



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON D.C. 20460

OFFICE OF THE ADMINISTRATOR
SCIENCE ADVISORY BOARD

October 22, 2004

The Honorable Michael O. Leavitt
Administrator
U.S. Environmental Protection Agency
1200 Pennsylvania Avenue, NW
Washington, DC 20460

Re: SAB Review of the Multimedia, Multipathway, and Multireceptor Risk Assessment (3MRA) Modeling System

Dear Administrator Leavitt:

A panel of the EPA Science Advisory Board (SAB) has reviewed the Multimedia, Multipathway, and Multireceptor Risk Assessment (3MRA) modeling system. The 3MRA system is intended to be used by the Office of Solid Waste in evaluating wastes for exemption from Subtitle C of the Resource Conservation and Recovery Act (RCRA). The panel review of the 3MRA system finds in particular that:

The 3MRA modeling system is a major step forward in providing a flexible and consistent tool for estimating the distributions of the probability of exceeding adverse effect benchmarks that result from various choices of exit thresholds. Used in conjunction with other factors, 3MRA provides a scientifically defensible framework that gives reproducible results for determining national exit levels for RCRA-listed hazardous wastes.

The manner in which 3MRA was developed, as a genuine cross-Agency effort forming a formal partnership between the Office of Solid Waste and the Office of Research and Development, is to be commended. It is clear that the developers of 3MRA were acutely aware of the need to address criticisms of previous modeling attempts.

To maintain the value, utility, and credibility of 3MRA, the Agency should support the continued development of the 3MRA modeling system; our comments contained in the panel's final report offer a number of specific recommendations.

In order to maximize the long term utility and vitality of the model, the panel recommends that the Agency articulate a plan for updating both the databases that

support the model, as well as the individual model components, as improved information and models are developed.

The panel wishes to commend the EPA scientists, and especially Mr. Barnes Johnson, Deputy Director, Office of Radiation and Indoor Air, and 3MRA team leader, for their extensive and invaluable support for this review.

We look forward to your consideration of and response to the enclosed report.

Sincerely,

/s/

Dr. William Glaze, Chair
EPA Science Advisory Board

/s/

Dr. Thomas L. Theis
Chair, SAB Review Panel

DRAFT

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Multimedia, Multipathway and Multireceptor Risk Assessment (3MRA) Modeling
System Review Panel**

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1.0 EXECUTIVE SUMMARY

The panel concurs that the 3MRA modeling system is a major step forward in providing a flexible and consistent tool for estimating the distributions of the probability of exceeding adverse effect benchmarks that result from various choices of exit threshold. **Used in conjunction with other factors 3MRA provides a scientifically defensible framework that gives reproducible results for determining national exit levels for RCRA-listed hazardous wastes.** It is clear that the developers of 3MRA were acutely aware of the need to address criticisms of previous modeling attempts to the problem posed by the HWIR. **The panel supports the current approach for establishing exit concentrations, and encourages its continued development for this and other uses.**

The panel also commends the manner in which 3MRA was developed, *i.e.* as a genuine cross-Agency effort that to a significant degree worked through the insular nature of individual units in a large organization, forming a formal partnership between the Office of Solid Waste and the Office of Research and Development, and encourages the Agency to maintain and extend the collaborative nature of this process as 3MRA is further developed. If the Agency does not continue to support the continued development of the various, source, fate and effects modules, assessment data and integrated system that comprise 3MRA, and the SuperMUSE computational system, the model will cease to evolve and its future value and utility will diminish. **In this context, the panel recommends that the Agency develop and articulate a plan for future upgrades and refinements of 3MRA and its databases.**

The panel endorses the Agency's use of the Beck, *et al.* (1997) validation protocol for evaluating the 3MRA modeling system. This approach represents a departure from traditional notions of data matching as the only criterion, to an inclusive view of validation as a process of model evaluation, rather than a state of model condition. This is a bold step, but one the panel believes is appropriate, certainly for the national risk assessment objectives of 3MRA, but in a broader context, for carrying the model evaluation debate forward as it pertains to regulatory environmental modeling. The Agency has provided, in 3MRA, perhaps the first case study of this model evaluation protocol. **While it carries some discomfort, e.g. limited data sets for module evaluation, and has been constrained, e.g. inadequate resources for implementing important peer review suggestions, the panel commends the adoption of this evaluation process for 3MRA, and urges the Agency to continue with its plan for 3MRA modeling system evaluation, particularly data-model and model-model comparisons.**

The panel agrees with the adoption of a Monte Carlo analysis (MCA) framework as an appropriate tool to use in examining a wide range of site, chemical, and exposure scenarios when setting national exit levels. The MCA provides an established science-based process to allow the Agency to identify a range of exit levels at defined levels of protection. While the MCA is an appropriate and useful tool for identifying risk management options to the decision-maker, it has important limitations. Even though the MCA results provide quantitative estimates of the probability of protection, the implied

level of confidence should be interpreted with caution. The Agency has recognized that a quantitative evaluation of the uncertainty of the variable (and uncertain) model input parameters (*i.e.*, input sampling error, or ISE) is not feasible with available data. **The panel agrees that such an analysis is impractical for the complete MCA, but the panel does make specific recommendations for a “focused ISE” uncertainty analysis.**

The panel acknowledges that 3MRA can be used today to support regulatory decisions for establishing national exit concentrations. However, it must be recognized that the model is built on limited data, pragmatic assumptions, and is the product of a collection of submodels, most of them extant legacy models, thus any regulatory decisions that rely on 3MRA will reflect the uncertainty and the limitations of these models. **The panel stresses the need for the Agency to make clear that 3MRA is to be used in conjunction with other tools and factors that also affect the setting of regulatory standards (e.g., economic implications, stakeholder input, etc.).**

The panel recognizes that the developers of 3MRA were required to balance the need to include the most advanced science in the model against the reality of the significant computational burden of the national assessment problem, forcing many difficult choices with respect to the level of model sophistication to be included in the 3MRA system. The panel notes with concern, for example, the incorporation of the ISCST3 air transport model (which does not distinguish among the physico-chemical properties of different chemicals), and the non-legacy Generic Soil Column Model (which contains questionable embedded assumptions). **The FRAMES architecture of 3MRA makes it possible to swap out and/or update modules with relative ease; the panel recommends that the Agency address these concerns before 3MRA is used to support regulatory decisions.**

The panel is also concerned about the lack of sophistication, in comparison with transport, fate, and exposure, of the treatment of toxicity in 3MRA, and with policy constraints placed on the application of 3MRA, *i.e.*, toxicological parameters are fixed at a single value rather than with a probability distribution, which the current 3MRA technology supports. **The panel strongly endorses the movement toward the inclusion of such an approach, one that uses the capabilities of MCA, into 3MRA as future versions are developed. Given the significant scientific limitations and difficulties characterizing uncertainty and variability in toxicological parameters, this goal can only be accomplished with a substantial commitment of resources for research.**

The application of 3MRA for site-specific purposes, in distinction to the setting of national standards, will foster continued evolution of the model. With significant expense and regulatory burdens at stake, stakeholders will seek to use 3MRA, and to provide feedback to the Agency regarding model assumptions and outcomes. In this respect, the panel finds that 3MRA omits certain pathways that may be important contributors to exposures at specific sites or regions. For example, some human exposure pathways (*e.g.*, vapor intrusion, dermal exposure) are not included, nor is the potential for

adverse effects beyond a two kilometer radius around WMUs (i.e., the attendant risks to human health and the environment associated with long-range transport and accumulation). Also, concurrent exposures to multiple contaminants in the waste are not considered. The panel understands that many of these exposure pathways were screened out of the modeling process because they were not thought to be significant contributors to the national risk/hazard problem. In addition, 3MRA does not include disposal options beyond land-based (e.g., incineration). Given the wide range of different chemicals and release scenarios that the model was developed to assess, and probable site-specific applications in the future, the panel believes that a more complete set of exposure pathways, and eventually disposal options, be built into the model. **If exposure pathways that are acknowledged to be of potential importance are to be excluded, the panel recommends that the Agency demonstrate, through appropriate analysis, that the results will still achieve the level of protection intended at the site level. In addition, the panel recommends that the implementation of the model for regulatory purposes include the flexibility for interested parties to provide additional data and new modeling approaches.**

3MRA processes and outputs very large quantities of information. **The panel encourages the Agency to continue development of mechanisms for meaningful interpretation of model output, currently underway for 3MRA version 1.x., and believes it is necessary that the version 1.x tools be completed prior to adopting 3MRA for site-specific applications. Similarly, the panel urges that the Agency complete the development and documentation of the Site Visualization Tool (SVT).** This tool shows significant promise for addressing panel recommendations to provide “intermediate” model outputs such as chemical concentrations in various exposure media, pathway-specific exposure, and so forth.

Finally, the panel recommends that the documentation for 3MRA undergo significant reorganization and revision with respect to the need for a readable summary, improved clarity of terms, concise descriptions of databases, and ease of implementation of the modeling system (i.e., a User’s Guide). Specific suggestions are provided in the report.

2.0 BACKGROUND AND CHARGE QUESTIONS

This chapter of the report provides the background, context, charge for the review and the procedural history. Specific responses to charge questions can be found in Chapter 3.

2.1 Background

2.1.1 *History of the 3MRA from HWIR to Development of the Integrated Research Plan*

There have been substantial efforts by Federal and State organizations and the private sector to develop risk assessment tools that include the evaluation of contaminants in different media and the integration of exposures across pathways to help establish an integrated risk-based assessment.

In December 1995, EPA's Office of Solid Waste proposed to amend existing regulations for disposal of listed hazardous wastes under the Resource Conservation and Recovery Act (RCRA). The December 1995 proposal (60 FR 6634, December 21, 1995) outlined the Hazardous Waste Identification Rule (HWIR) that was designed to establish constituent-specific exit levels for low risk solid wastes that are currently captured in the RCRA subtitle C hazardous waste system. Under this proposal, waste generators of listed wastes that could meet the new concentration-based criteria defined by the HWIR methodology would no longer be subject to the hazardous waste management system specified under subtitle C of RCRA. This would have established a risk-based "floor" for low risk hazardous wastes that would encourage pollution prevention, waste minimization, and the development of innovative waste treatment technologies.

In May and June of 1995, EPA's Science Advisory Board (SAB) reviewed the proposed HWIR methodology for calculating exit concentrations and in May 1996 published its findings in Review of a Methodology for Establishing Human Health and Ecologically Based Exit Criteria for the Hazardous Waste Identification Rule (HWIR) (EPA-SAB-EC-96-002).

In addition to this review, EPA's Office of Research and Development (ORD), and numerous industrial and environmental stakeholders, also reviewed the proposed methodology. While the SAB concluded that the methodology "lacks the scientific defensibility for its intended regulatory use," the SAB also made the following recommendations that, when addressed, should provide an adequate scientific basis for establishing a risk-based methodology applicable at the national level for the waste program:

- a) Develop a true multi-pathway risk assessment in which a receptor receives a contaminant from a source via all pathways concurrently, is exposed to the contaminant via different routes, and accounts for the dose corresponding to each route in an integrated way;

- b) Maintain mass balance;
- c) Conduct substantial validation of the methodology and its elements, against actual data derived from the laboratory or field, prior to implementation of the model;
- d) Conduct a systematic examination of parameters to ensure a consistent and uniform application of the proposed approach, and further, the full suite of uncertainties to be addressed for the final methodology;
- e) Discard the proposed screening procedure for selecting the initial subset of chemicals for ecological analysis and instead require that a minimum data set be satisfied before ecologically based exit criteria are calculated;
- f) Seek the substantive participation, input, and peer review by Agency scientists and outside peer review groups as necessary, to evaluate the individual components of the methodology in much greater detail; and,
- g) Reorganize and rewrite the documentation for both clarity and ease of use.

As a result of the methodology reviews, the Office of Solid Waste (OSW) collaborated with the Office of Research and Development (ORD) to develop and document a sound science foundation, supporting data for an assessment, and related software technology for an integrated, multimedia modeling system (entitled 3MRA) following the recommendations of the SAB and other reviewers. This effort was initiated with the peer review of an integrated research and development plan (ORD/OSW Integrated Research and Development Plan for the Hazardous Waste Identification Rule (HWIR), 1998, that describes the assessment methodology, the technical bases for the integrated multimedia modeling system, and quality controls to be followed during the developmental process.

2.1.2 The 3MRA Modeling System

The Multimedia, Multipathway, and Multireceptor Risk Assessment (3MRA) modeling system represents a collection of science-based models and databases that have been integrated into a software infrastructure that is based on the FRAMES (Framework for Risk Analysis in Multimedia Environmental Systems) concept, which provides a computer-based environment for linking environmental models and databases and managing the large amounts of information within the system, including the visualization of outputs. This integrated multimedia modeling system provides national-level estimates of human and ecological risks resulting from long-term (chronic) chemical release from land-based waste management units. The modeling system is described in greater detail in Section 2.3.2.

2.1.3 Peer Review of Modules within the 3MRA Modeling System

Over 45 experts participated in the peer review process of the underlying science within the 3MRA modeling system. The EPA plans to use the modeling system to help inform managers on a variety of decisions in the waste program, such as setting concentration-based exit criteria for wastes in the hazardous waste management regulations, or deciding whether technology-based standards are protective of human health and the environment.

2.2 Context

The EPA Office of Solid Waste (OSW) is responsible for managing solid and hazardous waste as specified by the Resource Conservation and Recovery Act (RCRA) of 1976 and subsequent legislation, such as the Hazardous and Solid Waste Act (HSWA) of 1984. These acts and the programs developed to implement them were designed to protect human health and the environment. Thus, many of the regulatory decisions within the RCRA programs are based, at least in part, on the human health risk and environmental impacts of the regulatory options under consideration.

As the RCRA program has evolved, and as new risk assessment methods have been developed, EPA's need for improved risk assessment models has greatly increased. The RCRA programs initially addressed only releases to ground water from land disposal operations and releases to air from waste incinerators and other types of boilers and industrial furnaces. However, the RCRA programs have expanded in scope over the years to encompass hundreds of constituents, thousands of waste streams, and many types of waste management practices, ranging from recycling and reuse to disposal and destruction techniques. Thus, new risk assessment models were needed to assess the types and magnitude of risks that fall under the broad purview of the RCRA programs.

In addition, in the mid-1990s, several groups within and outside of EPA came forward with recommendations or guidance for improving risk assessment methods. In 1996, EPA issued new guidelines for conducting exposure assessments and risk assessments that focused on improving the science underpinning the risk or exposure assessments that were being conducted, as well as improving the methods for characterizing the uncertainty in the risk estimates that are generated. In 1997, the Presidential/Congressional Commission on Risk Assessment and Risk Management (CRARM) issued a report on improving risk assessment methods used by the federal government. Also, EPA's Science Advisory Board reviewed and commented on a number of EPA risk assessments and models, including the dioxin and mercury risk assessments.

The 3MRA modeling system was developed as a predictive tool to provide risk assessment support for the types of risk management decisions that are made within OSW. OSW applies risk assessment modeling tools in a variety of situations; one application is the conduct of site-based national-level risk assessments to support rulemaking for the identification of hazardous waste. Consequently, the 3MRA modeling

system needed to be able to model waste management environmental settings that are representative of the range of environmental settings found in the United States, and within this broad range of settings, to simulate the release, fate and transport of many contaminants in waste undergoing a range of physical and biochemical processes. More than 400 constituents are regulated under the RCRA programs. EPA needs to consider the impacts of these released contaminants on humans and the environment within the broad range of environmental settings. This requires a modeling tool that encompasses releases to all media, transport within those media, uptake in terrestrial and aquatic food webs, and exposure of specific receptors to contaminated media and food items.

Together OSW and ORD intend to provide a base technology within which assessments can be conducted and science-based modeling experiments can be conducted.

2.3 Charge

The EPA asked the SAB to focus its review in the following four areas: assessment methodology, 3MRA modeling system, modeling system evaluation, and modeling system documentation. Some charge questions were modified slightly by the Panel in August 2003; their final language is used in Section 3 of this report. The original wording of the charge questions appears below.

2.3.1 Assessment Methodology

The 3MRA assessment methodology presents a strategy for estimating national distributions of human and ecological risks resulting from long-term (chronic) chemical release from land-based waste management units. The national distribution is constructed by performing “site-based” assessments at a significant number of randomly sampled hazardous waste site locations across the U.S. In the assessment methodology, a pollutant is released from a waste management unit to the various media (air, water, soil) according to its chemical properties and characteristics of the unit. The pollutant is transported through the media and exchanged between media via system linkages. Receptors are exposed concurrently to the pollutant via multiple pathways/routes resulting in an integrated dose.

The methodology describes a tiered approach for populating data files for each site evaluation. The approach is referred to as “site-based” because the assignment of data values for the site being simulated occurs according to a tiered protocol. Data values are filled first with data at a site level; when site data are not available, a statistically sampled value from a geographically relevant regional distribution of values are used; and lacking a representative regional distribution for the variable, a value from a national distribution is assigned.

The 3MRA methodology was designed specifically to include Monte Carlo simulation methods to address uncertainty and variability in the risk outputs. Statistical distributions for many modeling parameters were developed and upon implementation

provide a statistical measure of variability and uncertainty, i.e., the range and distribution of potential exposures and risks occurring at a site. When applied to the sites in a national assessment, the result is a statistical measure of variability and uncertainty, and national distributions of risks. The sites currently in the database are randomly selected from sites across the United States to represent the national variability in waste management scenarios and locations. The methodology for selecting the sites allows for measures of protection to be calculated at the site level and aggregated over all the sites to develop the national distribution of risks.

Charge Question 1: While the EPA had the assessment methodology peer reviewed prior to the development of the 3MRA modeling system, does the SAB have any additional comments about the methodology as implemented?

