

UNCERTAINTY ANALYSIS AND PARAMETER ESTIMATION: A MOU WORKING GROUP

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Abstract: An important issue facing the application of **multimedia environmental models** (MEMs) is the inherent uncertainty associated with their conceptual/mathematical model(s) and parameterization. Since many MEM applications involve an assessment of risk to the public health and/or environment, the use of uncertainty and risk analysis techniques and methods would enhance the insights and predictions derived from these models. A working group to examine uncertainty and risk analysis has been created under a Federal Interagency Memorandum of Understanding (MOU) on MEMs. The purpose of this MOU is to facilitate cooperative research on MEMs. Objectives of the working group include coordination of ongoing and anticipated new research on assessing uncertainty in the predictions of MEMs, development of a common understanding of various ways to address uncertainty, and the identification, evaluation, and comparison of tools for assessing uncertainty and risk related to MEM applications.

INTRODUCTION

A Memorandum of Understanding (MOU) has been established among eight United States Federal Agencies for the purpose of facilitating cooperation and coordination in the research and development (R&D) of multimedia environmental models. The MOU is intended to (1) provide a mechanism for the cooperating Federal Agencies to pursue a common technology in multimedia environmental modeling with a shared scientific basis; (2) reduce redundancies and improve common technology through exchange and comparisons of multimedia environmental models, software and related databases; and (3) facilitate the establishment of working partnerships among the cooperating Federal Agencies' technical staff and designated contractors in order to enhance productivity and mutual benefit through collaboration on mutually-defined research studies such as the development of a common model-data framework.

The working partnerships are established as formal working groups under the MOU. A working group is initiated by submitting a Phase I proposal to the MOU Steering Committee. The Phase I proposal is a brief statement of the purpose, goals, and objectives of the working group. Upon approval of the Phase I proposal, a more detailed Phase II proposal is prepared and submitted to the MOU Steering Committee. Approval of the Phase II proposal formally establishes the working group.

A working group on Uncertainty Analysis and Parameter Estimation has been established under the MOU. The objectives of the working group include coordination of ongoing and anticipated new research on assessing uncertainty in the predictions of MEMs, development of a common understanding of various ways to address uncertainty, and identification, evaluation, and comparison of tools for assessing uncertainty and risk related to MEMs applications. The approved Phase II proposal for the working group is provided below.

UNCERTAINTY ANALYSIS AND PARAMETER ESTIMATION - PHASE II PROPOSAL

Background:

An important technical issue facing the application of **multimedia environmental models (MEMs)** is the inherent uncertainty associated with their conceptual/mathematical model(s) and their parameter input estimates. Since many MEMs applications involve an assessment of risk to the public health and/or environment, the use of uncertainty analysis techniques coupled to more robust parameter estimation methods would greatly enhance the insights and predictions derived from these models. Decisions involved in selecting and applying these uncertainty methods support the need for (1) *a priori* strategy which would systematically identify the various sources of uncertainty [e.g., lack of knowledge, natural variability, measurement or sampling error, randomness in “real-time” processes (Kundzewicz, 1995)], and (2) *a posteriori* strategy for comparing relative uncertainty estimates (e.g., conditional uncertainty measures or ranking of uncertainties). Therefore, the establishment of a working group to examine uncertainty analysis and parameter estimation techniques could greatly assist many of the MOU participating organizations facing these problematic issues. Many of the MOU participating agencies, notably the USGS, ARS, USNRC, and EPA, are currently funding research studies related to this topic. Individually, these agencies also fund field studies, modeling assessments and training courses related to MEMs. Long-term support of a working group in this area would facilitate development of a common understanding and technical framework to address the issues of uncertainty and parameter estimation in the application of MEMs, and coordination of related Federally-funded research studies.

Objectives:

- To coordinate ongoing and anticipated new research that focuses on parameter estimation methods, and uncertainty assessment strategies and techniques that support MEMs. In pursuing this general objective, the following specific technical objectives are proposed:
- To develop a common understanding of the sources of uncertainty, and various ways to address uncertainty (e.g., strategies and methods for quantifying).
- To identify, evaluate, and compare, both strategies and tools presently available for assessing uncertainty, which may be useful for MEMs applications.

