist in the same modeling environment?

j. Should we develop tie-ins to existing systems (GMS, Surface Modeling System (SMS), and WMS)?

k. What are the existing sources of effects/toxicity databases?

(1) Public domain.

(2) File structure (cd, web, binary, bulletin boards, etc.).

(3) Proprietary

l. What is the desired modeling platform (i.e., personal computer, work \station, web-based . . .)?

2 Summary of Discussions

Introduction

The concepts and foundation for the development of both human and ecological risk assessment have been around for several decades. Past research efforts have yielded methodologies for conducting risk assessments, including exposure and effects assessment, as well as procedures for investigating uncertainty propagation through these models. The basic premise is to calculate risk as a function of both exposure, human or ecological, and effects resulting from exposure. The effects component can be acute or chronic. Therefore, the risk assessment paradigm is typically a problem formulation leading to both an exposure and effects assessment. The combination of the exposure and effect components results in a calculated risk characterization. Risk assessments are useful planning tools for the evaluation and determination of the impact of contaminants on both human and ecological resources.

From a military perspective, the contamination to air, surface water, and groundwater from MRCs has been of increasing concern in the past several years as the result of the closing of munition plants and bases. The assessment of the exposure to ecological units from the many mediums through the use of an exposure model is required to determine the risk associated with exposure to MRCs from these media. This assessment is valuable for permitting and planning activities, as well as for the possible cleanup operations of contaminated sites, should the risk to an ecological unit become too great (Deliman and Gerald 1998).

Background

Historically, there have been several options for conducting risk assessments. Perhaps the simplest of these involves direct field measurements to estimate exposure concentrations. These direct exposure estimates are then compared to effects data to estimate a risk, i.e., a risk quotient. One problem with this method is the assumption that the exposure concentration collected at the sample site is constant, both spatially and temporally. To gain an understanding of the time or spatial variance influence upon the estimated exposure concentration, a screening- or comprehensive-level model should be utilized.

Initially, when an indication of the level of risk associated with an exposure is desired, the use of a screening-level model will maximize the amount of information provided while minimizing the amount of effort required to obtain the necessary information to make a risk assessment. A screening-level exposure model refers to use of simplified, quantitative, predictive methods that minimize time and effort for implementation. Simplification is achieved by making assumptions that reduce the complexity of the predictive mathematical formulations and input data. If the results of the risk estimated by using screening-level exposure models indicate undesirable risk levels to either human or ecological resources, a more comprehensive exposure modeling approach should be employed. Comprehensive models being more physically based, both spatially and temporally, than the screening-level models can produce results which are more accurate and defendable. Selection of a comprehensive exposure model results in increased data and computing resource requirements.

During the workshop, the concept of the platform for the development of ARAMS was discussed. The three choices that were presented as viable alternatives were (1) personal computer-based, (2) workstation-based, and (3)web-based. Of these three, the web-based platform offered the most advantages, as well as combining the best of PC and workstation environments. The web-based system design was selected for ARAMS. The primary advantage of a web-based system is the ability to easily update and maintain databases which are required for both effect and exposure assessments. Users of ARAMS can access and search databases via the Internet by launching applets in the background. In addition, web-based systems offer the advantage of distributed computing. Distributed computing enables users without high-powered computing capabilities the option of running programs at remote locations. It is important to note that some security issues will have to be addressed for access to secure sites for some military applications.

The ARAMS will be developed for the purpose of conducting both screening- and comprehensive-level ecological risk assessments. Development of this system will incorporate current state-of-the-art modeling technologies and will further utilize concurrent research efforts in the U.S. Army Fate and Effects Research Program. The ARAMS will be a tool to characterize, integrate, and estimate ecological risk. The system will provide several tiers of complexity such that screening-level and complex models issues can be addressed. The system will include: (a) screening-level assessments based on simple exposure-response relationships and limited spatial and temporal scales, (b) an expanded assessment capability based on linkage of more rigorous exposure and ecological assessment techniques, and (c) linkage of ecological risk, comprehensive exposure models, and integrated temporal-spatial exposure, i.e., probabilistic estimate of exposure for individuals/population in time and space.