2.3.2 3MRA Modeling System

To implement the 3MRA methodology, the EPA chose to develop a comprehensive software-based modeling system, which facilitates the consistent use of sound-science models through a framework that controls model sequencing, facilitates data exchange, and provides data analysis and results visualization tools. Following modern Object Oriented software design and development principles and honoring the use of legacy models (i.e., fate and transport models that have a long history of use at the EPA), the EPA has constructed a modern modeling system that facilitates the consistent and reproducible application of the 3MRA modules and databases to problems requiring a national-scale assessment of site-based risks. The 3MRA modeling system is underpinned by a software infrastructure named FRAMES. FRAMES provides a computer-based environment for linking and applying environmental models and managing the large amounts of information within the system.

The 3MRA modeling system consists of: (a) 17 science-based modules that estimate chemical fate, transport, exposure, and risk; (b) 7 system processors that select data for model execution; manage information transfer within the system; ``roll-up'' site-based results into distributions of risk at the national level; and provide a visualization of the system outputs; and (c) multiple databases that (currently) contain the data for waste managements sites across the country as well as regional and national distributions of data values, (d) a software infrastructure (framework) based on FRAMES.

The 3MRA system was designed to provide flexibility in producing distributions of hazards or risks at sites that may manage exempted waste because the final regulatory decision framework for defining chemical-specific exit levels has not been formulated. The system is designed to allow the evaluation of human health impacts to the general population or selected subpopulations and the impact of varying the measures of protection at different probability levels. The system has similar capabilities with respect to evaluating the impacts on ecological systems.

Charge Question 2a: Does the 3MRA modeling system provide a tool for performing national risk assessments that facilitates consistent use of the science and provides a mechanism for reproducing results?

Charge Question 2b: Does the 3MRA modeling system provide decision-makers sufficient flexibility for understanding the impacts on potential chemical exemption levels by allowing varying measures of protection based on the number of receptors and/or number of sites protected, types of human and ecological receptors, and distance?

Charge Question 2c: Does the 3MRA modeling system provide appropriate information for setting national risk-based regulations for the waste program?

2.3.3 *Modeling System Evaluation*

In response to the SAB recommendation that substantial evaluation of the modeling system is essential to building confidence in the system, the EPA focused significant efforts to ensure the scientific integrity of the 3MRA system and its results during system development and post-development. The EPA designed and implemented rigorous quality assurance and quality control procedures for software development, data collection, verification testing, and peer review on the scientific components of the system.

The EPA implemented specific steps to build a level of confidence in the system to ensure that the system will present a reasonable estimate of nationwide risk for a national-level assessment.

First, the overall technical approach and each science-based module included in 3MRA have been peer reviewed. Teams of peer reviewers (at least three per module) provided critical feedback about the science-based modules. All told, over 45 independent experts reviewed the science modules to ensure that the theoretical concepts describing the processes within release, fate, transport, uptake, exposure, and risk components were adequate representations of the processes to be evaluated.

Second, all software components and databases underwent a series of tests to verify that the software and data were performing properly. At the heart of this protocol is the requirement that each component of the modeling system include a designed and peer reviewed test plan that is executed by both the model developer and a completely independent modeler (i.e., someone who did not participate in the original model development). These procedures, test plans, test packages, and test results are fully documented and available to the public.

Third, a comprehensive data collection approach was developed to parameterize the modeling system in accordance with the site-based approach described in the assessment methodology. This data collection plan described the general collection methodology for the major types of data (for example, facility location, land use, soil

characteristics, receptor locations), including quality assurance and quality control procedures and references for data sources.

Fourth, the 3MRA modeling system is currently undergoing a comparison analysis with EPA's Total Risk Integrated Methodology (TRIM) that is under development. The objective of the model comparison effort was to increase confidence that the 3MRA modeling system produces estimates consistent with other multi-media models.

While complete validation of a modeling approach would be the ultimate proof for a multimedia system like the 3MRA, the EPA did not find a multimedia data set to compare with the system's predictive outputs. In addition, the model comparison study was conducted using an actual industrial site where environmental monitoring data for mercury representing the relationship between contaminant source and environmental concentrations were available (albeit an incomplete set of observational data). Finally, a formal program focusing on sensitivity and uncertainty analysis for high-order modeling systems has been initiated at ORD. The early focus of this program is the investigation of parameter sensitivities and system uncertainties within the 3MRA modeling system. The SuperMUSE system has been configured to allow exhaustive experimentation with the 3MRA system in Monte Carlo mode. Initial results of these efforts have been documented.

Charge Question 3a: Is the software development and verification testing approach implemented for the 3MRA modeling system sufficient to ensure confidence that the modeling results reflect the modeling system design?

Charge Question 3b: Given the thorough evaluations that EPA has implemented using the available data resources and technologies, while also recognizing the real world limitations that apply to validating the 3MRA modeling system, have we reasonably demonstrated through methodology design, peer review, quality control, sensitivity analyses, and model comparison, that the 3MRA modeling system will produce scientifically sound results of high utility and acceptance with respect to multimedia regulatory applications?

2.3.4 3MRA Modeling System Documentation

In response to significant comments regarding the lack of clarity and transparency associated with documentation of the earlier modeling system the EPA has devoted significant time and resources to correcting this limitation. The 3MRA represents a comprehensive risk assessment capability and as such integrates the science from all contributing disciplines. Documentation is necessarily voluminous. In preparing the current documentation our intent is to provide different levels of presentation depending on the intended audience. The EPA has prepared a significant number of reports and documents at various levels of technical complexity that describe the 3MRA modeling system and the related HWIR application.

The review documents consist of a four volume set of documents, providing a comprehensive overview of the 3MRA modeling system. These documents are intended to be the primary means by which the general public would become familiar with the 3MRA system and are also intended to provide the level of information necessary for a risk assessor to make an informed decision regarding the applicability of the 3MRA modeling system to specific risk assessment problems.

Charge Question 4: Has the EPA made substantive progress, relative to 1995, in designing and preparing documentation for the 3MRA modeling system? Does the SAB have additional suggestions for improving the presentation of the comprehensive set of materials related to this modeling system?

2.4 Procedural History of the Review

2.4.1 Request and Acceptance

In May 2002, the Office of Solid Waste requested that the Science Advisory Board review the 3MRA modeling system in 2003. After considering all requests for 2003, the Executive Committee of the Science Advisory Board determined that the review should be conducted by a specialized panel. The Director of the Science Advisory Board Staff Office, in consultation with the Chairman of the Science Advisory Board, selected Environmental Engineering Committee member Dr. Thomas L. Theis, Director of the Institute for Environmental Science and Policy at the University of Illinois at Chicago, as chair of the panel.

2.4.2 Panel Formation

The panel was formed in accordance with the principles set out in the 2002 commentary of the Science Advisory Board, *Panel Formation Process: Immediate Steps to Improve Policies and Procedures* (EPA-SAB-EC-COM-02-003). A notice offering the public the opportunity to nominate qualified individuals for service on the panel was published in the Federal Register on April 11, 2003 (68 FR 17797-17800). Seventy-five (75) individuals were considered for membership on the panel. On the basis of candidates' qualifications, interest, and availability, the SAB Staff Office made the decision to put 35 candidates on the "short list". On May 29, 2003, the SAB Staff Office posted a notice on the SAB Web site inviting public comments on the prospective candidates for the panel.

The SAB Staff Office Director — in consultation with SAB Staff (including the DFO and the Acting SAB Ethics Advisor) and the Chair of the Executive Committee — selected the final panel. Selection criteria included: excellent qualifications in terms of scientific and technical expertise; the need to maintain a balance with respect to members' qualifying expertise, background and perspectives; willingness to serve and availability to meet during the proposed time periods; and the candidates' prior involvement with the topic under consideration. The final panel includes experts with

experience in academia, industry, research organizations, state agencies, non-Governmental organizations (NGOs), and consultant groups.

2.4.3 Panel Process and Review Documents

In summary, panelists were provided with the review materials prior to the first face-to-face meeting and asked to write down their preliminary individual responses to the charge questions. After briefings and public comment at the first face-to-face meeting, the panel articulated a set of consensus points to be used in drafting the report and coordinators were assigned to prepare responses to each of the four major charge questions using input from their colleagues on the panel. Although a draft was discussed at the second face-to-face meeting, much of the meeting was spent on additional Agency presentation and public comment, with a second draft being discussed by conference call on December 15 and January 16. New material was provided to the Panel during this time. Discussion of a third draft February 6 led to some further analysis and writing in specific areas to achieve clarity. The panel approved the final wording of its report March 18, 2004 after which it was forwarded to the Board for review and approval prior to transmittal to the Administrator.

The 3MRA modeling system is complex, the documentation extensive, and the review intense and time consuming. The Panel had two face-to-face meetings. These were held August 26-27 and October 28-30, 2003. These open meetings were supplemented by ten open conference call meetings: July 21, August 15, September 16, October 9, November 24, December 15, January 16 (2004), February 6, February 27, and March 18. Opportunities for written and oral public comment were provided at all of these meetings.

From time to time, a subset of the panel met with the Designated Federal Officer (DFO) to do planning, fact-finding, or other work preparatory for a subsequent open meeting. Each occasion was acknowledged at the following open meeting; a participant would summarize and answer questions and the DFO's notes were included with the relevant minutes. Such calls were organized around particular technical issues and include calls on validation on September 11 and 18; uncertainty September 12, September 19, December 4, and January 12; ecology and health October 8 and 15; on soils and source terms October 10; and the 2 km radius on January 9. In addition, the coordinators of the responses to the various charge questions met October 11 to discuss issues such as organization and format of the responses.

The primary review materials included a CD with four volumes of review materials and a user's guide for the model, a CD with the model on it. These were provided in July 2003 along with the website where the results of more than 45 previous peer reviews of parts of the modeling system are available, an e-mailed "Roadmap" from the Agency relating materials in the four volumes to the public comment received at the previous conference call.

The primary review materials were supplemented with additional information, almost always in response to requests from Panelists. In September, one panelist had requested and been sent the document, *Quality Assurance of Multi-Media Model for Predictive Screening Tasks* (EPA 600/R-98-106, August 1999). The Panel also requested and received *On The Problem of Model Validation For Predictive Exposure Assessments, published in Stochastic Hydrology and Hydraulics*, Vol. 11, pages 229-254, 1997, by M.B. Beck, J.R. Ravetz, L.A. Mulkey, and T. O. Barnwell and *Model Evaluation and Performance* by B. Beck, published in *Encyclopedia of Environmetrics* (ISBN 0471 899976) Volume 3, pp 1275-1279, edited by Abdel H. El-Shaarawi and Walter W. Piegorsch, John Wiley & Sons, Ltd. Chichester, 2002. In October, Robert Ambrose of EPA provided the Panel with a write-up on water balance. The Agency also provided a compilation and analysis of the 45 prior peer reviews. By December, the Agency had also provided a CD of new material with uncertainty analyses for seven chemicals, additional material relating to the General Soil Column module. In January, the Panel received additional material on uncertainty.

2.4.4 Review and Transmittal

During the course of the 3MRA review, the Science Advisory Board underwent a reorganization. The membership of the Executive Committee was broadened and it was renamed the Board. The mechanism for review of final products before transmittal to the Administrator was also modified. Under the previous organization, the Executive Committee had assigned vectors to review reports before transmittal; under the new organization a separate and specialized Quality Review Panel would be formed for the review of important reports. This Panel would meet separately, then report to the full Board. The 3MRA report was the first report to go through this new process.

The Vice Chairman of the Board, Dr. Domenico Grasso, Rosemary Bradford Hewlett Professor and Chair of the Picker Engineering Program at Smith College and former chair of the Environmental Engineering Committee, formed a Quality Review Committee (QRC) to review the 3MRA Panel's report. The review considered whether:

- a) the original charge questions were adequately addressed;
- b) there were any technical errors or omissions in the report or issues that were inadequately dealt with in the Panel's report;
- c) the Panel's report were clear and logical; and
- d) the conclusions and recommendations were supported by the body of the Panel's report.

After a review by the SAB's Quality Review Committee, the Board considered this report together with the evaluation of the QRC and decided and approved it for transmittal to the Agency. The Board expects that the Agency will provide a written response to this report.

2.4.5 References

Review of a Methodology for Establishing Human Health and Ecologically Based Exit Criteria for the Hazardous Waste Identification Rule (HWIR) (EPA-SAB-EC-96-002), Science Advisory Board, U.S. Environmental Protection Agency, 1996.

Panel Formation Process: Immediate Steps to Improve Policies and Procedures (EPA-SAB-EC-COM-02-003), Science Advisory Board, U.S. Environmental Protection Agency, 2003.

Integrated Research and Development Plan for the Hazardous Waste Identification Rule (HWIR), Office of Research and Development and Office of Solid Waste, U.S. Environmental Protection Agency, 1998.

<http://www.epa.gov/epaoswer/hazwaste/id/hwirwste/risk.htm>

3.0 RESPONSES TO CHARGE QUESTIONS

Charge Question 1. While the EPA had the assessment methodology peer reviewed prior to the development of the 3MRA modeling system, does the SAB have any additional comments about the methodology as implemented?

According to the Agency, the 3MRA assessment methodology as implemented contains several elements:

- Statistical sample of industrial sites
- Site-based human and ecological exposure/risk assessment
- Multi-contaminant, -media, -pathway, -receptor
- Tiered Data (site-specific, regional, national)
- Population-based site level risk estimates
- National roll-up of risks
- Alternative measures of protection
- Pseudo two-stage Monte Carlo
- Probability-based design to facilitate uncertainty analysis and sensitivity analysis
- Externally peer reviewed and independently tested

3.1 Panel Commentary

3.1.1 *Development of the 3MRA Modeling System*

The panel concurs that the 3MRA modeling system is a major step forward in providing a computer-based tool for estimating the distributions of the probability of exceeding an adverse effect benchmark that result from various choices of exit threshold, and provides a scientifically defensible framework for determining national exit levels for RCRA-listed hazardous wastes. The panel recognizes the rationale of a tiered set of data for conducting screening level assessments, and the use of statistical sampling and analysis that together define the approach for developing a national assessment methodology. In addition, the panel agrees that 3MRA is truly a multi-media, multi-pathway, and multi-receptor model that produces consistent and reproducible results. The panel supports the current approach for establishing exit concentrations, and encourages its continued development for this and other uses.

The panel commends the manner in which 3MRA was developed, *i.e.* as a genuine cross-Agency effort that to a significant degree worked through the insular nature of individual units in a large organization, forming a formal partnership between the Office of Solid Waste and the Office of Research and Development, and encourages the Agency to maintain and extend the collaborative nature of this process as 3MRA is further developed. The complexity of the technical and scientific issues involved makes an undertaking of this type extremely difficult. If the Agency does not continue to support the continued development of the various, source, fate and effects modules, assessment data and integrated system that comprise 3MRA, the model will cease to evolve and its future value and utility will diminish. In this context, the panel

recommends that the Agency develop and articulate a plan for future upgrades and refinements of 3MRA and its databases.

From a regulatory perspective 3MRA is a valuable tool and an important step forward for understanding the fate and effects associated with the disposal of chemicals in the environment. The panel acknowledges that 3MRA can be used today to support regulatory decisions for establishing national exit concentrations. However, it must be recognized that the model is built on limited data, pragmatic assumptions, and is the product of a collection of submodels, most of them extant legacy models, thus any regulatory decisions that rely on 3MRA will reflect the uncertainty and the limitations of these models. While the panel recognizes the benefits of building 3MRA on legacy models, it nevertheless stresses the need for the Agency to make clear that 3MRA is to be used in conjunction with other tools and factors that also affect the setting of regulatory standards (e.g., economic implications, stakeholder input, etc.).

An example of the panel's concern about the general applicability of legacy models is the ISCST3 submodel. ISCST3 is a steady-state Gaussian plume dispersion model originally designed for application to criteria air pollutants (CO, NO₂, Pb, PM₁₀, SO₂ and PM_{2.5}) for which the primary factors influencing atmospheric fate are advective flows and irreversible deposition. Such a model may not be ideal for chemicals that are not typically thought of as air pollutants. The panel agrees that the algorithms in ISCST3 have been extensively reviewed and evaluated for the criteria air pollutants and that the model has a long history of use by the EPA, but the panel also notes that because the model was developed for criteria pollutants, it does not account for differences in the physicochemical properties of volatile and semi-volatile organic pollutants. The panel cautions the Agency that "legacy" status does not necessarily mean a model is appropriate for all chemicals, particularly when the legacy model was designed for a specific purpose or chemical class. The Agency should demonstrate the adequacy of the air dispersion model for a wider range of physicochemical properties (see response to question 3b). This might be done by comparing results from 3MRA (over a relevant time period) with alternate models that have been developed specifically for multimedia fate modeling such as the Agency's TRIM.FaTE model or other Mackay-type fugacity models.

An exception to the use of legacy models in assembling 3MRA is the Generic Soil Column Model (GSCM), which is embedded within several of the transport modules of 3MRA. This model was written exclusively for 3MRA and does not appear to have been extensively reviewed or validated. The Agency has made a number of pragmatic assumptions regarding boundary transfer, local equilibria and solution methodology in order to ease the computational burden associated with this important module. It is incumbent upon the Agency to continue to test and evaluate the suitability of these approximations, as well as to explore more mechanistic treatments of the GSCM processes as they affect constituent fate and transport, in order to build confidence that the module is operating adequately and retains needed accuracy. Options for accomplishing this include additional data matching, comparison of results with other

accepted models, theoretical analysis, or error analysis. The panel's review of GSCM is presented in its response to question 3b and in appendix 3b.