- To develop, as needed, parameter estimation methodologies for use with available digital databases (e.g., available GIS-based datasets on the watershed scale).
- To establish the degree of applicability of existing and newly developed parameter estimation techniques to all MEMs, and where necessary, propose recommendations for enhancing their general utility.
- To assess, and where appropriate, test newly-developed techniques (e.g., the UCODE and PEST codes; MOCOM code developed at the University of Arizona; and the GLUE procedure designed at the University of Lancaster, UK) for parameter estimation and uncertainty analysis of MEMs.
- To facilitate exchange of newly-developed and tested parameter estimation, and uncertainty assessment strategies and methods, and to advance the knowledge in these fields by convening and conducting technical workshops, special sessions at professional meetings (e.g., AGU meetings), and training courses (e.g., USGS training facility at Lakewood, CO and USNRC Professional Development Center in Rockville, MD).
- To develop methods to better communicate uncertainty estimates to decision makers such as improved visualization techniques and decision-support system approaches.

Outcomes: A consistent and systematic basis for identifying and estimating uncertainty using tested methodologies, and improved (i.e., more robust) methods for estimating model parameters and boundary conditions (e.g., fluxes). These methodologies would include both strategies, and “tool boxes” of new methods and techniques for determining confidence limits on MEMS results. Strategies would include those presently under development and testing for hydrologic conceptual/mathematical model and parameter uncertainty. Tools would include both uncertainty assessment techniques, and sensitivity analysis and visualization methods. Techniques would be generally applicable to a wide range of field application problems and MEMs. Communicating uncertainty estimates to decision makers would utilize these techniques.

Activities: A number of activities are proposed for the working group over the 5-year lifespan of the MOU.

- Coordinate ongoing research studies in parameter estimation and uncertainty assessment using monthly working group teleconferences, e-mail correspondence, sharing of Web sites and updates on technical workshops, training courses, field studies, and code developments both within and outside of the working group purview . (To conserve travel funds, the working group will only meet at working-group-sponsored training courses, special sessions at professional meeting, and workshops.)
- Develop a summary of the uncertainty analysis and parameter estimation methods currently being used in the scientific modeling community. This summary would be tabularized and published on the MOU web site.

- Explore the development of comprehensive data sets in selected climatic and physiographic regions for model development and testing. Initial focus would be on the development of data sets representative of a humid site and an arid site. The development of synthetic data sets will also be examined.
- Review and assess strategies being developed and explore the possibility for peer review of uncertainty estimation strategies by working group members and collaborators.
- In conjunction with the *Framework Working Group on "Software System Design and Implementation for Environmental Modeling,"* examine the linking of multiple models which may perpetrate cascading errors through the MEMs thus contributing to the complexity of uncertainty assessments. (Although methods to address this issue are limited, some MOU participants have begun to address these cascading error and associated complexity issues in their modeling activities).
- Establish a working relationship with the *Framework Working Group* to facilitate the design and development of a generic "tool box" of uncertainty analysis, sensitivity analysis, and parameter estimation tools for use in the modeling frameworks being developed by MOU participants.
- Participate in the American Geophysical Union (AGU) 2002 Spring Meeting session "H07 Uncertainty Assessments for Environmental Modeling in the Unsaturated Zone" being convened by USNRC, DOE, and EPA to be held in Washington, DC, May 28-31, 2002.
- Host a special session on uncertainty analysis and parameter estimation at the 2nd Federal Interagency Modeling Conference to be held in Las Vegas, NV, July 28 - Aug 1, 2002.
- Enhance ongoing research studies that address parameter estimation and uncertainty assessments through coordination with working group members, and develop specific proposals to enhance existing parameter estimation methods and uncertainty techniques suitable for use in advanced decision support models (see *Attachment* from ARS for a specific proposal example).

Products: Products will include documentation of the aforementioned activities, preferably on the MOU Web site, and jointly coordinated strategies, methods and "tools":

- A directory, in tabular form, of existing Federal and non-Federal programs to include reports and related Web sites relating to parameter estimation and uncertainty assessments relevant to MEMs. This directory will be posted and maintained on the MOU Web site.
- A "tool box" of selected uncertainty analysis, sensitivity analysis, and parameter estimation methods will be developed for general application to a variety of multimedia

environmental models. The “tool box” will be developed in collaboration with the *Framework Working Group*.