ARAMS will contain the following components: (a) screening-level models, (b) comprehensive models, (c) population models, (d) an uncertainty component,

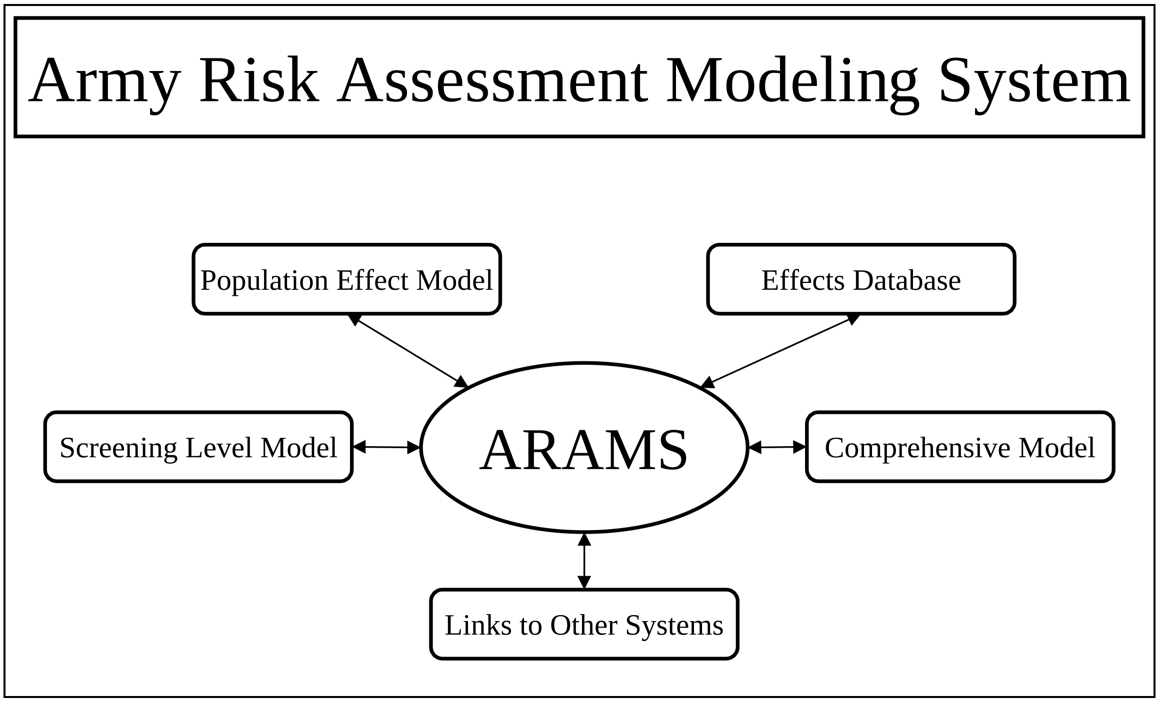

Figure 1. Schematic for the ARAMS

(e) bioaccumulation databases, and (f) effects databases (Figure 1). The uncertainty element will be built into each component of ARAMS. This feature permits users to quantify uncertainty and conduct sensitivity analysis at any point during a simulation. An additional feature of the system is that it will be linked to several systems and legacy codes.

Screening-level model

The screening-level component contained within ARAMS can be used for conducting simple or screening-level risk assessments. Simple risk assessment refers to exposure concentrations estimated from field data while screening level implies that the exposure concentrations are estimated from simple exposure models. Components of the screening-level module include a physico-chemical database, risk calculator, effects database, screening-level exposure models, and linkages to other fate and transport exposure models (Figure 2). To accomplish this objective, the workshop participants recommended the incorporation of FRAMES as the platform for the screening-level model (Whelan et al. 1999).

FRAMES was developed by Pacific Northwest National Laboratory for the DoE. FRAMES is an object-oriented model that is still under development. Within FRAMES will reside a collection of computer algorithms that will simulate the following elements of a transport, exposure, and risk assessment system: contaminant source and release to environment (including surface hydrology), overland flow transport, vadose-zone transport, food-supply