The ultimate results from 3MRA are expressed in terms of allowable concentrations of particular chemicals in a waste stream that may "exit" RCRA Subtitle C hazardous waste management facilities. Yet, the transport models used in 3MRA require as input the chemical concentration that enters a particular WMU (*e.g.*, a concentration in soil for land-based units). In 3MRA, the chemical concentration that actually is "applied" to a particular WMU is a function of two parameters: the modeled concentration in the waste (C_w) and the "fraction of waste," or f_{WMU} , term that defines the relative amount of waste in the waste stream applied to the WMU. The actual initial chemical concentration in the WMU is not C_w , but C_w reduced by a random fraction (f_{WMU}) between 0.01 and 1.0. For example, if an f_{WMU} value of 1.0 is randomly selected for any given simulation, this would equate to a "monofill" which receives 100% of a given waste compound. Because the value of f_{WMU} is selected randomly within the 3MRA Monte Carlo simulation structure, there is no way to determine the actual initial concentration that enters a WMU. The panel recommends that the Agency conduct an analysis of the 3MRA results in order to document the range of f_{WMU} values that ultimately are associated with the exit level results, for example are the exit levels typically associated with f_{WMU} values at the upper end of the range (*e.g.*, values near 1.0)? In addition, there does not appear to be any discussion or rationale in 3MRA for why the f_{WMU} term should be considered as a random variable, nor a justification for assigning it as a "uniform" random variable (a selection which implies very little knowledge of this parameter). As a direct scalar of the applied waste concentration, this single factor could potentially have a large impact on the 3MRA results. The panel suggests considering f_{WMU} as a decision variable, and modeling several discrete values.

During its development, 3MRA has become a sophisticated, computationally-intensive program. This has led to some confusion on the part of the panel about the intended users of 3MRA. On the one hand the Agency, in its regulatory role, can be viewed as the only valid user as they fulfill the requirements of HWIR in setting national risk-based exit values for subtitle C facilities. On the other hand, with significant expense and regulatory burdens at stake, stakeholders will seek to use 3MRA for various site specific purposes, and to provide feedback to the Agency regarding model assumptions and outcomes. The ready availability of extensive new data sets for incorporation into 3MRA is unlikely unless EPA seeks out appropriate data from the stakeholder community. As newer and more reliable data become available, and uncertainty is reduced, more realistic assumptions regarding the fate and effects of chemicals of concern on a site-specific basis should be incorporated into 3MRA. The application of 3MRA for site-specific purposes will foster continued evolution of the model. Therefore, the panel suggests that the implementation of the model for regulatory purposes include the flexibility for interested parties to provide additional data and new modeling approaches.

Early in its development the Agency made the decision to implement 3MRA on a Windows platform in order to facilitate its use in a PC-based computational environment.

(Indeed, during the familiarization period, panel members both individually and collectively at face-to-face meetings made several runs of the model on single PCs). However, actual use of 3MRA to assist in the setting of national exit levels is a much more complex application that greatly magnifies computational demands, thus necessitating the assembly and use of the SuperMUSE system. The panel recognizes the significant achievement that this represents, and expresses its support for maintaining this resource. The panel also recognizes concern on the part of the stakeholder community regarding the ease of use of 3MRA, and suggests that the Agency be cognizant of these concerns as future versions of 3MRA are developed and made available.

Although the national distribution of risks is clearly an important factor for decision makers who are responsible for setting exit levels, the panel is concerned that the exclusive focus on ecological and human receptors at specific points in space may not provide reasonable assurance that natural resources (aquifers, surface water bodies and agricultural soils) will be protected. To illustrate this concern, the Panel notes that the 3MRA modeling system only includes the groundwater pathways for receptor locations if the 1990 Census data indicate the presence of private wells in the particular Census block group. As a result, only ~35% of the population in the national assessment is exposed to groundwater. In addition, public water supplies, even those that originate from groundwater, are assumed to be treated so that exposure to groundwater is reduced even further. Although these may all be valid assumptions, the final result is that the spatial coverage around the national set of WMUs for exposure to groundwater is potentially small. As a result, an exit level C_w that is protective based on the national distribution of risk may result in a significant fraction of sites where contaminant levels in groundwater exceed levels set out in the National Primary Drinking Water Regulations. Similarly, contaminant levels in surface water bodies within the AOI may exceed the National Recommended Water Quality Criteria.

The panel notes that 3MRA already outputs specific media concentrations and the Site Visualization Tool (SVT) provides a means to access this data. These media-specific concentrations could be used to communicate to decision makers the potential for contamination of media around the WMUs. The panel recommends that the Agency include a summary table of abiotic media concentrations around the WMUs in the final model output. This will require continued development and documentation of the Site Visualization Tool (SVT), which is briefly described in Volume V, Section 4.3.2.1. Even in its “beta version” this tool shows significant potential for addressing panel recommendations to provide “intermediate” model outputs (this refers to such outputs as chemical concentrations in exposure media, pathway-specific exposure and so forth as given in the response to question 3). To be consistent with the other model outputs, the media concentrations might also be rolled up as percent of sites where NPDWR levels for groundwater, NRWQC levels for surface water and/or existing Soil Screening Guidance levels for soil are exceeded. Lacking a fully functional and documented SVT, the model results for the numerous output variables stored in the “GRF” files cannot be readily interpreted by anyone except the model developers. The panel recommends that completion and enhancement of the SVT should receive high priority (see additional recommendations in Appendix 4-1).

The panel is concerned about the lack of sophistication, in comparison with transport, fate, and exposure, of the treatment of toxicity in 3MRA, and with policy constraints placed on the application of 3MRA, *i.e.*, toxicological parameters are fixed at a single value rather than with a probability distribution, which the current 3MRA technology supports. In many cases, a significant degree of uncertainty in both the human health and ecological risk assessment protocols is associated with dose-response relationships. The panel feels that the Monte Carlo analysis should recognize these uncertainties as well as species response variability. The panel strongly endorses the movement toward the inclusion of such an approach into 3MRA, to the extent possible, as future versions are developed. Given the significant scientific limitations and difficulties characterizing uncertainty and variability in toxicological parameters, this goal can only be accomplished with a substantial commitment of resources for research. Lacking this, the panel recommends that sensitivity analysis include the dose-response for candidate chemicals. Another area where the modeling system appears to lack sophistication is with the assessment of potential ecological impact. The current approach in 3MRA, which uses simple protective criteria as benchmark comparative values, may not adequately characterize risk in ecological populations (see appendix 2b for additional details).

On September 14, 2004 the Chair of the Integrated Human Exposure Committee and the Environmental Health Committee presented a draft letter to Administrator Leavitt to the Board. After hearing a presentation on **An Examination of EPA Risk Assessment Principles & Practices (EPA/100/B-04/001, March 2004)**, the Committees wished to convey two messages to the Administrator. The second of these, the application of probabilistic methods for performing hazard and dose-response assessment, may be of interest to readers of this report. The 3MRA Panel did not consider this letter in its deliberations as it was drafted after the Panel had finished its work. The letter, when finalized, will be available at the SAB Web site: <http://www.epa.gov/sab>

The panel also finds that 3MRA omits pathways that may contribute to exposures. For example, some human exposure pathways (e.g., vapor intrusion, dermal exposure) are not included. Also, concurrent exposures to multiple contaminants in the waste are not considered. The panel understands that many of these exposure pathways were screened out of the modeling process because they were not thought to be significant contributors to the national risk/hazard problem. However, given the wide range of different chemicals and release scenarios that the model was developed to assess, and probable site-specific applications in the future, the panel believes that a more complete set of exposure pathways be built into the model. If specific exposure pathways are to be excluded, the panel recommends that the Agency demonstrate, through appropriate analysis, that exclusion of these pathways will still achieve the level of protection intended at the site level. Appendix 1-1 contains additional amplification from the panel on its concerns about exposure values. The panel also notes that several exposure parameters in 3MRA that co-vary with body weight are treated as independent. This may make the exposure appear more variable than it really is. Appendix 1-2 provides more detail on this matter.

The panel notes that the 3MRA modeling system does not address the potential for adverse effects in humans or ecosystems (and their components) beyond a 2 kilometer radius around WMUs. Therefore, it does not predict transport of chemicals beyond this region, nor was it designed to address the attendant risks to human health and the environment associated with long-range transport and accumulation (such as, for example, the atmospheric transport and deposition of chlorinated hydrocarbons in the Great Lakes). Thus care must be taken in the use of 3MRA as a regulatory tool to ensure that the risks associated with chemicals from medium to long-range transport beyond the 2 km region near a WMU are addressed via other means. The panel recommends that the agency account for those chemicals that are known to have risks of this nature, or are strong candidates for such risk pathways, and identify additional ways of assessing their potential for environmental harm in addition to the 3MRA analysis.

The 3MRA system is intended to rest on sound scientific principles, among them the conservation of mass. The panel is convinced that precautions have been taken to ensure that mass is conserved within the individual modules of 3MRA and during the transfer of information among linked modules. The panel notes in particular mass conservation within the source modules. Still, the panel is concerned that secondary sources of contamination, which are not presently modeled within 3MRA, may result in significant mass imbalances for certain chemicals, particularly over the long time scales used in the setting of national exit levels. Definitive demonstrations of acceptable mass balance are desirable, both for purposes of scientific integrity, and to promote confidence in the 3MRA system within the stakeholder community. Such demonstrations should include a suite of chemicals, particularly those that are highly partitioned between different media, and may take several forms, including summative inter-media mass calculations for the modules of 3MRA, comparisons among point estimates, comparisons with TRIM-Fate (a compartmental model in which mass is conserved), and heuristic calculations and arguments. The panel is aware that activities aimed at such demonstrations are underway, and encourages the Agency to complete these and make them public in a timely fashion.

The panel endorses the adoption of a Monte Carlo analysis (MCA) framework as an appropriate tool to use in examining a wide range of site, chemical, and exposure scenarios when setting national exit levels. The MCA provides an established science-based process to allow the Agency to identify a range of exit levels at defined levels of protection. In this manner, it provides useful results for risk management decision-making that provides an approximate quantitative estimate of the degree of protection (*e.g.*, 99% of population, at 95% of sites as one example) associated with alternative exit levels.

While the MCA is an appropriate and useful tool for identifying risk management options to the decision-maker, it has important limitations. Even though the MCA results provide quantitative estimates of the probability of protection, and thereby provide an associated degree of “confidence,” the implied level of confidence should be interpreted with caution. The Agency has recognized that a quantitative evaluation of the uncertainty of the variable (and uncertain) model input parameters (*i.e.*, input sampling error, or ISE)

is not feasible with available data. The panel agrees that such an analysis is impractical for the complete MCA, but the panel does make specific recommendations for a “focused ISE” uncertainty analysis (see question 2c). In addition, the Agency also recognizes that the MCA does not address model error (ME), another significant source of uncertainty.

Perhaps the most complex issue that the panel has faced in evaluating the 3MRA modeling system has been that of validation. 3MRA is a complex higher order model that does not lend itself to traditional methods of validation, *i.e.* in the sense of data matching. While such an approach can be achieved for some of the model components, such as waste management unit and fate and transport models, it is not possible to perform such a validation on the model as a whole for two reasons: (1) because a complete dataset that stresses all seventeen of the sub-models simultaneously does not exist and is unlikely to become available soon, and (2) because, ultimately, the purpose of 3MRA is to perform a *national* risk assessment. The Agency’s approach to this has been to develop a tiered validation protocol, based heavily on the work of Beck *et al.* (1997). In this scheme, validation is seen as a design problem with several elements:

- Quality of input data (volume 2 of the 3MRA material)
- Quality of model components (volumes 1 and 3)
- Quality of the modeling system (also in volume 3)
- Performance of the model as a reliable instrument for its assigned task (performance validity). Uncertainty and sensitivity analysis are central to the concept of performance validity, as is comparison with other models (e.g., TRIM fate), and matching against available but limited datasets (a chlor-alkali site). These are the subjects of volume 4.

The panel believes that the protocol that the Agency has developed and is following to gauge the acceptability of the 3MRA modeling system represents the state of the art for evaluating complex regulatory environmental models. Validation is achieved through completion of a series of well-defined tasks that must meet rigorous quality assurance evaluations of their outcomes. This approach represents a shift away from equating model validity with its ability to correctly predict the future, a future that in a scientific and policy context is fundamentally unknowable, to a focus on the quality and reliability of model forecasts (minimum risk of an undesirable outcome). In this context, the Agency has described in detail the problem that needs to be solved (national risk assessment), has designed a method for obtaining a solution (the 3MRA risk assessment methodology), and has generated a “solution” (the 3MRA model system). At present they are in the early stages of evaluating the performance validity of the modeling system for generating reliable forecasts. Thus in terms of the steps above, they have accomplished the first three and are engaged in the fourth.

The panel endorses the Agency’s use of the Beck, *et al.* (1997) validation protocol for evaluating the 3MRA modeling system. It represents a departure from traditional notions of data matching as the only criterion, to an inclusive view of validation as a *process* of model evaluation, rather than a *state* of model condition. This is a bold step, but one the panel believes is appropriate, certainly for the national risk assessment

objectives of 3MRA, but in a broader context, for carrying the model evaluation debate forward as it pertains to regulatory environmental modeling. The Agency has provided in 3MRA, perhaps the first case study of this model evaluation protocol. While it carries some discomfort, e.g. limited data sets for module evaluation, and has been constrained, e.g. inadequate resources for implementing important peer review suggestions, the panel commends the adoption of this evaluation process for 3MRA, and urges the Agency to continue with its plan for 3MRA modeling system evaluation.

It is clear to the panel that in each of the stages of model validation the Agency set forth extensive quality assurance procedures that include consensus on the model's intended use and performance criteria; incorporation, whenever possible, of legacy models with which the scientific community has considerable experience; independent peer reviews of model architecture and components; and verification of computer code and inter-model communication. Thus in evaluating 3MRA, the panel has had to first grasp the basis of the validation protocol, and then assess the degree to which the Agency has achieved what it set out to do. The panel believes that the final stage of the Agency's protocol, i.e., the performance evaluation, will be the most demanding and also the most informative. The Agency is still engaged in this effort so it is premature for the panel to make judgment about the ultimate acceptability of the modeling system at this stage. However, the panel believes the steps identified by the Agency for accomplishing this task are appropriate and the panel strongly encourages the Agency to continue these efforts with particular emphasis on evaluating mass balance, completing the development and application of the sensitivity analysis procedure, and continuing the data matching and inter-model comparisons activities.

The issues raised above are addressed in greater detail in the responses to charge questions 2, 3, and 4 below.

3.1.2 Additional Comments about 3MRA

The 3MRA system is based on the concept of acceptable risk. As a result, the model allows a contaminant to enter ecosystems, with some potential to adversely affect ecosystems and human health. Further, the system is based on the concept that the environment has an inherent assimilative capacity; that is, degradation, metabolism, transfer, or storage of contaminants within or outside of a WMU will occur and, as a result, will contribute to risk reduction.

The principal problem the designers of 3MRA set out to solve was that of the migration of listed hazardous waste streams from RCRA subtitle C to "ground based" subtitle D facilities (WMUs). This excludes other obvious waste management alternatives by adopting a conservative view that encompasses a limited range of final disposal options. This grows from the dependence on the inventory of candidate facilities dating back in the decade of the mid 1980s, and reflects the underlying influence of the Resource Conservation and Recovery Act on the motivation for developing 3MRA. Indeed, the Agency has embarked upon a thought process to reconsider the basis and

procedures of RCRA to make it more congruent with its original goal to encourage recycling and reuse of materials (Office of Solid Waste, 2003).

Because the FRAMES architecture allows for plug-in applications to suit specific needs, 3MRA can potentially have many other uses. The panel's view is that the present assessment methodology overlooks at least five strategies for releasing a waste stream from the rigors of Subtitle C: support for delisting of hazardous wastes, municipal waste combustors, detoxification of wastes, and pollution prevention and industrial ecology alternatives. By omitting such options, the 3MRA assessment methodology needlessly restricts the decision-maker's thinking by offering only the five classes of WMUs included in the simulation, when in reality the missing alternatives are readily implemented and officially encouraged under available contemporary practices. Appendix 1-3 contains more details about these options. The panel recognizes that the 3MRA modeling system has the capability of incorporating such alternatives, and recommends that Agency regulatory strategies take full advantage of this capability.

3.1.3 References

Beyond RCRA: Waste and Materials Management in the Year 2020
(EPA530-R-02-009), Office of Solid Waste, U.S. Environmental Protection Agency,
April 2003.

Charge Question 2a. Does the 3MRA modeling system provide a tool for performing national risk assessments that facilitates consistent use of the science and provides a mechanism for reproducing results?

3.2 Panel Commentary

3.2.1 General Comments

The panel finds that the 3MRA modeling system produces internally consistent and reproducible results. The 3MRA model development team has clearly succeeded in developing a national risk assessment tool that facilitates consistent use of the science incorporated in the 3MRA modeling system.

The panel recognizes that as with any model, the developers of 3MRA faced difficult choices in balancing the degree of scientific sophistication in the models adopted with practical real-world limitations due to computing power and data availability. The extensive peer reviews of the 3MRA modeling components have made it clear that scientific consensus about which models, modules or modeling components represent the "best" state of the science for fate, exposure and risk analysis is difficult if not impossible to fully achieve. Nevertheless, the panel believes that the choices made about the degree of scientific complexity to include in 3MRA modeling system were consistent and reasonable. Further, the modular "plug-and-play" design in 3MRA recognizes the fact that science, data quality and computing power will continue to increase and unlike most models, the 3MRA modeling system facilitates immediate access of new and/or alternate

components so that the model can systematically move forward with the advances in science.

As part of the model-model comparison process, one of the challenges in producing scientifically sound results is assessing how well the seventeen science modules that comprise 3MRA work together. As has been previously noted, not all models have been in use as long as others and thereby have not undergone the same degree of operational testing and peer review. The models employed by 3MRA range from the simplest of “screening” models, to advanced regulatory guidance modeling systems used for site-specific decision making, to more elaborate research-grade models. Therefore, when called upon for inclusion in a nationally applied comprehensive analysis, any of these models which are postulated as falling into a more advanced class of detail and sophistication may actually require application as a simpler model, due to the loss of key site-specific information normally relied upon to improve their scientific representation of the chemical and physical processes addressed. The concern, therefore, is that multi-part systems operate as efficiently and as effectively as their weakest component.