- Professional papers on the issues of uncertainty analysis and parameter estimation to be published in the technical proceedings report such as the *Proceedings of the 2nd Federal Interagency Modeling Conference*.
- Technical presentations and published abstracts for working-group-sponsored special sessions such as the upcoming AGU 2002 Spring Meeting.
- Published technical reports on development and testing of parameter estimation and uncertainty assessment strategies such as the USNRC supported research on parameter uncertainty at Pacific Northwest National Laboratory, and hydrogeologic conceptual/mathematical model uncertainty at the University of Arizona.

Resources:

USGS:

The USGS is collaborating with the ARS and the NRCS to integrate the USGS Modular Modeling System (MMS) with the ARS supported Object Modeling System (OMS) being developed by Dr. Olaf David from the Friedrich Schiller University, Jena, Germany. A part of this integration is the development of a set of uncertainty analysis and parameter estimation tools that can be used with any model developed within the OMS/MMS framework. These tools are also being developed collaboratively with the NSF funded “Sustainability of Semi-Arid Hydrology and Riparian Areas (SAHRA)” program at the University of Arizona and the Modeling research group at the University of Lancaster, UK. Personnel and financial resources among the collaborators are committed to this effort over the next 2-4 years. Documentation on the methods being developed will be provided for incorporation in the directory of methodologies being developed. The USGS is also a program chair for the 2nd Federal Interagency Modeling Conference and will provide the resources necessary to support the proposed special session on uncertainty analysis and parameter estimation.

Efforts to evaluate model uncertainty are pursued routinely in the USGS using traditional sensitivity analysis. Such analyses, however, only quantify uncertainty in a limited way. More useful methods are being developed both outside and within the USGS. The efforts within the USGS are diverse and this brief description cannot include all efforts, but a few highlights are provided. Richard L. Cooley (recently retired from the USGS) is considering expanded inferential statistical methods to quantify uncertainty in models of systems that are nonlinear in the parameters, as are most environmental systems of interest.

Reducing and quantifying uncertainty depends on the approaches taken and methods used over the entire model development process, which motivated Mary C. Hill (USGS) to develop a set of “Methods and Guidelines for Effective Model Calibration, USGS Water-Resources Investigation Report 98-4005” (Hill, 1998) (to view or download the report please go to the following Web site: <http://wwwbrr.cr.usgs.gov/projects/GW_Subsurf/mchill/pubs/method/

index.shtml>). These methods and guidelines have been applied to evaluate many field sites. Also, Mary C. Hill, in collaboration with Claire R. Tiedeman and D. Matthew Ely (Tiedeman and others, 2001; Hill and others, 2000), developed methods based on inferential statistics to evaluate the importance of observations and parameters in the context of predictions of interest. These methods can be used to plan future data collection and model calibration efforts to obtain additional observations, such as hydraulic heads, streamflow gains and losses, and concentrations from tracer tests, and to obtain additional information about other aspects of the conceptual/mathematical system, such as hydrogeologic framework, hydraulic conductivities, and recharge distribution. Monte Carlo efforts have been considered by J. J. Starn of the USGS's Connecticut District to investigate probable contributing recharge areas to wells, however, as related to ground-water systems, Monte Carlo methods have not generally been well developed or used extensively within the USGS.

USNRC:

The USNRC is funding work at the University of Arizona (UAZ) on hydrogeologic conceptual/mathematical uncertainty. The UAZ investigators have developed "A Comprehensive Strategy of Hydrogeologic Modeling and Uncertainty Analysis for Nuclear Facilities and Sites" which has been shared with the Federal working group participants, and was presented at USNRC headquarters in August 2001. This work will be completed in Fall 2002. The UAZ final research results including field application testing will be present to the working group on August 1-2, 2002 at NRC headquarters. Information on the UAZ related monitoring study with field datasets can be found at their Web site: <http://ag.arizona.edu/NRC/nrc.html>. A companion study at Pacific Northwest National Laboratory (PNNL) is developing a parallel methodology on parameter uncertainty. To date PNNL researchers have produced two reports (Meyer and Gee, 1999; and Meyer and Taira, 2001). Details on the PNNL study objectives, publications, test case problems and tools developed can be download at their Web site: <http://nrc-hydro-uncert.pnl.gov/code.htm> which is entitled "Hydrologic Evaluation and Uncertainty Assessment: Research Sponsored by the U.S. Nuclear Regulatory Commission." The USNRC researchers are planning to incorporate new studies on uncertainty into their research program as described in their recently released "Radionuclide Transport in the Environment."