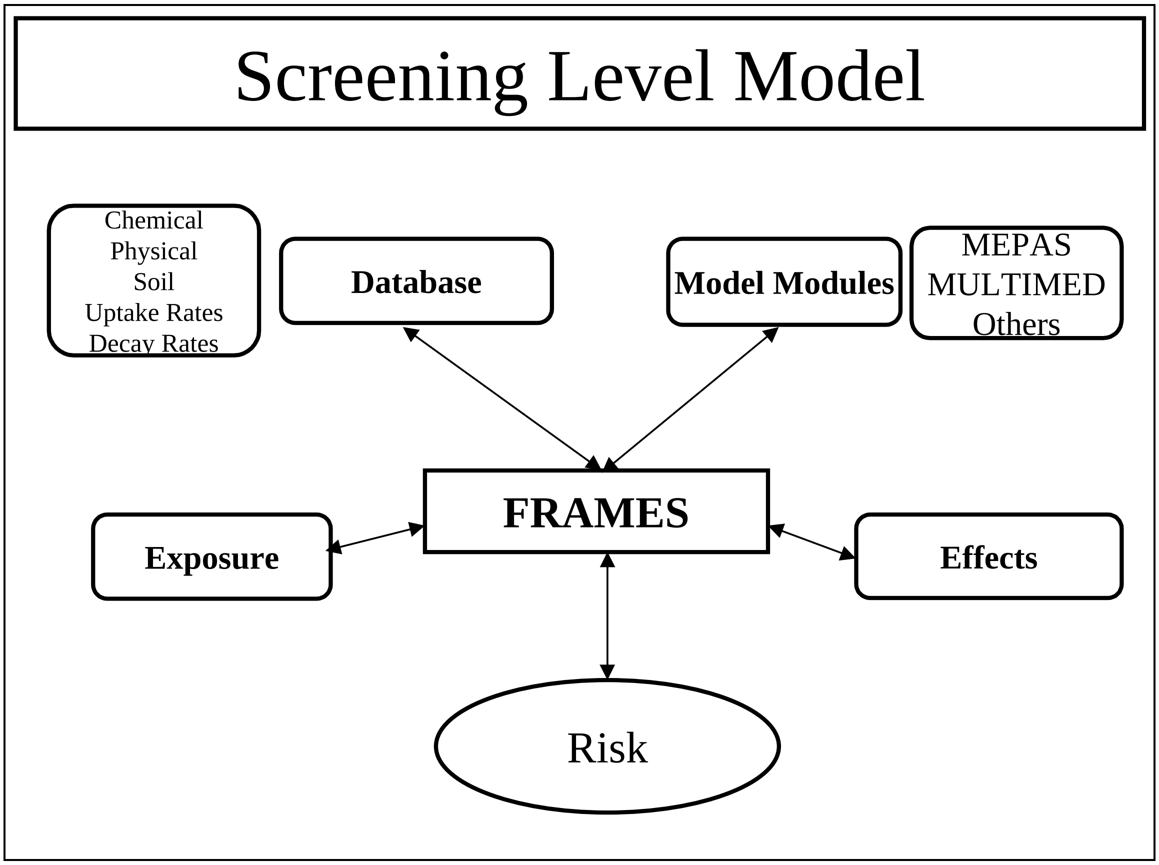

Figure 2. Screening-level model

transport (including animals and plants to humans), intake computation, and health impacts.

The database contained within the screening-level model provides chemical and physical properties, uptake and decay rates, as well as a soil properties characterization tool for input into the exposure modules. The exposure models currently contained within FRAMES are those developed for the Multimedia Environmental Pollutant Assessment System (MEPAS) and Multimedia Exposure Assessment Model (MULTIMED) (Buck et al. 1995, Salhotra et al. 1993).

The human health exposure components include the exposure pathways, the intake routes, and the human health effects database (IRIS and HEAT (Whelan et al. 1999)) containing noncarcinogenic and carcinogenic chemicals as well as radionuclides.

Models that will be included into FRAMES in the near future are RECOVERY and the Hydrologic Evaluation of Landfill Performance (HELP). RECOVERY is a sediment water interaction model to assess the impact of toxicants in the aquatic environment (Boyer et al. 1994). HELP is a landfill modeling tool to assess the movement of contaminants through contaminated soils and dredge material (Schroeder et al. 1994). It can be applied to evaluate landfill performance.

Comprehensive model

Similar to the screening-level model, the comprehensive model will have access to databases for physcio-chemical properties. The primary difference is that the comprehensive model (CE-QUAL-ICM/TOXI) (Wang et al. in preparation) can account for spatial and temporal variance in exposure estimation (Figure 3). Processes within the comprehensive model include chemical and solids transport in the water column and sediment bed, sorption to dissolved organic matter and three solids (sand, silt, and clay), chemical and biological degradation, and volatilization (Wang et al. in preparation). In addition, modules for addressing trophic transfer, bioaccumulation, and bioconcentration of contaminants will be available.