In order to clarify the relative strengths of the submodels used in 3MRA, the panel undertook an example model characterization/ranking exercise for 3MRA’s readily identifiable submodels. The exercise reinforced the impression of many panelists that one’s assessment of a model depends on the end-use. EPA has represented that 3MRA is currently being developed primarily for national regulatory policy analysis and implementation by regulatory specialists. However, the charges to the 3MRA review panel include a specific request for opinions and suggestions on “the best science” that may be presently included or readily added in the near future.

As such, two distinct rankings were created by the panel for each of the models employed by 3MRA with respect to the state of science (the scientist perspective) embodied in the module, and the level of regulatory practice with which each module is applied (the regulatory specialist perspective). A summary table, combining these findings along with background and details of the exercise, is presented in Appendix 2a-1, Table A2a-1.

While not a statistical assessment of model rankings (there were insufficient numbers of panelists), a pattern emerged when viewing the models from a regulatory perspective: voters biased toward the right (*i.e.*, they tended to rank models as more advanced) as compared to when panelists were wearing their “scientist” hat. From a “best science” perspective, the models tended to be ranked as less sophisticated. This qualitative exercise served only to highlight the challenge faced by the modelers when using models at different stage of maturity and linking them together.

3.2.2 Consistency

Consistency of scientific approaches is difficult to attain because of the disparate intrinsic time steps governing the chemical migration in different media; e.g., in air

changes are tracked over hours, but in groundwater, where migration is much slower, typical time frames of interest run into years. In a coupled multimedia-modeling system, any choice of time step results in significant compromises. The developers attempted to overcome this by altering the legacy models; for example, the sampling of hours in the air model instead of using the entire hourly meteorological record set, as well as the offline generation of short time-scale data (or intermediate calculations) to avoid rerunning the fully expanded model algorithms hundreds or thousands of times to represent the behavior of every single hour. For 3MRA's "sampling" approach to use of meteorological records as input for the ISCST3 air model, the EPA has presented results of specific sensitivity testing that demonstrates the effectiveness of this new method for reducing model run time without adding any significant margin of uncertainty to the analysis. This serves as an example of the type of continuing effort that should be employed to assess the additional uncertainties attendant to these necessary model changes (operational compromises). Perhaps an unavoidable set of inconsistencies occurs, because the degrees of advancement and validation differ widely among the module algorithms (as illustrated in Appendix 2a-2).

3.2.3 Reproducibility of Results

The panel also believes that the 3MRA modeling system provides a mechanism for reproducing results, particularly when used by trained technicians and scientists who are familiar with the system. The panel recognizes that for every model run a very large amount of information/data is generated, transferred and consumed by the various modules in 3MRA and the panel commends the agency for the approach that they developed using dictionary files of metadata to insure that various attributes of the information being passed through the modeling system remain consistent and correctly applied.

3.2.4 Potential Inconsistency in Model Uses

While the panel recognizes that 3MRA was developed specifically for Agency use, we note that with significant expense and regulatory burdens at stake, stakeholders will also seek to use 3MRA to confirm agency results, apply it for site-specific assessments, and provide feedback regarding model assumptions and outcomes. Even with the moderate amount of user guidance that is already provided in the documentation, users who are new to the model will make mistakes.¹ Thus, the greatest potential source of differences and inconsistencies in modeling results will be due to mistakes made during model setup and execution. This is not unusual for a model that is as complex as 3MRA, but to help minimize this type of inconsistency the panel recommends that the revised user manual be explicit in describing the steps in conducting a model run, e.g. clearly identify steps that are required versus those that are recommended. Furthermore, the panel recommends that training workshop be developed and presented at select

¹ As an example, refer to the "Second Evaluation of 2003 3MRA" prepared by AMEC where the modeler seemed to be getting different results from run to run and it was later determined that the model user was not running the batch file to clear results from previous runs before performing a new run. This inconsistency occurred even though the user was experienced and had reviewed the user guidance material.

scientific meetings (e.g., Society of Environmental Toxicology and Chemistry; Society for Risk Analysis; Society of Exposure Analysis and Environmental Epidemiology, etc.). The panel further suggests that the Agency should extend the existing benzene example to several other chemicals and scenarios so that interested model users can start with a realistic amount of information, setup and run the model, and then verify their results against simulation outcomes provided by the Agency.

Charge Question 2b. Does the 3MRA modeling system provide decision-makers sufficient flexibility for understanding the impacts on potential chemical exemption levels by allowing varying measures of protection based on the number of receptors and/or number of sites protected, types of human and ecological receptors, and distance?

3.3 Panel Commentary

3.3.1 General Comments

The panel believes that 3MRA provides sufficient flexibility to model the local impacts of waste management units with a reasonable level of detail sufficient for its primary intended use -- to develop national concentration thresholds for wastes that would be exempted from the hazardous waste regulatory rigors of RCRA. The decision as to the appropriate level of detail to include in a modeling effort is a trade-off between increased complexity (and flexibility) and manageability of the modeling effort. The exit level processors of 3MRA are especially important innovation that should assist the user in interpreting results.

The 3MRA modeling system uses more than 700 variables to describe a site's setting. These include human and ecological receptor locations and physical characteristics of WMUs that are site-specific, as well as regional and national input parameters relating to hydrogeologic factors, human exposure factors, *etc.* The spatial input parameters included in the 3MRA modeling system consist of the location and type of the waste management unit, the surrounding environment (including lakes, streams, and wetlands), and the location and type of human and ecological receptors. The model incorporates site-specific data on the location of human receptors and local land uses. These are based on U.S. Census block data for residents and home gardeners, and urban and agricultural census data for land use. Census data include the number and location of households with private wells. These locations are included in the modeling effort. Farm number and sizes are based on agriculture census data. In addition, every farm is assumed to be on a private well. Census data provide estimates of urban, rural-farm, and rural-non-farm recreational fishers as a percentage of the total state population. These percentages are used to calculate the recreational fisher population within the study site.

Ecological habitats and receptors are based on site-specific land use. Fourteen representative terrestrial, wetland, and margin habitats have been developed for use in the 3MRA modeling system. Ecological receptor species can be selected to represent ecological regions throughout the United States. Other inputs used are watersheds and

water sub-basins; local lakes, streams, and wetlands; and information regarding surficial aquifers (unconfined ground water sources near the surface) and vadose zone data. These parameters provide considerable flexibility for modeling the migration of chemicals from waste management units and their subsequent uptake by ecological and human receptors.

While 3MRA appears to incorporate significant flexibility in the derivation of exit levels, the panel cautions that this doesn't necessarily lead to an adequate understanding of the impacts that these levels may exert on human health or ecological systems. It is possible to incorporate a great deal of flexibility in the selection of protection levels, whether based on the number or types of receptors, the number of sites protected, or distance from the WMU. However, the selection of an exit level cannot be rationalized by flexibility. Rather, it must be based on the adequacy of the underlying biology, ecology, and toxicology and on an appropriate level of confidence that exit levels will be fully protective of human health and the environment.

For the purpose of generating an exit level, a model user or risk manager must select a suite of choices in the exit level processor, e.g. percent sites protected, population protection, risk level, hazard quotient, receptor, cohort, pathway, radius of the area of interest, etc. It would be expected that by selecting, for example, 99% population protection at a risk level of 10^{-6} and a hazard quotient of 1, the processor would return an exit concentration that would result in 99% of the selected receptors in the specified area of interest having a calculated risk of $\leq 10^{-6}$ and a hazard quotient of ≤ 1 at the specified percentage of sites. However, that would not necessarily be the case. Instead, those selections would mean that 99% of the selected receptors in the specified area of interest would have a calculated risk of $\leq 2.5 \times 10^{-6}$ and a hazard quotient of ≤ 5 at the specified percentage of sites. The panel recommends that this type of potential misunderstanding be remedied by changing the bin boundaries so that the upper limit for the bins corresponds with the risk and hazard levels in the exit level processor.

In many cases, the largest degree of uncertainty in both the human health and ecological risk assessment protocols is associated with the selection of "adverse effects concentrations." EPA has made substantial efforts to estimate the uncertainty associated with the parameters that affect exposure estimates; however, no attempt to evaluate the uncertainty associated with effects parameters has been made. Unless the issue of uncertainty associated with the effects equation is addressed quantitatively, statements about the degree of certainty cannot be reliably made. Notwithstanding Agency policy to exclude toxicological response distributions in risk analysis, the panel feels that the Monte Carlo analysis should recognize these uncertainties as well as species response variability. Therefore, the panel strongly endorses the movement toward the inclusion of such an approach into 3MRA modeling system as future versions are developed. Given the significant scientific limitations and difficulties characterizing uncertainty and variability in toxicological parameters, this goal can only be accomplished with a substantial commitment of resources for research.

The panel is concerned about the use of annual average exposure concentrations, which are likely to underestimate risks to ecological receptors leading to a decision that

may be under-protective in delisting of wastes. The use of average annual values tends to “smooth” the estimated exposure concentrations used in the risk assessment. Instantaneous exposure concentration estimates will vary around the mean in terms of magnitude, duration, and frequency and may be high enough to cause acute or sub-chronic toxicity even though the average annual concentration is below a level of concern. Therefore, the panel recommends that the Agency consider and if possible demonstrate, through appropriate analysis, that the approach implemented in the 3MRA modeling system achieves the desired level of protection to ecological receptors.

Additional detailed technical comments regarding effects on ecological systems and human health are provided in Appendix 2b.

3.3.2 Site Specific Use of the 3MRA Modeling System

The panel believes that additional factors that should be incorporated into 3MRA before it is applied to site-specific assessments. One exposure pathway that is not considered, and for which the Agency and a number of States have begun to take into account with respect to environmental impact, is volatilization of groundwater contaminants into indoor air. Because 3MRA considers groundwater as a potential source only when drinking wells are found to be in use, the drinking water and shower inhalation exposures are the only resultant pathways considered. However, if groundwater is impacted it is possible that even if it is not used as a source of potable water, vapor intrusion can be a potential source of exposure. There are, of course, numerous factors that contribute to the vapor intrusion pathway that will only add to the complexity of the model. At the moment, it is unclear how to strike a balance between comprehensive consideration of exposure pathways and modeling burden. At the very least, this should be addressed in the text.

The 3MRA documentation clearly acknowledges that dermal exposure is not considered in the model. Yet, efforts at EPA and elsewhere have been conducted since 1995 to assess and predict dermal exposure and its effects (its contribution to aggregate or cumulative exposure and risk). Olin (1999) concluded that “it is fairly easy to develop estimates of body burden from a dermal exposure.” The 3MRA system should be updated to address this deficiency by including dermal exposure in the human exposure component of the model before assessment of specific sites.

Charge Question 2c. Does the 3MRA modeling system provide appropriate information for setting national risk-based regulations for the waste program?

3.4 Panel Commentary

The panel concurs that the Monte Carlo Analysis used in 3MRA is an established science-based process that allows the Agency to identify a range of national exit concentrations at specified levels of protection. In using this process, 3 MRA provides useful information for risk management decision making in the form of an approximate quantitative estimate of the degree of protection (*e.g.*, 99% of population, at 95% of sites)

associated with alternative exit levels. In addition, the panel wishes to emphasize that the framework represented by 3MRA serves as an excellent foundation for integrating new science and information as it becomes available.

While the MCA is an appropriate and useful tool for identifying risk management options to the decision-maker, it has important limitations. Even though the MCA results provide quantitative estimates of the probability of protection, and thereby provide an associated degree of “confidence,” the implied level of confidence should be interpreted with caution. The Agency has recognized that a quantitative evaluation of the uncertainty of the variable (and uncertain) model input parameters (*i.e.*, input sampling error, or ISE) is not feasible with available data. The panel agrees that such an analysis is impractical for the complete MCA, but does make specific recommendations for a “focused ISE” uncertainty analysis (see below). The MCA also does not address variability/uncertainty associated with the toxicity component of the risk analysis (a component of ISE), which the Panel believes is a significant limitation in the 3MRA analysis. In addition, the Agency also recognizes that the MCA does not address model error (ME), another significant source of uncertainty. Appendix 2c-1 provides greater detail on the use and interpretation of MCA within the 3MRA modeling system.

The MCA provides an efficient mathematical means to iterate the model outcomes many times to generate “probabilities” of associated outcomes, however these probabilities must be interpreted within the narrow context of the system that is modeled. The magnitude of the uncertainties that are not modeled remains undefined. It is the sense of the panel that these unaccounted for uncertainties may in fact be more significant than the range of uncertainty currently modeled, in which case the probability of achieving the desired levels of protection remain unknown. Furthermore, model uncertainty is not accounted for in the MCA, and is unlikely that it can be addressed in any quantitative fashion. As a result, it is potentially misleading to interpret the exit levels as though they provide A% protection at G% of the sites with H% certainty without carefully qualifying such statements. Without a rigorous sensitivity/uncertainty analysis, the degree to which the exit levels are “protective” will remain unquantifiable.

While the panel supports the use of MCA in 3MRA, it is not convinced that the procedures adopted in 3MRA represent a discernable “second dimension” of uncertainty analysis, as the “pseudo 2-D” terminology implies. In the panel’s assessment, the regional and national data distributions do not represent only variability as suggested in 3MRA. Many fate, transport and exposure parameters, for example, are uncertain as well as variable. Yet, the uncertainty in the selected distributions is not modeled or quantified in 3MRA. Statements regarding the “confidence” or “level of certainty” in the outcome can be misunderstood because the 3MRA analysis ignores significant contributors to the overall uncertainty – ISE and ME (and uncertainty in the toxicity component which is a component of ISE). The panel believes that a more accurate statement of the MCA results would be:

“For the sites and conditions modeled, the exit levels ensure that no more than A% of the population near a WMU will have a specified incremental human

lifetime cancer risk above CR* or non-cancer Hazard Index above HI* (where CR* and HI* are both Agency defined guidelines), and these levels of protection are met for G% of the WMUs modeled. Similarly, for the conditions modeled, no more than D% of the estimated exposure concentrations exceeds ecological benchmark concentrations for G% of the WMUs modeled.”

Accordingly, the panel has developed the following recommendations on the use of MCA in the 3 MRA modeling system:

- The panel recommends reconsidering the use of the “pseudo 2-D” terminology. Given that the “two dimensions” of risk analysis in 3MRA appear to revolve around dual protection metrics of population protection and percent of sites meeting this population protection, the Panel suggests using terminology that more accurately reflects these dual protection criteria (*e.g.*, “Dual Population Protection” MCA). Furthermore, as described in response the Charge Question 4, the panel recommends that the documentation describing the Monte Carlo Analysis in 3MRA be significantly revised in order to describe the analysis more succinctly.
- It is suggested that the Agency modify the method of processing the MCA results. The panel finds that the current approach lacks transparency, and appears to discard valuable information. The panel understands that this proposed change may impact the storage requirements for the MCA results, depending on how the results are stored, and has offered a possible means to address this issue. Appendix 2c-2 contains further details.
- The “resolution” of the modeled C_w range should be addressed. In some instances, two orders of magnitude separate C_w intervals, which will inevitably lead to crude interpolation of the exit levels (with unknown biases). One possible approach to do this would be to conduct an initial set of model runs in order to determine an approximate C_w range for the exit concentrations. Once an approximate concentration range is identified, the range of C_w 's within this narrowed range could be selected such that the interval between each successive C_w is less than an order of magnitude.
- Sensitivity analyses planned for 3MRA model/exposure parameters will no doubt reveal those that have very large impacts on model output. The panel recommends that the Agency conduct a 2nd order MCA analysis using a manageable number of such key parameters (*e.g.*, say less than 20 input parameters for example), for a subset of chemicals, one or two WMU types, and a reasonable subset of sites. Such an analysis would provide a more quantitative assessment of the degree to which uncertainty in key input distributions in turn impacts the exit levels. To be clear, the panel is not recommending that this 2nd order, or 2-D, analysis be conducted on a “national” scale but rather for a manageable number of sensitive model parameters for which sufficient data (or professional judgment) allow for the assignment of a PDF representing uncertainty. This analysis could be conducted by conducting a “1-D” analysis for a particular WMU and a

particular site using the current 3MRA distributions. The “focused 2-D” analysis would apply to the same site/WMU, simply adding the 2nd dimension uncertainty PDFs. If this were done for a small number of site/WMU combinations, and on the order of three chemicals, the results would provide insight into the degree to which input parameter uncertainty gives rise to large, modest, or relatively small changes in the upper percentiles of risk for the modeled scenario. This information would then provide a semi-quantitative context for interpreting the degree to which the inability to model ISE impacts the overall degree of “confidence” that the national exit levels are “protective.”

The panel recommends extending the MCA to include the uncertainty/variability of chemical toxicity factors within the analysis. As has been noted previously, toxicity parameters are treated as fixed when, in fact, they are both variable (not everyone’s threshold is the same) and uncertain (most criteria are based on laboratory animal data). On the one hand, this has the effect of artificially narrowing the distribution of risk and percent population protection. However, because the fixed values are upper-end estimates, the distribution of risk versus probability is artificially shifted to the right. Ideally, toxicity parameters should be entered as distributions, like other variable and/or uncertain parameters. It should be a long-term goal to develop distributions for toxicity parameters. While the Agency has indicated it does not intend to adopt such an approach, at the very least, the documentation should make it clear that the risk and hazard estimates corresponding to the exit levels are exaggerated on the basis of the selection of high-end toxicity factors. However, even if the Agency will not incorporate toxicity variability/uncertainty in the derivation of the exit levels, such an analysis could and should be conducted on a subset of the chemicals that are being modeled as part of the uncertainty/sensitivity (UA/SA) analysis. The panel recognizes that probability distributions for toxicological parameters cannot always be characterized with confidence and precision. Published studies describing possible approaches that could be considered for this analysis are listed in appendix 2c-3.