EPA:

EPA is developing uncertainty and sensitivity assessment methods for the Multimedia, Multipathway, Multireceptor Risk (3MRA) Assessment model. 3MRA is an important software code being used by EPA's Office of Solid Waste for risk assessments of RCRA sites. 3MRA is a forward-calculating analysis that evaluates the multiple exposure pathway risks to human and ecological receptors. A forward-calculating analysis starts with a chemical concentration in a waste management unit, estimates the release and transport of the chemical in various environmental media, and predicts the exposure and risk that result from those concentrations. Comprised of 25 individual software components representing 17 source-term and media/pathway/receptor modules, 3MRA represents an integrated set of environmental models designed within the more robust Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) modeling framework system.

The 3MRA model provides a state-of-the-science environmental modeling technology that simulates multimedia (air, water, soil, sediments), multipathways for exposure (food ingestion, water ingestion, soil ingestion, air inhalation, etc.), multireceptors for exposure (resident, farmer, gardener, fisher, ecological habitats and populations, etc., with various cohort considerations), risk assessment (human cancer and non-cancer effects, ecological population and community effects), and an overall national assessment (e.g. strategy used to inform regulatory decisions). Key aspects of 3MRA include an overlay of site-based, regional, and national databases, with actual site data representing 201 national waste disposal sites and 419 site-waste management unit combinations; cumulative exposures across pathways and time; conservation of mass in source terms; and an inherent probability-based risk assessment design that allows the modeler to address key aspects of input data variability and uncertainty. 3MRA allows for evaluation of 5 waste management unit types (i.e. landfill, waste pile, aerated tank, surface impoundment, and land application unit).

The development of 3MRA has been driven by its initial intended application to a nationwide risk assessment underpinning EPA's Office of Solid Waste's proposed Hazardous Waste Identification Rule (HWIR). The HWIR is designed to identify which waste streams can safely be released from existing hazardous waste disposal requirements under Subtitle C of the Resource Conservation and Recovery Act (RCRA). The rule is designed to evaluate "mixture and derived from" waste streams associated with regulated "listed" hazardous wastes. The mixture and derived-from rules are a key part of the RCRA rules that define when wastes are regulated as hazardous wastes. Under the mixture rule, a listed hazardous waste remains regulated as a hazardous waste when it is mixed with a non-hazardous waste. Under the derived-from rule, waste generated from the treatment, storage, or disposal of a listed hazardous waste also remains regulated as a hazardous waste. "Mixed and derived from" hazardous waste streams with constituent chemical concentrations less than "exit" levels calculated by 3MRA could be reclassified as nonhazardous solid waste. 3MRA represents a software development endeavor never before undertaken on this scale by EPA's Office of Research & Development, while achieving an operational status that directly meets program office evaluation needs.

Please see the Web site at <<http://www.epa.gov/OSWRCRA/hazwaste/id/hwirwste/risk.htm>> for a more detailed description of the 3MRA modeling system, and go to the following Web site which contains documentation for the 3MRA Software at <<http://www.epa.gov/ceampubl/hwir.htm>>.

EPA's National Exposure Research Laboratory is currently working to identify and develop appropriate approaches, methods, and guidance for conducting uncertainty and sensitivity analyses (UA/SA) on multimedia models such as 3MRA. EPA has identified significant needs to conduct research in these areas, in the long-term and in the short-term. Long-term research goals in UA/SA have identified an overall need to develop tools and associated guidance to support various (future-concept) multimedia modeling systems and applications. Short-term UA/SA research needs are driven by a requirement to facilitate productive peer review of the 3MRA-HWIR assessment strategy by EPA's Science Advisory Board. An aspect of EPA's research program includes construction of a 270 GHz PC-based supercomputer cluster. For more detailed discussion of USEPA/ORD/NERL/ERD's activities please refer to Attachment 3.