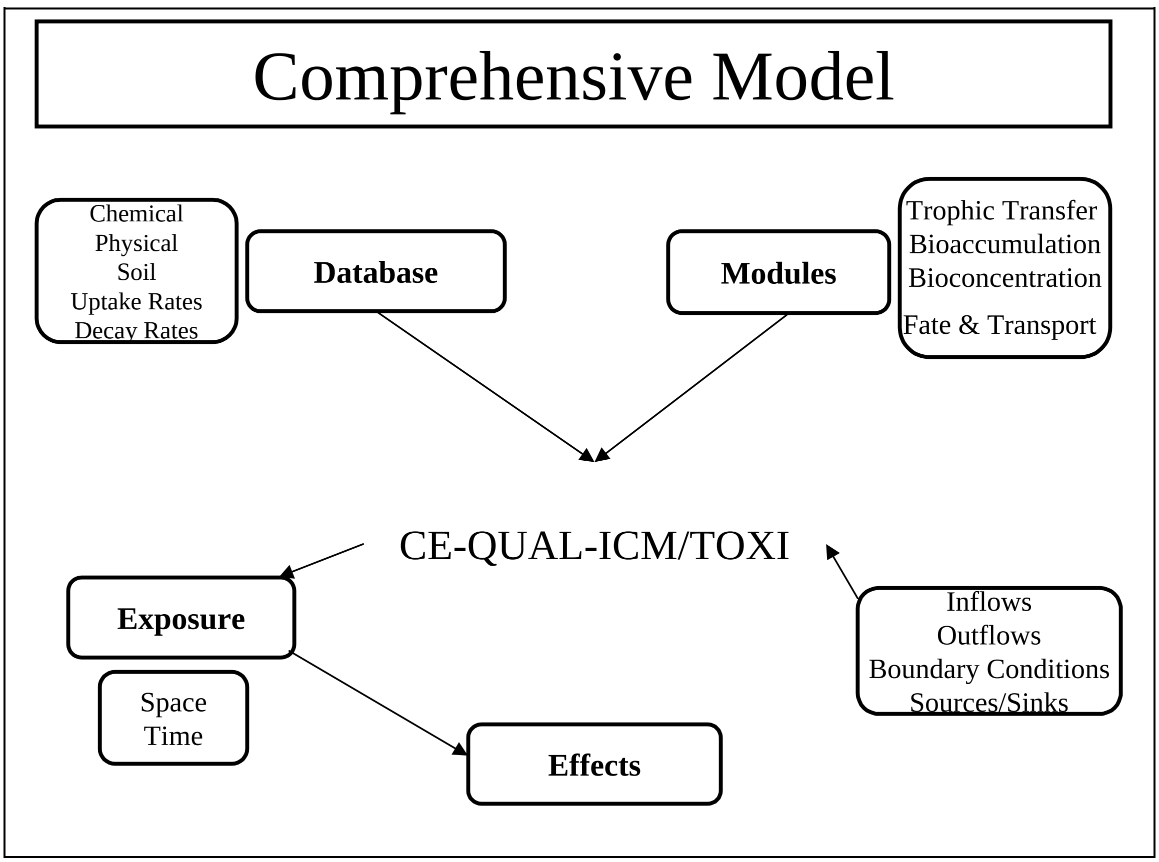

Figure 3. Comprehensive model

CE-QUAL-ICM/TOXI (Wang et al. in preparation) must be linked to comprehensive hydrodynamics codes such as CH3D and RMA10 (Environmental Modeling Research Laboratory 1998b) that compute the input required to run the water quality and contaminant transport model. In addition, the user has to provide extensive input relating to contaminant boundary conditions, sources and sinks, and contaminant inflows and outflows.

The model produces exposure concentrations in the water column and sediment bed over time and space (one-, two-, or three-dimensional (1-D, 2-D, 3-D)). This information can be exported to other ARAMS modules or can be coupled with the effects database to estimate a comprehensive human or ecological risk assessment.