Charge Question 3a. Is the software development and verification testing approach implemented for the 3MRA modeling system sufficient to ensure confidence that the modeling results reflect the modeling system design?

3.5 Panel Commentary

This question asks whether the 3MRA modeling system code implements a quantitative calculation that is consistent with the model conceptual design and whether EPA has “verified” that the code computes what it is intended to compute. The panel agrees that the Agency has made a significant effort to verify that the 3MRA modeling system functions according to its design. The special attention given to the development team communication and “top-down” code design, as well as conduct of QA/QC testing according to a pre-planned testing strategy (as presented in Vol. 3 – Section 3.1 of the documentation) are particularly notable. Also, the individual modules and the feed-

forward connections between modules have been verified with respect to data and information transfer.

Two advancements in model development and application that the agency has made during the 3MRA development and verification process represent a major contribution to the modeling community and warrant special commendation. First, the use of the FRAMES architecture is a remarkable mechanism for making the model more adaptable to future modifications, with less repetition of structural testing. Second, the significant efforts that the Agency expended to develop hardware and supporting software tools for the SuperMUSE windows-based parallel computing framework have greatly facilitated the verification process, not to mention the capability to conduct sensitivity and uncertainty analyses heretofore impractical with a model of this complexity. Also, the fact that the SuperMUSE system is scalable to any number of networked computers allows stakeholders with a range of available resources to conduct national scale analyses with 3MRA.

There are two concerns relative to verification of the modeling system that the panel would like to suggest be investigated during the ongoing sensitivity and uncertainty analysis. As the current verification process now stands, each of the algorithms and calculations for the human risk module have been checked with respect to their intended functionality individually. The first concern arises out of a desire by the panel to have data consolidation understood with respect to its impact on under- or over-estimating risk. The ELP1 and ELP2 capture all the different combinations of human cancer risk and non-cancer health impact producing up to 21,840 separate exit levels for a given population percentile and percent sites protected. As pointed out in Section 4.6.2, Volume 4, the decision-maker will need to narrow his or her focus to a smaller set of national exit levels. Selection of the specific exit level construct or scenario is a matter of policy. It is here that 3MRA output, in the form of preliminary analyses, can provide the decision-maker with adequate background information to determine what the driving concerns for each chemical and each WMU are. In 3MRA's effort to be manageable with respect to data storage and run-time for PC-based applications, these preliminary analyses are designed so the system can aggregate results into four composite receptor categories (resident, resident gardener, fisher, and farmer) to develop cumulative population frequency histograms and critical years (of maximum risk). 3MRA has a dual classification capability and can provide risk/HQ information on individual pathways as well as aggregation across pathways. The $T_{crit\ max}$ (for aggregated data) and T_{crit} value (for individual pathways) may not be the same values. The panel recommends that these values be cross-checked to ensure that cumulative risk is being adequately captured. It is conceivable that the "trueness" of risk of the specified percent population protected, because it is population based, in actuality relies on the quality of the census data.

The second verification issue is related to the quantification of biases in model results based on the propagation of module assumptions/limitations (i.e., process/loading assumptions, module structure, etc.) through the system. Limitations and potential biases of individual modules have been qualitatively described for each module and in some cases the direction and approximate magnitude is presented. It would be desirable to

attempt to make estimates of biases for all modules more quantitative. Also, it is important for model developers to estimate how the module biases are propagated through the integrated system. In other words, does the risk bias inherent in the known module limitations tend to accumulate (positive or negative direction) or do some biases increase risk while others decrease it, thus offsetting each another? This concern could be evaluated through an appropriately designed sensitivity analysis.

Charge Question 3b. EPA has implemented thorough evaluations using the available data resources and technologies, while also recognizing the real world limitations that apply to validating the 3MRA modeling system. Have we reasonably demonstrated through methodology design, peer review, quality control, sensitivity analyses, and model comparison, that the 3MRA modeling system will produce scientifically sound results of high utility for use in multi-media regulatory applications?

3.6 Panel Commentary

3.6.1 General Comments

This question deals with the ability of the 3MRA modeling system to reproduce actual system responses relative to risks to human and ecological receptors caused by chemical releases from WMUs. This capability is necessary for decision-makers to confidently use the model to inform decisions regarding national-scale, contaminant-specific solid waste risk assessment. In recognition of the virtual impossibility of conducting a traditional validation for 3MRA, the panel agrees with the adoption by the 3MRA modeling team of the validation protocol suggested by Beck *et al.* (1997) for evaluating higher order models such as 3MRA. This protocol recognizes other means of model performance evaluation. It includes two basic model features: 1) assessment of the theoretical and numerical construction of the model (essentially an internal measure of validity); and 2) the demonstrated performance of the model in terms of its design purpose (essentially an external measure of validity). The Beck *et al.* (1997) paper also correctly contends that the question of “model validation” in the context of predicting risk to natural environmental systems does not really have a “yes or no” answer. The best we can do is gain sufficient confidence in the model to support decision-making in the specific domain for which it was developed. Part of the “internal” measure of model validity rests in its design and code verification, which has been dealt with in question 3a above. With regard to the other aspects of model validation, the panel believes that the Agency has made every attempt during the developmental phases of 3MRA, given the limitations imposed by available resources and programmatic considerations, to follow the set of principles for validation discussed by Beck, *et al.* (1997).

In spite of the panel’s general agreement with the process being followed for 3MRA validation, there are several concerns and recommendations relative to what has been done and what is ongoing with regard to this question.

3.6.2 Model-Data and Model-Model Comparison

The panel believes that careful comparison with as many actual datasets as possible, even if they are incomplete, is an important way to build confidence in use of the 3MRA modeling system for its stated purpose. The panel applauds the effort that has been initiated for mercury at a former chlor-alkali site, but encourages the location of additional, albeit partial, site-specific datasets involving other contaminants that can be used for model-data comparison. Perhaps a good source of such datasets would result from a post auditing of sites where 3MRA has been applied and a decision has been made. Of special concern are data that stress the source modules of 3MRA. Also, waste disposal sites for which data are available on a single major exposure pathway would provide a useful field test for 3MRA. Such an approach is useful for determining biases of 3MRA and its databases, and will assist in the interpretation of results. The more of these data comparison exercises that EPA can perform, the more transparent the model will become and the more confidence the public will have that 3MRA produces reasonable predictions of risk on a national basis.

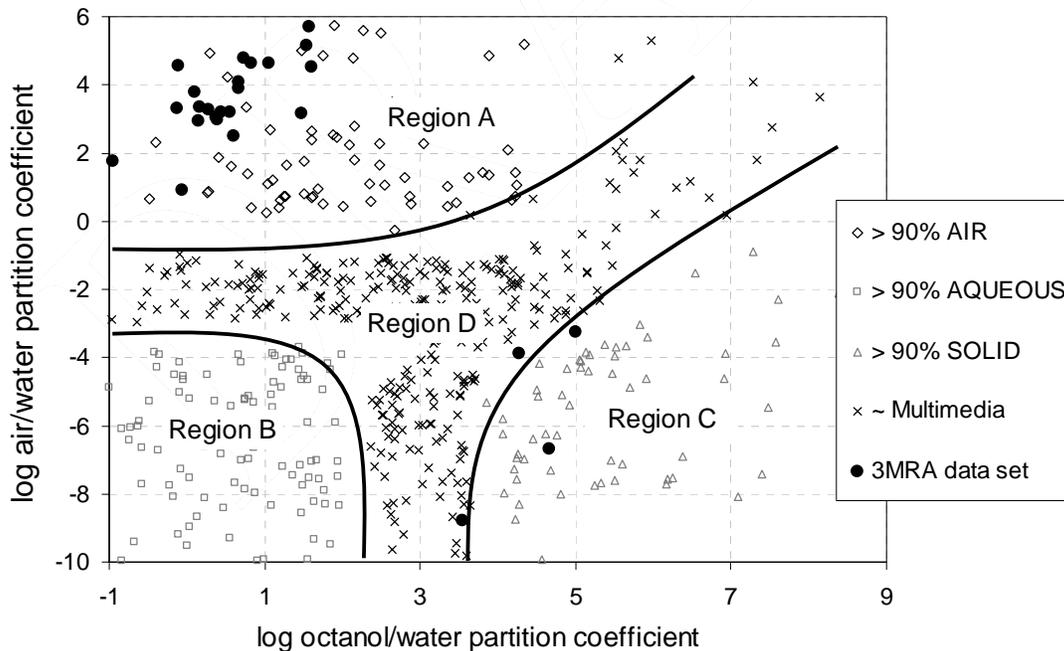
The chlor-alkali facility appears to be one of the few cases where a site exists with available information for both model-model and model-data comparisons. The panel supports the efforts of the Agency thus far in comparing 3MRA with TRIM.fate and with site data on mercury exposure and effects. However, it is apparent that the model to data comparison at the chlor-alkali site is not expected to be very meaningful given the long (and unknowable) history of releases from the site, and the fact that mercury can be transported long distances in the environment making it difficult to determine the original source loading to the area.

Making model-model comparisons and model-data comparisons and explaining differences using knowledge of model process formulations and assumptions is another valuable exercise in building confidence in 3MRA. For example, in the 3MRA – TRIM.fate comparison the 3MRA modeling system takes a linked media receptor-based approach while the TRIM.fate model takes a fully coupled media area-based approach. Recognizing these model differences provides a unique opportunity to test and compare some of the underlying assumptions that these models are based on. For example, the higher concentration of mercury in soil worms in 3MRA versus TRIM.fate at the chlor-alkali site might be explainable by the deeper mixing (and thereby more diluted exposure) of surface soils in TRIM.fate. The agency should endeavor to understand other comparison differences, such as the surface water mercury concentrations and chemical speciation.

Regarding the appropriate chemical space over which 3MRA should be tested for multimedia modeling performance, the panel would certainly recommend retaining the metals and pH dependent chemicals that are currently among the 46 constituents selected to develop and test the 3MRA modeling system. However, among organic constituents, it is important to have chemicals representing the four general areas of solubility parameter space. One approach for describing this solubility space is illustrated in Figure 3-1 where a set of 300+ chemicals are plotted based on their octanol/water partition coefficient and air/water partition coefficient. Regions of the plot are identified where

chemicals partition primarily into a single media (air, water, solid)². The fourth dimension that should be considered when constructing a test set of chemicals for a multimedia model is environmental persistence. The panel notes that the existing set of chemicals in the dataset that is planned for use in testing the model is clearly biased towards chemicals that partition into the air. The panel recommends that the existing set of chemicals be augmented to more fully represent both the potential solubility space and environmental persistence for organic chemicals; and especially recommends adding chemicals that do not partition greater than 90% in any single medium.

The panel recognizes other model analysis efforts to address various validation questions that have arisen. For example, the panel acknowledges EPA's analysis of ISCST3 with regard to its sensitivity to distance from the source. This was an attempt to address the question regarding implications of the 2 km boundary for site definition. The analysis showed that annual average vapor concentrations approach zero within a range of 1-4 km from the edge of each of 20 HWIR sources tested at 10 sites. However, the panel cautions that 3MRA will not capture the cumulative risk potential of chemicals with long-range atmospheric transport potential. While the panel recognizes that the 2 km radius was chosen largely on the basis of limiting the cost of data acquisition, it is recommended that the Agency identify those classes of chemicals for which other tools in addition to 3MRA may need to be applied to assess cumulative risks at longer transport distances.



² The idea of using solubility space to evaluate multimedia behavior comes from Wania, F. (2003) "Assessing the Potential of Persistent Organic Chemicals for Long-Range Transport and Accumulation in Polar Regions" ES&T. 2003, 37,1344-1351 although earlier papers and authors have also used this approach.

Figure 3-1.

Example of solubility parameter space and how it influences partitioning in the environment (generated with the CalTOX model). Region A of the plot includes chemicals that partition primarily into air. Region B includes chemical that partition primarily into water. Region C includes chemical that partition to solids (soil or sediment) and Region D includes chemicals that partition into multiple environmental media. The plot also shows the current list of 3MRA chemicals (solid dots).

While the preliminary results of the ongoing model-data and model-model comparison exercise seem promising, the panel recommends that EPA look for opportunities for additional such validation exercises in order to provide increased confidence in using 3MRA. In looking for additional comparisons, the panel recommends selecting simpler site layouts so that a better site characterization is available. In conducting these exercises, the panel urges that quantitative criteria for evaluating the performance of 3MRA be established. For example, “satisfactory” model-data comparisons might mean that model state variables are within a factor of 2-5 of field observations. Finally, the panel also suggests that any model-model comparison exercise should also include a comparison of model sensitivities for each of the estimation endpoints.

Given the complexity and broad scope of the 3MRA framework and the resulting difficulty in performing traditional data-matching validation of the model prior to using it as a management tool, the panel suggests that a complimentary approach be considered, *i.e.* to ask if the use of the model leads to “correct” management decisions. In fact, this assessment is consistent with the principle stated by Beck, *et al.* (1997) that the best validation of a policy model is “whether the model can perform its designated task reliably, *i.e.*, at a minimum risk of an undesirable outcome.” Given the long history of RCRA and Subtitle C (> 25 years), it may be possible to pose questions where the answers are actually knowable. For example, are there chemicals where a consensus on exit levels has been reached through some other process? Of course, if these chemicals are not already in the 3MRA database, it would be necessary to determine their physical-chemical and toxicity properties and potential source rates so that they could be modeled by the 3MRA system to compute exit levels.

Another possible confidence building exercise would be to show that the relative partitioning of chemicals into different environmental media predicted by 3MRA is reasonable. This can be accomplished by comparing 3MRA model results with those obtained using fugacity models.

3.6.3 Conservation of Mass

An important internal measure of model validity is its ability to conserve both water and chemical mass. As noted in charge question 1, the panel agrees that precautions have been taken to ensure that mass is conserved within the individual

modules of 3MRA. The panel notes in particular that mass is conserved within the source modules, a response to previous criticism.

Still, the panel is concerned that feedback (secondary) sources of contamination, which are not presently modeled within 3MRA, may result in significant mass imbalances for certain chemicals. The panel recognizes that 3MRA contains strictly feed-forward transport of mass from one module to the next. This assumption, although it reduces runtime, may be invalid for certain chemicals and certain media configurations. For example, in 3MRA volatilization loss from surface water or terrestrial plants is a loss of mass from the entire system rather than a contribution to the air compartment. At the same time, volatilization loss is not balanced by gas phase absorption (volatilization is treated effectively as a first-order loss rate based on the single medium concentration). It must be demonstrated using mass conservation analyses that computing air-water or air-plant exchange on the basis of the inter-media concentration gradient (this would require some level of module coupling that allows inter-media feedbacks that are time-dependent) is not a necessary part of the 3MRA system for all chemicals of concern. For example, the screening calculations of air-leaf transfer of chemicals conducted by Ambrose (personal communication, November 20, 2003) does a reasonable job of demonstrating that this partitioning does not impact the air compartment mass balance by more than 5%. The panel is appreciative of this sort of analysis, and recommends continued thinking along these lines to address mass balance questions.

Another mass balance concern in 3MRA deals with the assumption that biota in the system are not included in the mass balance for a given medium; that is, chemical taken up by biota in the food web bioaccumulation modules for water and land becomes an unaccounted-for loss from the entire system. If, in reality, this is a significant transfer of mass, then 3MRA is failing to balance mass by whatever fraction of the total mass is entering the biota. This would be a fairly simple assumption to check; at a given point in time one could multiply the 3MRA-computed biota chemical concentration by the model-assigned biomass for that organism within a given media segment (or segments). One would then compare this mass with the mass of chemical (computed in the same way) in the abiotic portion of that media segment. Probably the simplest media-biota check would be to look at fish in surface water segments.

3.6.4 Peer Review

The panel finds that the level of peer review that the individual science modules received has been impressive, however it is noted that many of the concerns identified by the reviewers, although acknowledged by the Agency, have not been implemented in 3MRA. The panel recognizes that resource limitations may have prevented the Agency from implementing many of the peer review suggestions. We further concur that overt model errors identified through peer review have been corrected through the verification process. Still, concerns persist about the continued implementation of reviewer suggestions such as those related to the GSCM module, secondary sources, and human and ecological exposure issues.

With regard to the GSCM the panel recognizes the key role it plays in three of the five 3MRA source modules. The land-based source modules that use the GSCM are the following WMUs: landfills, waste pits, and land application units. Those not dependent on the GSCM are surface impoundments and aerated tanks. For the 3MRA predictions to be reliable these five source modules must accurately launch the chemical masses on their multi-pathways through the ecosystem delivering quantities that eventually impact biological targets. The panel is concerned that this module, which is not a legacy model with a long history of peer review and field-testing, has not received the same degree of scientific scrutiny as other modules. Of particular concern with this model are its method of mass transfer from wastes to environmental media (air and vadose zone) and the assumption of local equilibrium among phases.

Given that the GSCM is relatively untested and has some potential theoretical inadequacies it is incumbent upon the agency to demonstrate that the GSCM affords a level of accuracy commensurate with the legacy models being used in the 3MRA system. This analysis should be done using data matching under a wide range of conditions and chemicals, comparison of results with more robust models, and theoretical or error analysis. The LAU Module, which contains GSCM, has been compared to experimental data obtained on organic chemicals during application of municipal wastewater onto soil (Schmelling *et al.* 2003). Five factors were tested: volatilization, first order chemical decay, appropriateness of the quasi-analytical solution, LAU thickness, and temperature. The volatilization rate was reported to be in the “right order of magnitude” for all categories of compounds. However, for the highly volatile chemicals the model was consistently lower than observed. In another validation exercise for the LAU module, measured half-lives of dioxin in sewage sludge were compared. Remaining concentrations at equivalent human health risks were calculated for the LAU in order to estimate the half-lives. Results were stated as: “The range of half-lives over the selected percentiles was 20 to 48 years, which is in reasonable agreement with the observed half-lives at several monitored sites.” However, the numerical range was not reported; and the number of monitoring sites not in agreement was not reported. The panel also recognizes the model comparison effort between GSCM and MODFLOW-SURFACT that has recently been made by EPA (December, 2003 communication). Several insights were gained through this exercise, including an explanation for why GSCM gives higher volatilization fluxes in the first several years of a simulation – it solves for fluxes sequentially with volatilization computed prior to leaching. While these validation exercises are the type of activities that the panel believes are needed for GSCM, the panel recommends a more rigorous model-data validation analysis, perhaps using well-controlled lysimeter experiments, that identifies the conditions (chemical and site-specific) under which GSCM fails. As part of this analysis, quantitative criteria need to be established that are consistent with those used for assessing the WMU legacy models. If the GSCM does not meet these criteria, the panel strongly recommends that the model be revised to remedy the shortcomings. The outcomes of this validation process and model revisions should be documented.