EPA's Office of Radiation and Indoor Air (ORIA) is working with other Federal agencies on the Interagency Steering Committee on Radiation Standards's (ISCORS) to develop a Federal-wide parameter database for multimedia environmental models. Projects related to the MARPAR effort may ultimately include (a) a catalog of currently available sources of parameter values and distributions, both in the open-literature and in the "grey literature"; (b) guidelines on parameter QA; (c) a catalog of resources determining site-specific parameters; (d) a catalog of modeling scenarios; and (e) the development of consensus databases of parameter values and distributions. Because of the movement towards probabilistic risk analyses, any catalogs, guidance, or databases developed through ISCORS will need to include information on parameter uncertainties. Coordination with this Workgroup is therefore essential.

Another EPA project is an enhancement to the FRAMES Sensitivity/Uncertainty Module that allows the direct use of databases containing parameter distributions in Monte Carlo calculations. In addition, ORIA has sponsored a two-volume report on "Understanding Variation in the Partition Coefficient, K_d " for radionuclides (see <http://www.epa.gov/radiation/technology/partition.htm>).

DOE:

DOE is supporting related uncertainty work within the *Environmental Management Science Program* (basic and applied research), the *Subsurface Contamination Focus Area* (technology development and deployment), and through compliance model development (e.g., RESRAD code). Throughout the DOE Complex, there are six Environmental Management (EM) clean-up sites. Within these six sites, designated DOE national laboratory and contractor staff support the clean-up mission through development of site-specific predictive models including uncertainty and parameter estimation tools. DOE headquarters EM and Environmental Health (EH) staff can represent participation of R&D, compliance and field site code development as appropriate and needed.

ARS:

ARS's Salinity Laboratory over the years has developed a large number of models for predicting water, heat and/or solute movement in the vadose zone. Especially significant has been the development of the windows-based (MS Windows 95, 98, 2000, XP, and/or NT environments) modular HYDRUS-1D and HYDRUS-2D software packages addressing one- and two-dimensional flow and contaminant transport problems, respectively. The HYDRUS codes use the Richards equation for variably-saturated flow and Fickian-based convection-dispersion equations for both heat and solute transport. The flow equation considers water uptake by plant roots as well as hysteresis. The solute transport equations include provisions for nonlinear sorption, one-site and two-site non-equilibrium transport, and the transport of solute decay chains. The software packages come with Levenberg-Marquardt type nonlinear parameter optimization modules to allow estimation of a variety of soil hydraulic and solute transport parameters from experimental data. Unknown hydraulic parameters may be estimated from observed water contents, pressure heads, and/or instantaneous or cumulative boundary fluxes during transient flow by numerical inversion of the Richards equation. Additional retention or hydraulic

conductivity data, as well as a penalty function for constraining the optimized parameters to remain in some feasible region (Bayesian estimation) can be optionally considered. The procedure similarly permits solute transport and/or reaction parameters to be estimated from observed concentrations and related data.

Details of the ARS programs, and selected applications, can be found on ARS's Salinity Laboratory Web site: <<http://www.ussl.ars.usda.gov/MODELS/MODELS.HTM>>. Agricultural applications include irrigation and drainage design, salinization of irrigated lands, pesticide leaching and volatilization, virus transport in the subsurface, and analysis of riparian systems, while typical non-agricultural problems include the design of radioactive waste disposal sites, contaminant leaching from landfills, design and analysis of capillary barriers, transport and degradation of chlorinated hydrocarbons, and recharge from deep vadose zones.

As increasingly sophisticated computer models are being developed to simulate fluid flow and contaminant transport in the vadose zone, application of those models to real-world situations requires the estimation of a large number of input parameters. Especially challenging is the acquisition of accurate estimates of the unsaturated soil hydraulic properties (water retention, hydraulic conductivity) that determine rates and directions of water flow in the vadose zone. Because of their highly nonlinear nature, direct measurements of these properties are very time-consuming, costly, and often subject to many experimental limitations.