Population-effect model (PEM)

Population-effect models will be included in ARAMS to estimate the risk to single organisms, populations, and ecosystems. Both aquatic and terrestrial effects components will be incorporated. The first step is the determination of the effect on a single organism. Once this is achieved, the population models can be utilized to estimate the overall effect on a given population. For example, effects that can be seen in the environment can correspond to reduction in fertility, survival of young and adults, and susceptibility to predation. Initially, the metapopulation effect models included in ARAMS will be for an estuarine amphipod and a marine polychaete (Figure 4). The coupling of these and other metapopulation modules will allow for an evaluation of the interactions of population groups and the effect of contaminant exposure within a given population, resulting in an ecological risk assessment.

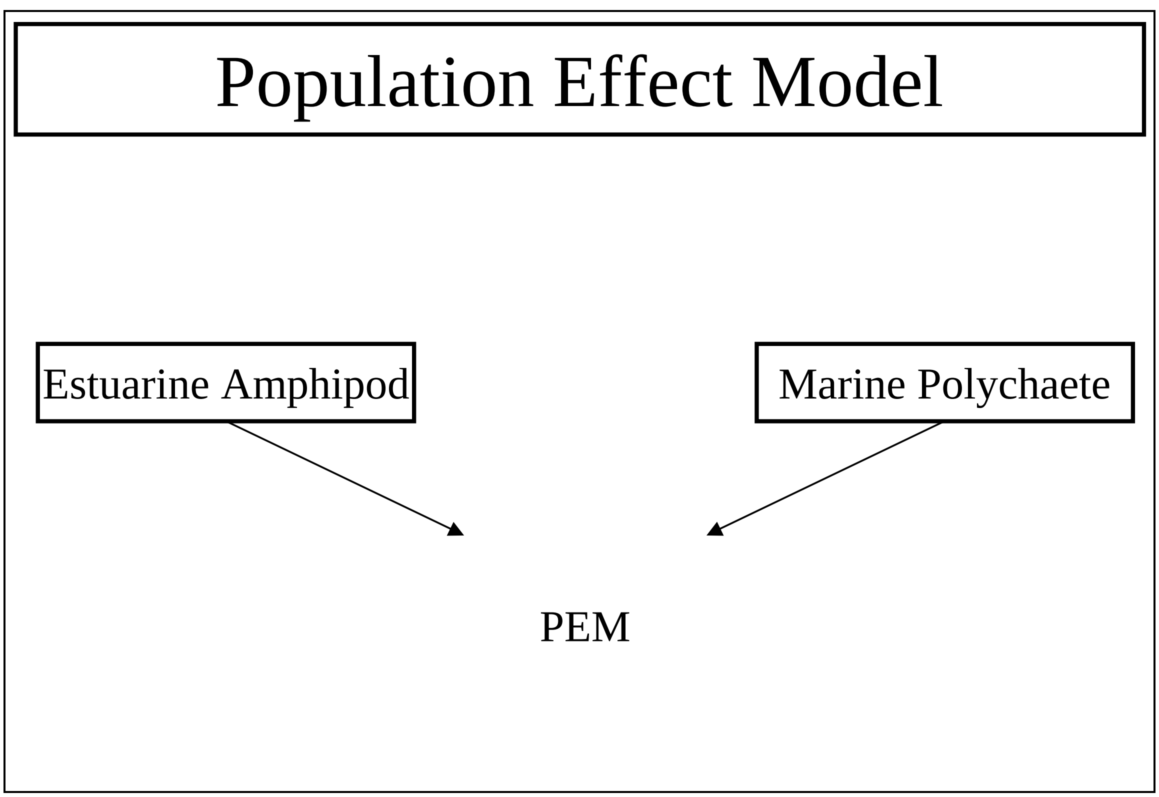

Figure 4. Population-effect model

Another component of the population-effect model will be the incorporation of food chains or food webs. This feature will allow for the evaluation of trophic transfers of contaminants in the ecosystem. Coupling these population effects models with the exposure data predicted from the comprehensive models will provide a comprehensive environmental risk assessment.

Effects database

An integral part of any risk assessment modeling system is the effects database. The effects database provides the relationship between the exposure concentration and the effects to individual organisms. The effects database in ARAMS will contain the Environmental Residue-Effects Database (ERED) and the Biota-Sediment Factor Database (BASF) (Figure 5). ERED is a compilation of literature data where both biological effects and tissue contaminant concentration were simultaneously measured in the same organism. Biological effects refer to a measured or observed effect such as reduced survival, growth, reproduction, etc. Currently, the biological effects within an organism are limited to those linked to specific contaminants observed in the tissue.