A more detailed discussion, review, and recommendations for improvement of the GSCM module are presented in Appendix 3b.

3.6.5 Sensitivity Analysis

The panel believes that sensitivity analysis is a critical part of the validation process for 3MRA. Although a model sensitivity analysis is not a direct measure of its reliability, there are indirect indicators of problems with model validity that can be obtained through a sensitivity analysis. The sensitivity analysis results can identify and prioritize areas of concern that require model modifications or additional data collection. For example, a model whose predictions vary greatly in response to minor changes in key parameters, especially parameters with high uncertainty, would be a cause for more detailed investigation of its validity. Although the Agency has demonstrated their understanding of existing techniques, the documentation fails to adequately explain – or demonstrate through an illustrative case study – how an actual sensitivity analysis of a 3MRA application will be performed and how the outcome will be presented to the decision-makers and stakeholders. The panel strongly encourages the Agency to complete a sensitivity analysis in 3MRA that covers the chemical space displayed in Figure 3-1 so that each “national assessment” for the list of chemicals for which data are available can be accompanied by a sensitivity analysis using a stochastic basis for risk parameters.

In summary, the panel agrees with and commends EPA’s defined series of model validation tests that 3MRA must pass prior to acceptance for use in the HWIR national risk assessment. The panel recognizes that completion of the very important performance validity tests is ongoing. Indeed, the panel understands that models and sub-models are continually evolving and improving as we expand our knowledge base and acquire new data, made easier in 3MRA by its innovative design and construction within FRAMES. In this regard, the panel recommends use of 3MRA for its stated purpose of supporting the establishment of national exit levels pending completion of the Agency’s planned performance validity tests. However, the panel strongly recommends that the 3MRA modeling team continue to evaluate and upgrade the 3MRA model and to clearly communicate the results of this work to the stakeholder community along with commensurate statements regarding model limitations and caveats for its use.

3.6.6 References

- Ambrose, R.B., Jr. “Screening Analysis of Air to Canopy Pollutant Mass Balance,” personal communication to the 3MRA panel, November 20, 2003.
- Beck, M.B., J.R. Ravetz, L.A. Mulkey and T.O. Barnwell. 1997. On the problem of model validation for predictive exposure assessments. *Stochastic Hydrology and Hydraulics*. 11:229-254.
- Schmelling, S., M. Wang and K. Liu. 2003. Proceedings The Air and Waste Management Association: National Mtg., Washington, D.C.

Charge Question 4. Is the documentation for the 3MRA Modeling System adequately designed and prepared? Does the SAB have additional suggestions for improving the presentation of the comprehensive set of materials related to this modeling system?

3.7 Panel Commentary

3.7.1 General Comments

In general, the panel finds the documentation for 3MRA (five volumes) to be well presented, and reasonably well organized. Several panelists with familiarity with the earlier 1995 HWIR documentation that preceded 3MRA have indicated that the 3MRA documentation is a significant improvement over the HWIR materials prepared in 1995. It seems clear that many earlier criticisms about the clarity and completeness of the deficiencies in the HWIR documentation have been taken as constructive criticism by the EPA authors.

Given the challenging volume of material included in the 3MRA modeling system, it is generally readable if taken in modest doses. The level of detail provided helps the reader to understand both the strategic thinking that went into its planning, development, and testing. The organization of the material, with detailed tables of contents, makes it relatively easy to limit reading to the subjects of greatest concern. The document also provides numerous helpful graphical depictions of model components to aid the reader's understanding of this complex modeling system.

For the reader who is deeply interested in the model framework, the development and verification history, or the specific modeling algorithms used in the 17 simulation models, the documentation is well designed. However, for those most interested in applying the model, the current documentation could be improved. The panel recommends reorganization and revision with respect to the need for a readable summary, improved clarity of terms (especially those related to the treatment of uncertainty in 3MRA), and more concise descriptions of databases. In addition, for users of the model (beyond the model developers), a revised User's Guide should be considered that better focuses on implementing the model and processing the results, rather than the model theoretical framework.

There are several areas that require clarification, and even significant revision, in order to make the 3MRA documentation clear, transparent, and more understandable in order to facilitate stakeholders outside the Agency in their ability to understand and run the model. The panel provides the following general recommendations.

3.7.2 Recommendations

The panel recommends that the Agency develop a more "digestible" summary that describes the 3MRA in more understandable terms. The sheer volume of material,

combined with technical jargon covering many disciplines, makes for a “dense” read for even a technical audience.

The concept of “population protection” is central to the development of national exit levels, yet this concept does not receive adequate attention in the documentation. The document should provide a very simple and clear example of how population protection is calculated, using a graphical depiction, and then how these results for a particular site/simulation are “rolled up” into a calculation of the percent sites protected. As it stands, the documentation tends to describe the mechanics of the approach relying on 3MRA “jargon” (such as ELPI, ELPII, RSOF, *etc.*), which does not provide the typical reader with an intuitive understanding of the approach. The document should provide very concrete examples of a probability distribution of population protection with well-labeled graphs, using an example of a single chemical/concentration simulation. The figures in Volume 1 describing these concepts are not clearly labeled and do not convey the concept of population protection adequately. Not only does population protection (and percent sites protected) require better definition, at present the text gives the impression that 3MRA will provide outputs of the “nationwide distribution of risks” for receptors (see, for example, pp. 1-15). Yet, it is the panel’s understanding that the risk results themselves are not stored in 3MRA, and instead “risk bins” are used to estimate the distribution of nationwide WMU sites that achieve a specified value of population protection (in question 2c, the panel recommends that 3MRA actually store the calculated risk outcomes at each site.)

From public meetings/conference calls with the Agency, the panel understands that there are internal “check points” in the 3MRA calculations such that particular sites are “excluded” from the percent population protected calculations if an adequately sized human population does not exist within the radius of interest examined in 3MRA (the Agency indicates that all sites have ecological receptors within the specified area of interest). The documentation should include a discussion of this, and also indicate for how many site/WMU combinations this in fact occurs. The documentation should be very clear in terms of the minimum threshold population size within the radius of interest, or within census blocks if that is how the calculations are performed, that is required to be included in the 3MRA percent population protection and percent sites protected calculation.

As noted previously, the number of operational input parameters that go into the 3MRA is very large, such that it is quite difficult for someone not fully versed in the model details to grasp those that are based on empirical data, those that are based on professional judgment, and those that are “operational” assumptions. It appears there are key variables that are based on operational assumptions (for example the “fraction hazardous waste,” or f_{wmu} , term) that are not clearly articulated in the documentation. It is essential that EPA summarize these more concisely, perhaps developing a parameter matrix and categorizing them as suggested here (empirical, professional judgment, and operational), in order to provide a more intuitive understanding of how the operational parameters influence the model formulation and results.

The discussion of uncertainty, variability, and sensitivity concepts relating to the Monte Carlo analysis (Volume IV) fails to explain adequately what was done to address variability and uncertainty in the 3MRA. The explanations in Volume IV require significant revision in order to make the actual Monte Carlo Analysis implementation of the 3MRA understandable and transparent (see Appendix 4-1 for additional suggestions). In addition, for reasons further explained in question 2c, the panel recommends that the document avoid the “pseudo 2-D” terminology used in reference to the MCA, as the terminology invites misinterpretation of the results.

The panel encourages the Agency to continue development of mechanisms for meaningful interpretation of model output, currently underway for 3MRA version 1.x. While the Agency has indicated that Version 1.x provides the ability to store detailed output results for some of the underlying governing model parameters, only the Agency has access to the version 1.x “tools.” The panel believes it is incumbent upon the Agency to complete the version 1.x tools prior to adopting 3MRA for site-specific applications, as without these tools, the public is left without the ability to examine the results in a meaningful fashion.

The adoption of the FRAMES modular architecture with the inclusion of legacy modeling codes, offers the flexibility to “swap out” modules as improved models/data are available. In addition, the means of passing input and output parameters from one module to another in the form of SSF and GRF files is one of virtues of the 3MRA/FRAMES construct. As recognized by the Agency, this structure offers the flexibility and ability to turn certain modules “on” or “off” and even substitute certain components (*e.g.*, source terms) as information allows. While the panel strongly endorses this architecture and believes the Agency should be commended for its design, at present the documentation necessary to take advantage of this flexible design is insufficient for anyone but the model developers. The panel therefore encourages the Agency to provide adequate documentation of (1) how to substitute or turn off certain modules, and (2) provide a more detailed data dictionary and description of the SSF and GRF data files. Without these two critical elements, it is at present infeasible for the public and stakeholder community to harness or test these elements of the 3MRA.

The panel is confused over the Agency’s use of the term “screening level” with respect to 3MRA. Is this meant to convey that the mathematical models within 3MRA are considered “simple” based on conservative assumptions? Alternatively, the term screening level in the 3MRA context could be viewed instead as a collection of models (of varying complexity) that are assembled in 3MRA for excluding (“screening”) listed hazardous wastes. It is recommended that the 3MRA documentation provide a clear definition and consistent use of this term.

The remaining panel comments on the 3MRA documentation are provided as “specific comments” in Appendix 4-1. Several that are not specific to a particular volume are presented first, followed by comments that are directed toward recommendations for specific volumes. Appendix 4-2 contains a candidate outline for a possible revision to the 3MRA User’s Manual. Finally, while it was not the panel’s

intent to review the document in terms of style, grammar, or typographical issues, to the extent we have input, these comments are noted in Appendix 4-3.

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APPENDICES

Appendix 1-1 Exposure Duration

Exposure duration is input as a constant value in 3MRA, neither variable nor uncertain. This fixed value fails to capture the upper end of the distribution. For example farm families in particular often spend their whole lives at one residence. This lack of variation may distort the output distribution, making it appear narrower than it really is. This may tend to underestimate risk or hazard at the upper end of the distribution. Since 3MRA addresses farmers specifically, a distribution of exposure duration applicable to farm families should be used or, at a minimum, the general exposure duration distribution should include farm families. Inclusion of upper end values will ensure that subpopulations that tend to reside in one location for an extended time are protected.

Appendix 1-2 Correlated Variables

Several exposure parameters in 3MRA that co-vary with body weight are treated as independent. This makes the exposure appear more variable than it really is. For example, respiration rates are not normalized to body weight, nor are they apparently correlated to body weight. This means that body weights and respiration rates are selected randomly and independently from their distributions for each model realization. The result of this approach is that the largest adult (660 lbs) is just as likely to be paired with the minimum breathing rate (1 m³/day) as with the maximum breathing rate (50 m³/day). This is also true for the smallest adult (33 lbs). This means that the breathing rate can cover the implausible range from 3.3 L/kg/day to 3,300 L/kg/day. (The occurrence of such implausible combinations can be studied by storing individual iterations of the model Ranking them according the resulting risk or hazard and examining the results in the tails of the distributions.) Ideally, respiration rates would be expressed as a function of body weight to the 0.7 power. Other examples of variables incorrectly treated as independent of body weight include fish consumption and drinking water consumption. Again, the problem is similar: when the exposure to contaminants in the fish or in drinking water is expressed in mg/kg/day, the range of exposure rates is exaggerated because the model allows, for example, a 10 kg child to eat 1500 g fish or drink 2100 ml of water per day.

The panel recognizes that extremes in the tails of the distributions are not picked very often, so absurd pairings will be rare. Still, 3MRA exposure factors are based on sources (e.g., the 1997 Exposure Factors Handbook) that were not designed with stochastic analysis in mind. If mid-range body weight and breathing rates for an adult are chosen for a deterministic analysis, then it does not matter if normalization to body weight is done or not. But when parameter values are allowed to vary within their ranges, it is essential to control how they co-vary. The assumption of independence is not justified in this case.

Appendix 1-3 Alternative Waste Management Options

The focus in 3MRA on only land-based facilities has some intrinsic limitations; for example, the landfill prototype and the surface impoundment WMU are put down on native material without the benefit of liners, gas collection systems or leachate treatment systems. It is unclear to the panel how many facilities fitting these descriptions are still allowed to operate even considering the range of regulatory oversight under state jurisdictions, but in any case the panel feels that some representative range of modern technology should become available to the 3MRA user. This becomes especially important as the uses of 3MRA are extended to include evaluation of individual facilities (for example for delisting purposes), or designs for proposed facilities. In addition, the consequence of allowing relatively unsophisticated protective designs is the influence on exit levels, which may turn out to be unrealistically restrictive thereby defeating one of the major purposes for developing 3MRA, the perception of overly stringent regulation. In order to treat the case of a modern Subtitle D landfill, there will need to be sub-models to determine gas generation, collection and utilization, contaminant levels in fugitive emissions of uncollected gas, pollutant partitioning in cover soil, and failure mode analysis of these processes.

The panel's view is that the present assessment methodology overlooks at least five strategies for releasing a waste stream from the rigors of Subtitle C: support for delisting of hazardous wastes, municipal waste combustors, detoxification of wastes, and pollution prevention and industrial ecology alternatives. By omitting such options, the 3MRA assessment methodology needlessly restricts the decision-maker's thinking by offering only the five classes of WMUs included in the simulation, when in reality the missing alternatives are readily implemented and officially encouraged under available contemporary practices. These alternatives are amplified below.

An immediate application of 3MRA would be to support de-listing petitions. For this use it needs to be set up in such a way that site-specific data can be readily entered to supplement the existing databases, and enough iterations run for a single site to give reproducible results. Beyond this, there is potential for assessment of risk at contaminated sites, and risk-based support of permitting decisions. Because the FRAMES architecture allows for plug-in applications to suit specific needs, it can have many other uses. The panel supports the use of this model with some enhancements for the intended purpose and its continued development for other applications.

Considering that, after materials recovery, 21% of US municipal waste is handled by municipal waste combustors (MWCs), it is surprising that this diversion alternative is not included in 3MRA. Preliminary studies have suggested the favorable feasibility of destroying household hazardous waste in MWCs considering the temperature-time characteristics of MWC furnaces. Very effective destruction and removal efficiencies are available in the MWC even for such refractory compounds as CFCs. In its present form, the 3MRA modeling system has all of the modules needed to assess risks of air emissions and ash disposal from MWCs, and sufficient data exist to support a combustion

alternative that can be evaluated on a national scale. Emission rates and configuration parameters (e.g., stack characterization: height, diameter, temperature, velocity and base elevation) are available for the US population of MWCs, although the range of receptor domains would need to be enlarged for each source because of emissions at higher elevations. All of the algorithmic mechanisms for handling deposition and indirect pathways are already embodied the present version of the 3MRA so that only the source and receptor files need to be modified.

A second type of WMU alternative that 3MRA might address are pollution prevention/detoxification schemes involving stabilization of a hazardous waste in a product stream. An example of this is the exemption of petroleum coke quenched with oily refinery sludges from the standards, record keeping and labeling requirements of RCRA. Since the early 1970s some refineries have blended API separator sludges, tank bottoms and biological solids in the water stream used to cool petroleum coke at the end of a delayed coker cycle. Presumably contaminants such as metals or polycyclic aromatic hydrocarbons bind to the carbonaceous substrate of coke particles. This technique has been embraced by the European Commission in its catalog of Best Available Technologies, but it is doubtful that any occupational or community health risk assessment was ever performed. Evaluation of exemptions such as this should have a clear place in the 3MRA assessment methodology. A generic module with adjustable input/output structure might be contemplated in anticipation of problems like this. As further encouragement to the user, some synthetic case studies might be packaged in with the software as a means of demonstrating the flexibility of 3MRA.

The third example is taken from the industrial ecology field: the use of a waste stream from one process as a raw material for another. Many industries, long accustomed to seeking out profits from their own waste products, have embraced this concept enthusiastically. There are numerous present-day examples of such approaches ranging from the use of more environmentally benign materials in processing, pollution prevention, products designed for reuse, and materials recycling. Such approaches are viable when they retain embodied value within the manufacturing system, or when they help in the avoidance of waste management costs. On a larger scale, the co-location of compatible (in terms of waste reuse) industries in eco-industrial parks has gained wide recognition as a viable waste management option in many areas, including the United States. A recent report by the SAB has documented the advantages of the industrial ecology approach, and summarized research needs in this area (Thomas *et al.* 2003). Flexible access to a tool such as 3MRA, suitably modified to incorporate industrial ecology strategies, could be quite useful in quantifying comparative risk among traditional and forward-looking management strategies. A synthetic demonstration study would encourage users to consider other possible waste management scenarios.

Reference

Thomas, V., T. Theis, R. Lifset, D. Grasso, B. Kim, C. Koshland, and R. Pfahl (2003). Industrial Ecology: Policy Potential and Research Needs. *Environmental Engineering Science*, 20(1): 1-9.

Appendix 2a-1 Classification of 3MRA Submodels

The 3MRA review panel and the Agency both recognize that it is common risk assessment practice to consider a series of graded steps or “tiers” to distinguish between models used to make judgments about output information applied to environmental risk analyses. These range from the simplest of “Screening” models to advanced regulatory guidance modeling systems used for site-specific decision making to more elaborate research-grade models. The panel also recognized that the use of the terminology “tiers” could often mean different things to different model users depending upon the intended application. For instance, those who are most concerned about the use of the “best current science” might have a different perspective about the needs for relative ease of use, understandability to the broader public, or verification history than someone who is tasked with using the information to formulate policy. The regulatory officials are charged (and challenged) with making credible decisions in an “immediate” time frame, based on modeling results likely to have a reasonable level of acceptance by the stakeholders in the pending decision.