One alternative to direct measurement is the use of pedotransfer functions (PTFs) to indirectly estimate the hydraulic properties from more easily measured and/or readily available data such as soil texture and bulk density. The Salinity Laboratory recently developed a windows-based software package, Rosetta that may be used for this purpose. The PTFs in Rosetta are based on a combined bootstrap-neural network procedure to predict water retention parameters and the saturated and unsaturated hydraulic conductivity, as well as their probability distributions. The PTFs were calibrated on a large number of soil hydraulic data sets derived from three different databases, including the UNSODA unsaturated soil hydraulic database developed at the Salinity Laboratory which are described at ARS's Web site: <http://www.ussl.ars.usda.gov/models/unsoda.HTM>). Rosetta offers a hierarchical set of five PTFs to predict van Genuchten type parameters from limited information (textural classes only) to more extended sets of data (texture, bulk density, and one or two water retention points).

ARS researchers consider one attractive feature of Rosetta is that it provides uncertainties in its parameter estimates. Uncertainty estimates are generated with the bootstrap method and are given as standard deviations around the estimated hydraulic parameters. The uncertainties, which depend on the invoked PTF model and its input data, are useful in cases where few or no hydraulic data are available, for example in Bayesian studies of parameter uncertainty. The uncertainties can also serve in risk-based simulations of water and solute transport. Rosetta is available for the Windows and Linux operating systems and can be downloaded from ARS's Salinity Laboratory Web site: <<http://www.ussl.ars.usda.gov/models/rosetta/rosetta.htm>>.

ARS is actively developing and maintaining the codes and databases described earlier. ARS has developed a specific proposal described in Attachment 1 to cooperatively pursue this work with

the other working group partners and to enhance these products according to the uncertainty and parameter needs.

USACOE

The US Army Groundwater Modeling Technical Support Center, part of the Corps of Engineers' Engineer Research and Development Center (ERDC), has developed and continues to enhance the Groundwater Modeling System (GMS). GMS is a comprehensive graphical user environment for performing groundwater simulations, site characterization, model conceptualization, mesh and grid generation, geostatistical interpretation and post-processing. GMS is developed through the collaborative efforts of 15 different government research labs and offices within the DoD, DoE, EPA, and NRC as well as participation from 20 universities and private industry. Model calibration is an important aspect of the groundwater modeling process. A number of calibration tools are provided in GMS for the trial and error method of model calibration. Interfaces to two inverse models are contained in the GMS. These models, UCODE and PEST, provide a means to automate the parameter estimation process. Uncertainty estimations of the parameter are incorporated into these parameter estimation programs. ERDC provided research support for the development of the program UCODE. For data interpolation, there are several techniques including ordinary, universal, and zonal kriging, plus tools to evaluate the sensitivity of individual data points. (For more GMS information please go to the following Web site: <<http://chl.wes.army.mil/software/gms/>> or <<http://www.ems-i.com>>).

Currently a transitional probability/Markov approach to geostatistical simulation of variables is being added to the next release of GMS. This research supported by ERDC provides a method that is more conducive to integration of geologic interpolation. Three-dimensional Markov chains are developed to yield conceptually simple yet theoretically powerful models of spatial variability for hydrostratigraphic architecture. The geostatistical conditional simulation algorithms of sequential indicator simulation and simulated quenching are modified to yield more realistic results by considering spatial cross-correlations and locally variable anisotropy directions (Carle, 1996 and 1998). There are a number of risk analysis capabilities being incorporated into the future releases of GMS. The reader is referred to the above web sites for the latest information.

The numerical model that we like to use is FEMWATER which is a variably saturated flow and transport model. One area that has become important is surface water groundwater interaction. Currently we have development a new code called GSSHA and are evaluating this plus another code to determine the appropriate tool for the surface water groundwater interaction applications.

The Corps has incorporated parameter uncertainty into the evaluation of dam rehabilitation. The uncertainty due to parameters plus the uncertainty of a particular high water event are incorporated to develop a priority list for decision makers to allocation rehabilitation funds.

The participating Federal agencies will need to commit both staff years (SY) and funds to pursue the activities described. Of particular need will be travel funds and cooperative funding for preparing, convening, and publishing joint reports for technical workshops and training courses.

QA/QC: Each Federal agency has their own QA/QC guidelines to conduct their research studies. Common QA/QC criteria are the requirements for peer review, and to inform the public of their research findings through public meetings (e.g., technical conferences, meetings and workshops), and through agency and professional publications. The QA/QC procedures used by the individual participating agencies in their research studies will be shared with the other working group participants along with their research products.

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