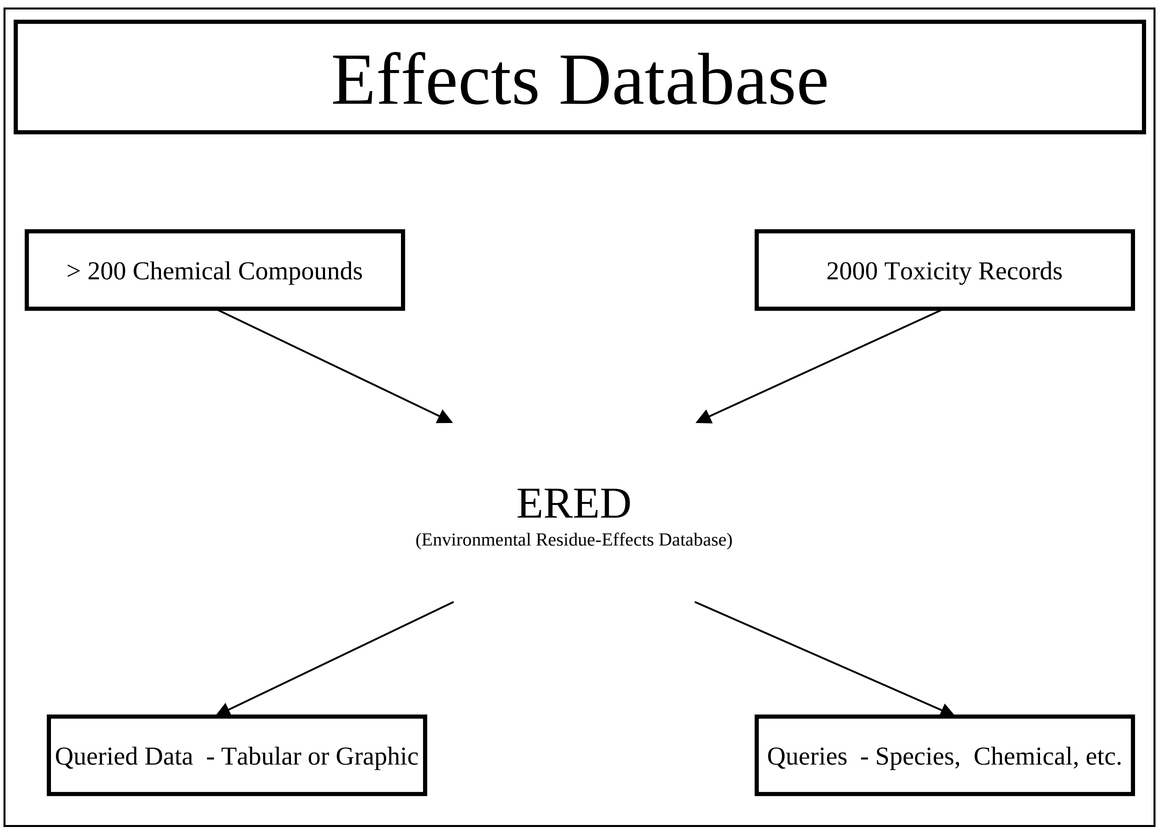

Figure 5. Effects database

The ERED database contains some organism bioaccumulation data, although bioaccumulation is a measurable phenomena rather than an effect. The measured or predicted level due to bioaccumulation is not sufficient information to conclude that the contaminant will produce an adverse effect. The key is to compare the level due to bioaccumulation to a measurable biological effect like those in the ERED database.

The BASF database is a collection of laboratory and field generated BASF numbers. The database also contains lipid values for numerous organisms which can be used in lieu of actual organism lipid content. BASF numbers are used to predict more environmentally realistic bioaccumulation levels when using the Thermodynamic Bioaccumulation Potential (TBP) formulation. The TBP estimates the bioaccumulation potential directly from the contaminant sediment concentration, organism lipid content, contaminant BASF, and sediment organic carbon.

Links to other systems

Based on workshop consensus, it was decided that the ARAMS would provide links and hooks to access legacy codes and other modeling systems. This component of ARAMS maximizes the use of existing codes with minor development of linkages. Linkages will be developed for transferring input and output between the modules and/or components. Initially, systems that will be linked into the ARAMS will include the three DoD modeling systems which provide a comprehensive graphical user environment (Figure 6). All three DoD modeling systems can be characterized as comprehensive components of ARAMS.