A further challenge arises when multiple models, of varying complexities, are linked together, as is the case with 3MRA. Often, a multi-part model may be only as strong as its weakest component in terms of the validity, reliability, and reproducibility of its output. Therefore, to help clarify understanding of the 3MRA system of models, the panel undertook a simple characterization exercise. Panel members were asked to rank the relative level of sophistication and validation experience observed for each of 3MRA’s sub-modules, considering both the “state of science” embodied in the module and the level of “regulatory practice” with which each module has been applied.

To support this effort, outlined below are some common characteristics used to classify models according to their varying “Tiers” of sophistication, and demonstration of performance acceptability by those in the regulatory and risk analysis research communities. Initially, two separate model characterization matrices were proposed for panel members. Each of these tables contains the same set of models and Tier classifications to register panel member opinions. However, one version of the table was to characterize the relative Tier levels on the basis of “best science” employed by the individual components; while the other table was to characterize how the individual components typically are used in the regulatory arena.

Any such listing is necessarily affected significantly by the experience of the authoring group. For that reason, the panel has made this model ranking demonstration a

“group effort” to ensure that they would reflect some of the diverse experience of panel members. As this model characterization effort developed, it became evident that the detail level presented below in order to help standardize the assessment framework could only be maintained when a member was intimately familiar with a model’s design and application history. Therefore, most participating panel members simplified their representation of the detailed characteristics and presented assessments that clearly categorized a submodel as falling into one, or possibly two Tiers. After the assessments were submitted, the panel’s task force editors tallied the (sometimes split) votes and further simplified the presentation of results to present them in a single tabulation (Table A2a-1). At the end of the table are listed the three versions (1.0, 1.X, and 2.0) of the entire 3MRA modeling system that the EPA now has under development. Without presenting details of version differences in this appendix, the assessment of panel members is presented to reflect their overall opinions of the Tier-status of each of these versions. As noted in the table, the assessments for “best science” are labeled as “s”, and for “regulatory application” as “r”. To give readers a sense of the “mode” of their distributions, these symbols are capitalized when two or more total assessments (summing split and whole assessments) were tallied for a particular Tier classification.

This model classification effort commenced early in the panel’s review efforts. As the review continued, a number of the steps already taken by the Agency earlier in its 3MRA development planning became more evident. The panel appreciates the very significant progress already made by the Agency in reaching the present level of 3MRA development. The panel trusts that the characterization scheme identified here will not only have been useful to the panel in its own deliberations about the state of 3MRA development; but may also assist the Agency in establishing priorities for the continuing that progress as it strives to make the best use of the present version(s) of this landmark risk assessment modeling system.

The 3MRA Submodel Classification Process

Beyond the simplicity of the present characterization, the models/modules of multi-pathway risk modeling systems range widely in their level of sophistication and applicability. They may start with a very simple screening model (Tier 1) used to make initial “back of the envelope” estimates. These Tier 1 models predict chemical concentrations in various media for instant comparison with benchmark concentration levels or risk levels; and they are often based on use of generic national or “worst case” input parameters.

At the next, more refined level, (Tier 2), more sophisticated and complex models/modules consisting of “stand-alone” environmental release, dispersion, environmental transport and fate, and exposure/uptake/risk models are frequently used by the EPA for advanced screening assessments, or basic site-specific studies. Finally, for advanced risk assessments (Tier 3), usually performed on a local or site-specific basis, some of the same models, employing more representative local (or regional) input parameters will be applied to more advanced risk assessment studies. For many of the most sophisticated models, however, the detail and quantity of input data may be

demanding. In these latter cases, the unavailability of representative and detailed local data can make a Tier 3 model inaccurate and ineffective; and in those cases, either the Tier 1 or Tier 2 models may be preferred. That is why many of the Tier 1 and Tier 2 models are most often broadly recommended by regulatory agency “guidance.”

Initially the panel also discussed the potential role of research-grade models, of which there are many, to allow analysts to address special chemical fate and transport or environmental transformation and uptake processes. Although these models can be considered when needed to address information gaps that are recognized in the 3MRA system, particularly model verification comparisons; the selection, application and interpretation of this last set of modeling tools relies heavily upon professional judgments made by the model users, most often for site-specific rather than national “screening” contexts. (The panel has seen EPA’s consideration of the many alternatives in its careful selection of a set of models that will, in the Agency’s view best meet the regulatory application objectives established for the 3MRA system).

For these reasons, the following outline defines, for the present 3MRA submodel classification context, a set of characteristics that the panel members have used for determining the herein-defined “Tiers.” (Note that, for considerations of “best science”, these Tiers necessarily differ from the Tier systems specified in various regulatory federal and state agency guideline documents; but for the current listing of “Regulatory Application” tiers, they could be tailored in the future to match a particular reference guideline document if desired). As defined below, Tier characteristics are separated into traits that are usually important for judging the level of achievement/applicability based on “best science” or “regulatory application.” In all cases, it is assumed that the output information is either exposure point concentrations in various media, or the risks calculated by immediate application of widely published risk (or Hazard Quotient/Index) factors to these media concentrations.

TIER I – SIMPLE SCREENING MODELS

- **Qualitatively**
 - (a) **Box Models** - based upon experience with more refined models applied to a range of site specific cases, but in present case applied to a geographical, physical, or chemical environment setting about which very little information is available.
 - (b) **Environmental Compartment (e.g., fugacity) Models** – basic versions, when sufficient information about application environment is known to derive estimates of potential fluxes between compartments, but scale of application may lead to very low precision due to inclusion of numerous regimes or ranges of variation of key variables for the environment of the particular screening application.
 - (c) **Simple Dispersion or Linear Transport Models** – based on models with either (1) modest history of application and little verification/validation data; or (2) better history of validation and acceptance, but applied in a situation in which key

underlying theoretical assumptions are known to be violated--making the representativeness/accuracy/precision historically associated with the model all highly suspect.

- (d) **Advanced Dispersion or Complex Transport and Fate Models** – based on use of scientifically advanced (perhaps newest) models that include much of the known science on transport and fate processes, but applied in situations for which many key model input parameters must be based on “generic” default values because no comparable data are available to represent/describe the particular location of the application. [For example use of national average values for all input parameters without any information available to judge how to potentially “adjust” the results to the specific situation(s)].
- (e) **General Concerns:** (1) validation/verification history of less concern at this level due to inherent questions raised by magnitude/impact of simplifying assumptions; (2) reproducibility is enhanced by simplicity of formulation; (3) history of use, especially in regulatory context, can add importantly to credibility of screening decision outcome, even at a Tier 1 level of application.

- **Quantitatively**

- (a) Typically deterministic “point”-estimate models may provide estimates for a number of case-specified locations or situations, but normally do not include any stochastic sampling routines/elements.
- (b) May be “pre-solved” lookup tables based on distillations of analysis results from families of existing or hypothetical situations. (E.g., engineering nomographs for range of typical situations).
- (c) Large Margin of Uncertainty due to anticipated wide range of variability in model input data and large uncertainties about model representativeness. (Depending on application uncertainty may be 10 to 10,000-fold).
- (d) Use in decision-making virtually always “one-way”: If results, with consideration of all conservatively-biased input data estimates, indicate “no possible problem”, then no further analysis is necessary and results are considered “acceptable.”
- (e) Simplicity ensures quantitative reproducibility and easy understanding of limitations of application results.

TIER II – REFINED SCREENING MODELS

- **Qualitatively**

- (a) **Box Models** – advanced versions, more in the sense of their calibration or verification history and their representativeness of the particular application/location; may also be derived from statistical (e.g., epidemiological) studies in which the coefficients for the particular application have been estimated from an empirical study that include relevant parameters.
- (b) **Environmental Compartment (e.g., fugacity) Models** – more advanced versions, when sufficient information about application environment is known to derive estimates of potential fluxes between compartments, and scale and specificity of application allows “reasonable” (moderate) precision due to availability of environmental media concentration data (supplemented by “proven” models) and limitation to known regimes or ranges of variation of key variables for the environment of the particular screening application.
- (c) **Simple or Advanced Dispersion or Linear Transport Models** – based on models with “solid history” of application, including moderate to good verification/validation data; but applied in a situation in which key underlying theoretical assumptions are known to be reasonably applicable, or at least not seriously violated, so that the representativeness and accuracy/precision associated with the model are more acceptable to both scientists and regulators.
- (d) **Advanced Dispersion or Complex Transport and Fate Models** – based on use of scientifically advanced (including perhaps the newest) models that include much of the known science on transport and fate processes, but applied in situations for which many key model input parameters can be supported by a combination of parameter values demonstrably specific to the application, with modest reliance upon “generic” default parameter values when necessary. [For example, replacement of national average values for all key input parameters with regional or local (site-specific) values to potentially “adjust” the results to the specific situation(s)].
- (e) **General Concerns:** (1) validation/verification history of more concern at this level, but due to inherent questions raised by magnitude/impact of simplifying assumptions; and the typical “one-way” decisions made, not necessarily crucial (2) reproducibility may be a significant issue for the more complex models, as more technical skill and frequent use of “professional judgment” is required; (3) history of use, especially in regulatory context, can also add importantly to credibility of screening decision outcome .

- **Quantitatively**

- (a) Typically deterministic “point” estimate models may provide estimates for a number of case-specified locations or situations. However, more advanced screening models but may include a stochastic “shell” sampling routines/elements to enhance analyst’s ability to evaluate uncertainty of model predictions by allowing repeated simulations to vary input values over anticipated ranges that could be applicable to the particular situation of interest. [Normally Monte Carlo or Latin Hypercube sampling is performed on a One-dimensional basis at this level and thus does not attempt to separate effects of parameter “variability” from measurement or estimation “uncertainty”].
- (b) Unlikely to be “pre-solved” lookup tables based on distillations of analysis results from families of existing or hypothetical situations, unless the method is supplemented by algorithms that can be evaluated with site-specific information to over-ride the original “generic” results. (E.g., engineering nomographs for interactive range of specific situations).
- (c) Reduced Margin of Uncertainty due to better-understood and more limited range of variability in model input data and smaller uncertainties about model representativeness. (Depending on application uncertainty may still be 10 to 1,000-fold—individual media concentrations may be within 5 to 500-fold).
- (d) Use in decision-making usually “one-way”: If results, with consideration of all conservatively-biased input data estimates, indicate “no likely problem”, then no further analysis is necessary and results are considered “acceptable”.
- (e) Greater complexity suggests specification of benchmark problems or test cases to be run by model user to ensure quantitative reproducibility and to promote better understanding of limitations of application results.

TIER III – ADVANCED MULTIPATHWAY RISK MODELS

- **Qualitatively**

- (a) **Box Models** – advanced versions may still be used to fill in gaps not addressed by other modules. In this case, simplicity and direct specificity (and perhaps comparison to site-specific data gathered for the purpose) for the particular application are essential to replace the absent calibration/verification history—to demonstrate representativeness and likely accuracy/precision for the particular application/location; may also be “supported by” data/results derived from statistical (e.g., epidemiological) studies in which the coefficients for the particular application have been estimated from an empirical study that include relevant parameters. In general, usually replaced or augmented by more complex deterministic and/or stochastically enhanced modules.
- (b) **Environmental Compartment (e.g., fugacity) Models** – may be compared with more detailed deterministic model results by regulators, but less likely to serve as

- primary tool for regulatory decisions, except at the global, or perhaps national policy level. In this latter situation, the most advanced model versions (along with their validation history for situations in which they have been optimally applied and compared with available measurement data) would be used to judge whether the predictions of future balances between environmental compartments, and estimates of potential fluxes between compartments, are credible for the application of interest.
- (c) **Simple or Advanced Dispersion or Linear Transport Models** – based on models with “solid history” of application, including previous regulatory application precedent and moderate to good verification/validation data. Once again, acceptability depends upon model application in a situation in which key underlying theoretical assumptions are known to be reasonably applicable, or at least not seriously violated, so that the representativeness and accuracy/precision associated with the model are more acceptable to both scientists and regulators. [Often the use of a more advanced model, especially one which is based on stochastic procedures for producing distributions of outcomes, will be required to be compared with results from a simpler “legacy” regulatory model to provide a regulatory context that is best understood by all stakeholders in the particular regulatory decision].
- (d) **Advanced Multi-pathway Dispersion and Complex Transport, Fate, and Exposure Models** – based on use of a combination of scientifically advanced (including perhaps the newest) models that include much of the known science on transport and fate processes, but applied in situations for which many key model input parameters can be supported by a combination of parameter values demonstrably specific to the application, with modest or minimal reliance upon “generic” default parameter values when necessary. [For example, replacement of national average values for all key input parameters with regional or local (site-specific) values to potentially “adjust” the results to the specific situation(s), to the limits of application-specific data].
- (e) **General Concerns:** (1) validation/verification history of highest concern at this level, but due to inherent questions raised by the complexity of the combination of models/modules it is likely (as stated in the present 3MRA documentation) that it may never be possible to test all of the components of any available multi-pathway environmental risk assessment model.--at least, not while they are functioning in an integrated manner, unless a major verification experiment is undertaken with that goal as the organizing principal for the experiment. The extraordinary cost and complexity of such an undertaking would suggest that it would likely take at least several years to accomplish. In the meantime, the regulatory agencies have many risk management decisions requiring decisive action in a shorter time frame. Thus, in the interim the best situation that may be achievable would be that resulting from critical review of the currently available modeling tools, with an ongoing commitment to a maintaining a “best practical application of the best science” culture; (2) reproducibility will certainly be a

significant issue for the most complex models, as much technical skill and frequent use of “professional judgment” is required (see need for benchmark testing, below); and (3) history of use, especially in regulatory context, but also with independent verification of important results by other stakeholders will determine the ultimate credibility of risk management decisions based on employment of these most complex regulatory modeling tools .

- **Quantitatively**

- (a) Typically deterministic “point” estimate models may provide estimates for a number of case-specified locations or situations. However, the most advanced multifunctional multi-pathway models like 3MRA will increasingly rely upon the supplementary perspectives provided by the ability to properly apply stochastic “shell” sampling routines/elements. Eventually the availability of 2-D (and perhaps 3-D) stochastic modeling routines as shells will not just provide an important “diagnostic” tool for the model development team. Instead, these tools will also allow the well-trained user to demonstrate the differences between uncertainties that are due purely to “variability” and the relative magnitude of the residual “uncertainties due to measurement or estimation or model representativeness (from 3-D tests).
- (b) Potential to reduce, or at least better diagnose, Margin of Uncertainty due to better-understood and more limited range of variability in model input data and smaller uncertainties about model representativeness. (Depending on application residual uncertainty in components of primary interest may still be 10 to 1,000-fold—individual media concentrations may be within 3 to 100-fold).
- (c) Use in decision-making is improved for drawing more reliable conclusions about alternative situations that yield competitive risk results; comparisons can suggest which of potential future situations is likely to be associated with reduced risk to the designated parties. (E.g., more confidence (with quantitative statement of level) that one result differs by a quantifiable magnitude from the alternative).
- (d) Greater complexity suggests specification of benchmark problems or test cases to be run by model user to ensure quantitative reproducibility and to promote better understanding of limitations of application results.

Detailed Model Characteristics to Consider for Tier Selection

Table A2a-1 presents the combined matrix for both the “Best-Science” (S) and “Regulatory Application” (R) attributes for the 3MRA submodels, and the entire model (three versions). Capitalization of symbol S or R indicates that 2 or more panel members voted for the particular classification of the sub-model. Lower case = < 2 votes, some members split votes. This summary tabulation notation differs from the detailed notation method initially recommended to Panel members for the first draft of the model characterization/ranking procedure. That initial procedure was quite detailed (see below), and then streamlined slightly to make it easier for those relying on 3MRA documentation

as much as their own experience to draw conclusions on model features. These detailed attributes are the descriptors of process simulation details included in each model.

- 1) **PU** = **P**rocess **U**nderstanding (detail)
- 2) **SR** = **S**patial **R**esolution (1-D, 2-D, 3-D)
- 3) **TS** = **T**emporal **S**tructure (static equilibrium or dynamic)
- 4) **MS** = **M**athematical **S**ophistication (e.g. box, multiple layer, Gaussian or Lagrangian model)
- 5) **H** = **H**istory of **U**se (validation, verification, and regulatory use)
- 6) **ID** = **I**nter **D**ata (age, quality, & representativeness of information)
- 7) **UR** = **U**ncertainty of **R**esults (model output)

Initially, a blank “A” and “B” versions were circulated to panel members to acquire separate votes for ‘Best Science’ and for expected best “Regulatory Practice”, respectively. The Agency has represented that 3MRA has been developed primarily for national regulatory policy analysis and implementation by regulatory specialists. However, because the utility of this set of modeling tools may be attractive for more extensive applications, some future users are likely to be by non-Agency personnel, and the context may be different. Thus, the 3MRA review panel was charged with a specific request for suggestions on the “best science” that may be presently included or readily added in the near future. (It was assumed that some of the descriptors might not be applicable in both matrices, and panel members only voted on models for which they felt they had enough information to support an opinion).

Streamlined Alternative Model Ranking Scheme

Many panel members considered the use of the mnemonic (two letter) coding scheme identified above for all 7 listed characteristics a bit too complicated for the current demonstration exercise, and the following improved summary method was proposed. As noted above, all votes were ultimately translated into integrated scores that could be summed and represented by either an “S,” “s,” “R,” or “r” symbol on the final Table A2a-1, with capitalized symbols indicating two or more total votes for the particular table entry.