The WMS is used for performing hydrologic and water quality analysis and supports several legacy codes including HEC1, TR-55, CASC2D, and HSPF (Environmental Modeling Research Laboratory 1998a). These models represent both widely used lumped parameter models, as well as more advanced 2-D distributed parameter watershed models. Models contained in the WMS can be used to address the terrestrial component for exposure assessments.

The GMS is used for performing groundwater simulations, site characterizations, model conceptualizations, and geostatistical interpretation (Environmental Modeling Research Laboratory 1999). GMS supports several legacy codes including MODFLOW, FEMWATER, MT3D, RT3D, and SEAM3D. These models represent more advanced 3-D water and contaminant transport models for exposure for human (drinking wells) and ecological exposure (groundwater-surface water interactions). Models contained in the GMS can be used to address the groundwater component for exposure assessments.

The SMS is used for performing model conceptualization, mesh generation, statistical interpretation, and visual examination of surface water model

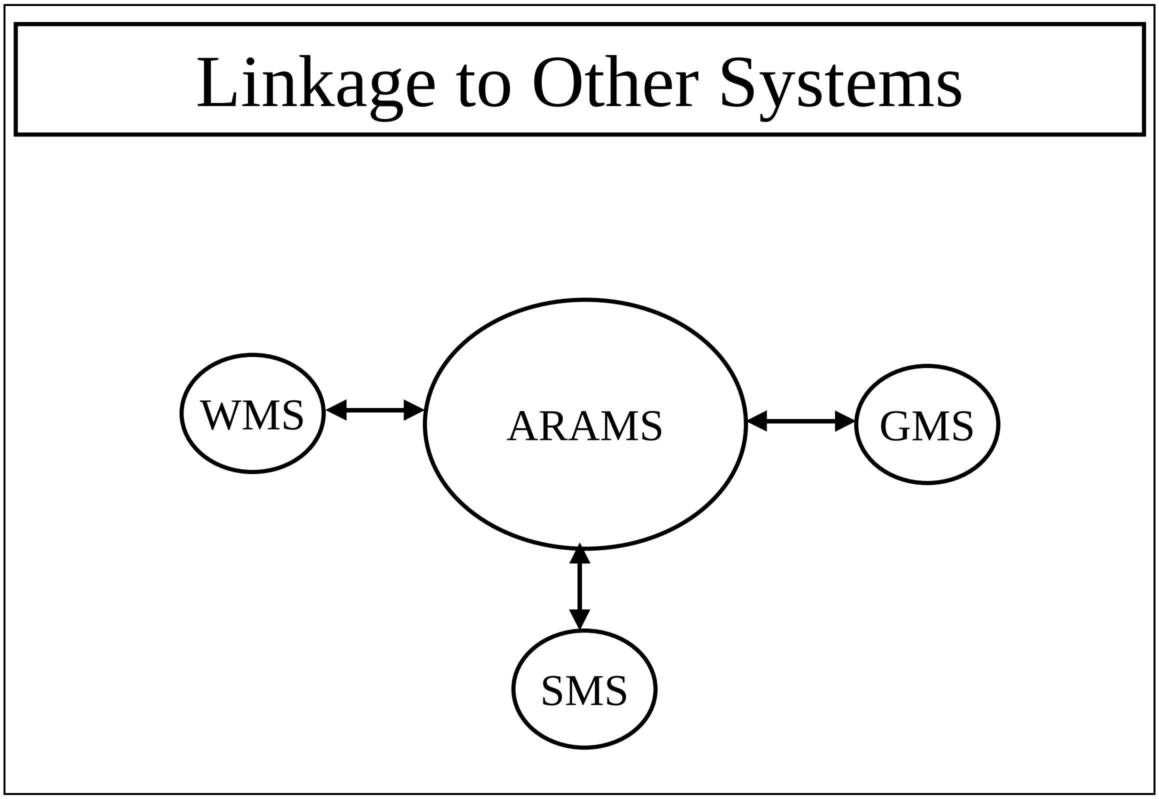

Figure 6. Linkage of ARAMS to existing comprehensive modeling systems

simulations (Environmental Modeling Research Laboratory 1998b). SMS supports several hydrodynamics and water quality legacy codes including RMA10, TABS-MD, CH3D, and CEWES-ICM (Wang et al. in preparation). Models contained in the SMS can be used to address the aquatic component for exposure assessments including both water column and bottom sediments.

Future efforts will include linkage of additional legacy codes from the EPA, USGS, DoE, and universities. The ARAMS flexible design will allow implementation of other systems and legacy codes without the burden of maintenance. This is accomplished through the ARAMS by providing only the linkage to these systems. Code maintenance will be the responsibility of the owners of the legacy codes and modeling systems.

3 Workshop Recommendations

During the workshop a list of system attributes was developed for ARAMS. The list was made in an effort to provide a flexible framework that would allow for adaptation of emerging technologies as well as provide the users seamless access to databases contained at web-site locations. For ARAMS to be successful, the consensus was that the following points would have to be addressed by the system:

- Web-Based, Network Services
- Ecologically Oriented and Spatially Explicit
- Contains Components for Both Human & Ecological Risk
- Standard Hooks Between Models
- Integration of Legacy Models
- Modular to Include New Models, Science
- Couples Exposure, Fate, Effects, Uncertainty, Economics - Risk vs Cost
- Launches Off User's Desktop, Probably in Windows NT, Supports UNIX, PCs
- Transport Use if Used for High Performance Computing (HPC)
- Data Standards to Allow as Seamless as Possible Data Access
- Client/Server Relationships to Access Remote Data, Simulations
- Multimedia from Outset
- Differing Levels of Tools From Screening to HPC

- Leverage Funding from Other Federal Sources
- Self Defensive Software - Units, Range Checking
- Security “Black Box” - For Certain Military Applications
- Smart - Adaptive Software

The development of ARAMS is anticipated to take several years to complete. One last major point discussed at the workshop was the necessity of choosing a proper location to test the system. A site would have to be chosen with a plethora of data such that screening- and comprehensive-level approaches for risk assessment for both ecological and human risk could be validated.

References

Boyer, J. M., Chapra, S. C., Ruiz, C. E., and Dortch, M. S. (1994). "Recovery, a mathematical model to predict the temporal response of surface water to contaminated sediments," Technical Report W-94-4, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Buck, J. M., Castleton, K. J., Whelan, G., McDonald, J. P., Droppo, J. G., Sato, C., Strenge, D. L., and Streile, G. P. (1995). *Multimedia environmental pollutant assessment system (MEPAS) application guidance*. Pacific Northwest National Laboratory, Richland, WA.

Deliman, P. N., and Gerald, J. A. (1998). "Development of a multimedia exposure assessment model for evaluating ecological risk of exposure to military-related compounds (MRCs) at military sites," TR-IRRP-98-9, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Environmental Modeling Research Laboratory. (1998a). *Department of Defense watershed modeling system - reference manual & tutorials.* WMS V 5.1, Brigham Young University, 368B CB, Provo, UT.

__________. (1998b). *Department of Defense surface water modeling system - reference manual & tutorials.* SMS V 5.0, Brigham Young University, 368B CB, Provo, UT.

__________. (1999). *Department of Defense groundwater modeling system - reference manual & tutorials.* GMS V 3.0, Brigham Young University, 368B CB, Provo, UT.

Salhotra, A. M., Mineart, P., Sharp-Hansen, S., Allsion, T., Johns, R., and Mills, W. (1993). "MULIMED, the multimedia exposure assessment model for evaluating the land disposal of wastes - model theory," NTIS Report PB93-186 252/AS, National Technical Information Service, Springfield, VA.

Schroder, P. R., Dozier, T. S., Zappi, P. A., McEnroe, B. M., Sjostrom, J. W., and Peyton, R. L. (1994). "The hydrologic evaluation of landfill performance (HELP) model: Engineering documentation for version 3," EPA/600/9-94/168b, U.S. Environmental Protection Agency Risk Reduction Engineering Laboratory, Cincinnati, OH.

Wang, P. F., Martin, J. L., Wool, T., and Dortch, M. S. CE-QUAL-ICM/TOXI, "A three-dimensional contaminant model for surface water: Model theory and user guide" (in preparation), U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Whelan, G., Buck, J. W., Gelston, G. M., and Castleton, K. J. (1999). *Framework for risk analysis in multimedia environmental systems - Training manual*. Pacific Northwest National Laboratory, Richland, WA.