Tier Ranking Level:	Tier I	Tier II	Tier III
Process Understanding	Low	Medium	High
Space, Time And Structure	Steady State, Equilibrium Single Box.	Space, <u>or</u> Time Resolution, Multiple Boxes.	Space and Time Resolution Continuous Coord.
Mathematical Level	Algebra, Deterministic (no	Ordinary Diff. Eqns. Some Statistics	Partial Diff. Eqns., Multiple Statistics

	statistics)	(e.g., 1-D)	(e.g., 2-D)
H istory of Use/Acceptance	New and Untested	Emerging, Incomplete, Promising	Time tested, Much used, Extensive validation

Key: Enter alphabetic codes that correspond to the attribute that exists for the model at the corresponding tier level. Some models can span more than one tier, depending on the layers and corresponding level of sophistication. See below for further notes on definition of the streamlined attributes for model characterization:

P = The level of Process understanding attribute ranks the degree/state of scientific development of the combined physical, chemical and / or biological mechanisms within or across the natural media systems.

ST = The Space (x, y & z), time (t) and structure attribute ranks the degree to which the state variable(s) need to be described in the respective media in order to capture the most realistic behavior patterns of the processes.

M = The Mathematical level attribute reflects the types of coupled deterministic and stochastic algorithms that are needed to capture the process space, time and structure elements in order to realistically quantify the state variable(s).

H = The History attribute reflects an integrated, weight-of-evidence ranking that combines the time-period of use, data/validation issues and consensus/acceptance of the final algorithm.

Results and Conclusions

Review of Table A2a-1 indicates the diversity of opinion among the participating panelists. Due to the small number of individuals casting opinions for any individual model, this may not be too surprising. The panel members were selected by the EPA SAB to represent a diverse set of experienced scientists who have experience with either model development or model application. Most often panelists have modeling experience primarily in subject areas most closely associated with a particular environmental science, or with the biological aspects of risk assessment, without equal experience in other specialty topic areas, thus the sum of the team responses often includes between two and five individuals with special expertise in any given model or submodel topic area. This limitation of sample size must be remembered when reviewing the overall results.

The results in Table A2a-1 indicate a few general trends, in spite of the small sample sizes. Although there are a few elements in which the panelists agreed that the science was already effectively at an “advanced” Tier 3 level, the majority of the transport models varied between Tier 2 and Tier 1. Generally, the opinions on “regulatory applicability” and “best science” did not differ very much. One minor trend was noted: the “center of mass” of the R, r scores tended to lie slightly to the “right”; that is, toward the more advanced analysis cases, than the S, s scores. More noticeable, however, was the fact that “best science” scores were higher (more advance) for the models that were devoted to characterizing basic chemistry, air modeling, and basic hydrological processes compared with more complex exposure modeling and risk assessment details. That trend seemed consistent with many of the panel discussions in meetings. The results, perhaps supplemented by further EPA analysis of submodel precision and accuracy, may help the EPA decide on which improvements in the science may offer the greatest enhancement in ultimate accuracy and precision of the final risk estimates. In turn, these continuing improvements will positively affect the value of the other statistical decision-support parameters calculated by 3MRA.

**TABLE A2a-1
Tier-Ranking Matrix for 3MRA Submodel Assessment**

3MRA Constituent Models:	Tier I Simple Screening *	Tier II Refined Screening *	Tier III Advanced Risk Analysis *
* S = best science; R = good for regulatory applications			
Capitalization of symbol “S” or “R” indicates that 2 or more panel members voted for the particular classification of the sub-model. (Lower case = < 2 votes, some members split votes).			
<u>Chemical Properties Data:</u>			
SPARC		s	S, r
MINTEQ_2		s	S, r
<u>Sources:</u>			
<i>Wastewater Modules: (SI and AT)</i>			
CHEMDAT8		s	s , r
EPACMTP	s	r	S
<i>Land-based Source Modules: (LF, WP, and LAU)</i>			
GSCM		s, r	S
Local Watershed Model	s	S, r	s
Particulate Emissions Model	S	r	R
Hydrology Model	s	s, r	s
Regional Baseflow (STORET-30Q2)		r	S
<u>Media Fate & Transport:</u>			

3MRA Constituent Models:	Tier I Simple Screening *	Tier II Refined Screening *	Tier III Advanced Risk Analysis *
* S = best science; R = good for regulatory applications			
Capitalization of symbol “S” or “R” indicates that 2 or more panel members voted for the particular classification of the sub-model. (Lower case = < 2 votes, some members split votes).			
<i>Air Module:</i>			
ISCST3 Enhanced by: area sources, SCIM input, dry/wet deposition, terrain & new plume depletion.	s	S	R
<i>Watershed Module:</i>			
GSCM		s, r	S
30Q2	s	s	
MUSLE	s	s, r	S
<i>Surface Water Module:</i>			
Waterbody Network	s	S	S
EXAMS II	s	S	S, R
<i>Vadose Zone & Aquifer Modules:</i>			
EPACMPT		S	
1-D Vadose Zone Model		s, r	
~3-D Aquifer Model	s	s	R
Food Webs			
<i>Farm Food Chain Module:</i>			
Air-to-Plant	s, r	s, r	
Plants in Soil	S, r		
Beef and Milk	s, r	s, r	
<i>Terrestrial Food Web Module:</i>			
Soil Concentrations	s	s, R	
Plant Concentrations	S, R		
Soil Invertebrates	S, R		
Vertebrate Prey	S, R		
<i>Aquatic Food Web Module:</i>			
Food Webs for Waterbodies	s	r	
Dietary Matrix	s	s, R	
Concentrations in Food Web	s	s, r	
Consumed Fish (Concentrations)	s	S, R	
Exposures (Doses)			
<i>Human Exposure Module:</i>			
Ingestion of soil	S, r	S	R
Ingestion of groundwater	S	r	R
Inhalation of shower air	r	S, r	
Inhalation of volatile emissions	s, r	S, r	
Inhalation of particulate	s, r	S, r	
Ingestion of produce	s	S, R	

3MRA Constituent Models:	Tier I Simple Screening *	Tier II Refined Screening *	Tier III Advanced Risk Analysis *
* S = best science; R = good for regulatory applications			
Capitalization of symbol “S” or “R” indicates that 2 or more panel members voted for the particular classification of the sub-model. (Lower case = < 2 votes, some members split votes).			
Ingestion of beef & milk	s	S, R	
Ingestion of fish	s	S, R	
Breast Milk Exposure to PCDD/F		S, R	
<i>Ecological Exposure Module:</i>			
Direct Exposure: surface water	s, r		
Direct Exposure: sediment	s, r		
Direct Exposure: soils	s, r		
Indirect Exposure: surface water	s, r		
Indirect Exposure: sediment	s, r		
Indirect Exposure: food	s, r		
<u>Risks/Hazard Indices</u>			
<i>Human Risk Module:</i>			
Risks	s	s, r	r
Weighted Population Risk	s, R	s	
Hazard Index	s	s, r	r
<i>Ecological Risk Module:</i>			
Benchmarks	S	r	
Stressor Limits	S, r		
Hazard Quotients	s	s, r	
<u>3MRA</u>			
VERSION 1.0	r	s, r	s
VERSION 1.X		s, R	S
VERSION 2.0		R	S, r

Appendix 2a-2 Comments on Embedded Assumptions and Default Values

The level of peer review that the individual science modules received while the model was under development was impressive and the table of comments that the review produced represent a significant resource and guide for continued development and enhancement of the model. It is unfortunate that time and resources did not allow more of the comments to be explored in more detail and implemented where appropriate. The panel recognizes the need for making tradeoffs or simplifications during the model development process but we caution that some of these simplifications may lead to unexpected inconsistencies in model performance.

For example, there are currently two alternate methods used in 3MRA to estimate the concentration of constituents in aboveground vegetation, Cp. A deposition-based approach is used for chemicals with log Kow less than 5 and a partitioning-based

approach is used for the more lipophilic compounds. The partitioning-based approach uses an empirical air-to-plant bio-transfer factor (ChemBv) to relate the concentration of the constituent in air to that in aboveground vegetation. As discussed in Volume 2 Section 10.0, there are currently three chemicals classified as “special chemicals” and of these only Benzo(a)pyrene is assigned an empirical ChemBv value (4.7E+4). The other two special chemicals, Bis (2-ethylhexyl) phthalate and Dibenz (a, h) anthracene, are assigned ChemBv values of 1 because, as the documentation points out, “There are few experimental determinations of ChemBv.”

The panel is concerned that arbitrarily assigning a value of 1 for the ChemBv of lipophilic compounds can lead to inconsistencies in the modeling results both across chemicals that have similar physicochemical properties and even from run-to-run for the same chemical if uncertainty in Kow is considered. To illustrate this point, consider that Bis (2-ethylhexyl) phthalate has a log Kow reported in the 3MRA documentation of around 4 but other sources put the values above 5. Thus, it is conceivable that a user might select a log Kow that is on either side of the threshold that is used to change calculation methods. It is also feasible that a distribution might be assigned to this input that crosses the threshold.

If a log Kow value of around 4 is used then the model would default to the deposition method (Eq. 10-2). Using forage as the vegetation type and assuming wet deposition is negligible for lipophilic chemicals as stated in the first paragraph on page 10-7 then the resulting Cp is about $4 \cdot C_{va}$. (Note that Cva is the vapor concentration in ug/m³ and Cp is in mg/kg[DW]). If the model user selects a log Kow value of 5 and the ChemBv of 1 is used then the model would default to the bio-transfer factor approach (Eq. 10-3) resulting in a Cp of approximately $8.4E-4 \cdot C_{vap}$. Further, if the ChemBv was assigned a value similar to that of BaP (4.7E+4) then the resulting Cp comes back up to approximately $40 \cdot C_{vap}$. Thus, there is potential for almost 5 orders of magnitude variation in Cp cause by a relatively small change in Kow. It is not clear how this might influence the overall model outcome because the chemicals in question may not be present in the vapor phase of the air but this would need to be confirmed using sensitivity analysis.

Another imbedded assumption that may lead to discontinuities in the results can be found in the calculation of bio-concentration factors for milk and beef (ChemBa). The values are calculated using an empirical function on Kow but the calculation defaults to a value of 1 outside the range of the original data (see Figure A2a-2-1). The panel appreciates the concern for not wanting to extrapolate beyond the range of an empirical relationship but simply defaulting to a value of 1 may not be appropriate. For chemicals with log Kow between 1 and 3 or between 6 and 7, a small change in Kow can result in a significant change in the resulting ChemBa value.

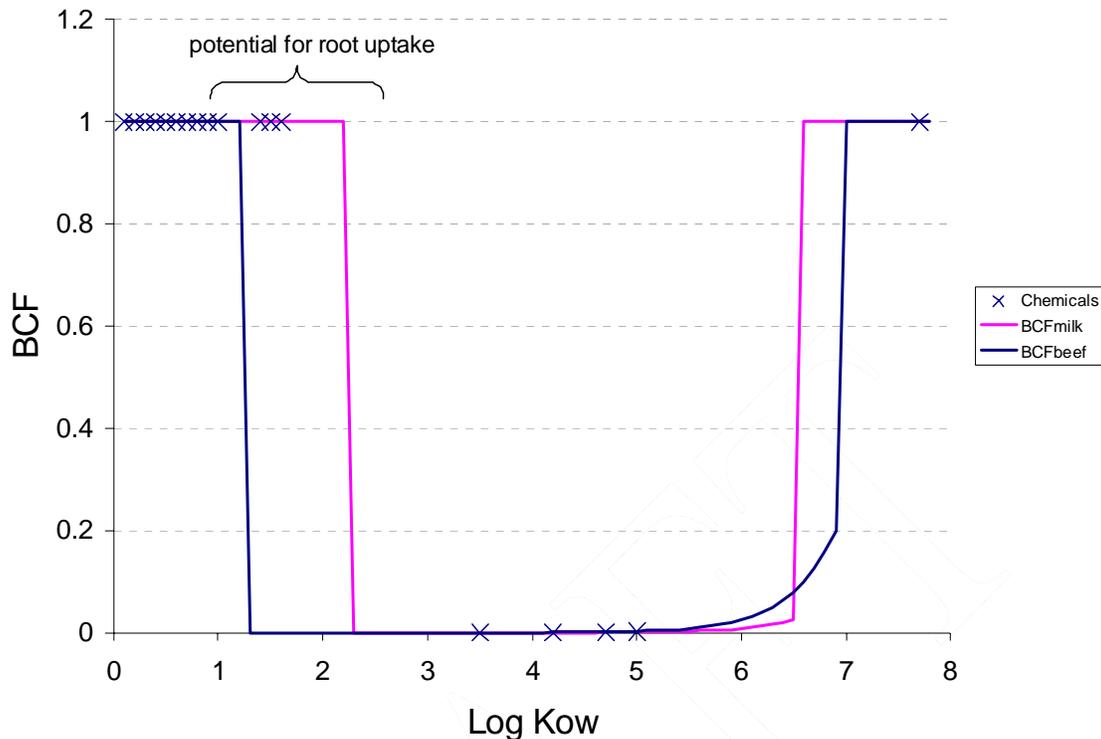


Figure A2a-2-1

Illustration of 3MRA prediction of bio-concentration factors for beef and milk as a function of log Kow. The imbedded assumption in the farm food chain module assigns a value of 1 to BCF for chemicals with logKow outside the range of the empirical relationship. Chemicals in the current data set are plotted on the chart showing that the majority of these chemicals are assigned the default of 1. This figure also shows that lipophilic chemicals, those that are most likely to interact with lipid phases in the model (soils, biota, and sediment), are under represented in the current data set.

Appendix 2b Benchmarks of Human and Ecological Effects

The 3MRA system uses a Hazard Quotient (HQ) approach to risk assessment, comparing predicted environmental concentrations with risk levels drawn from a variety of EPA programs. For example, the system uses ambient Water Quality Criteria as protection benchmarks for effects in aquatic systems. These criteria are intended to protect 95% of the species in a selected database, 95% of the time, from adverse effects of chronic exposure to a single toxicant. Exceeding a criterion does not necessarily portend an adverse effect (Spehar and Carlson 1984, Brungs *et al* 1992), nor does staying below a criterion ensure that aquatic ecosystems and their components will be protected (Suter *et al* 1987). There is an inherent uncertainty associated with any benchmark of environmental effect such as AWQC that will lead to that benchmark being potentially over- or under-protective. This uncertainty should be addressed through the sensitivity analysis planned for 3MRA.

Development of an HQ for aquatic life based on ambient Water Quality Criteria incorporates one level of protection (95% of the species in the database 95% of the time), which is then layered upon (or within) another level of protection for site selection (e.g., 3MRA can select exit levels based on a percentage of sites protected). As a result, application of exit levels at the 90% level of site protection combined with ambient WQC that protect 95% of species, and which may result in adverse effects at a much higher level, may not ultimately be protective of populations of aquatic organisms or aquatic systems.

The approach to ecological risk assessment and to the development and use of HQs is compromised further as ecological risks are calculated without assessment of the risks and impacts associated with concurrent exposure to multiple contaminants, and without assessment of the influence of multiple chemical and non-chemical stressors. There is abundant evidence that the toxicity of chemicals with similar modes of action act in an additive fashion, and that failure to incorporate additivity in an ecological risk assessment will result in under-protection of organisms, where they are exposed concurrently to more than one toxic chemical. It has also been recognized (Foran and Ferenc 1999, Ferenc and Foran 2000) that a variety of chemical and physical stressors act and interact to influence organisms, species, populations, and communities in both aquatic and terrestrial systems. Without consideration of these multiple stressors and their incorporation in ecological risk assessment, single, chemical-specific risk assessments may not be adequately protective.

Effects on Human Health

The 3MRA system uses a risk-based approach to assess exit levels for their potential to pose adverse or unacceptable risks to human health. It relies on U.S. EPA threshold numbers (RfD) for non-cancer effects, and on risk levels derived from EPA's slope factors for cancer. While the use of the RfD and cancer risk levels draw on standard methods for their derivation and use, the human health risk component of the 3MRA system has three important deficiencies.

The 3MRA documentation clearly acknowledges that dermal exposure is not considered in the model. Yet, efforts at EPA and elsewhere have been conducted since 1995 to assess and predict dermal exposure and its effects (its contribution to aggregate or cumulative exposure and risk). Olin (1999), in work sponsored by the U.S. EPA, concluded that "it is fairly easy to develop estimates of body burden from a dermal exposure." The 3MRA system should be updated to address this major deficiency by including dermal exposure in the human exposure component of the model.

The 3MRA system does not consider concurrent human exposure to multiple contaminants, and the risks that result from these exposures. The U.S. EPA has incorporated the concept of concurrent human exposure to multiple contaminants in a number of its risk-based documents and decisions, recognizing the potential to underestimate risk without incorporation of this concept. The 3MRA system should be revised to address this major deficiency, at least by incorporating the concept of additive

risk in the model, and ultimately by incorporating a more thorough assessment of cumulative risks from multiple chemical exposures in the model.

Finally, the 3MRA system appears to discount cancer risk where exposure occurs only for a portion of the lifetime. However, less than full lifetime exposure should not be discounted for some chemicals such as vinyl chloride, particularly where exposure occurs in childhood. Ginsberg (2003) has developed a list of chemicals for which this approach is appropriate and a thorough discussion of why this approach is appropriate. The 3MRA system must incorporate flexibility that allows the calculation and use of non-discounted cancer risks for vinyl chloride and other chemicals as appropriate.

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Appendix 2c-1

Discussion of 3MRA Monte Carlo Analysis

The 3MRA system relies upon a Monte Carlo simulation framework as a critical component of developing chemical-specific national exit levels. As defined in Volume 4 of the 3MRA documentation, the general national risk assessment problem statement is designed to establish exit levels such that a given exit level ($C_{w,EXIT}$) will:

1. Protect A% of the human population (within specified distance and at defined risk/hazard thresholds).

2. Protect D% of the ecological habitats (within specified distance and defined hazard quotient).
3. Provide these levels of protection at G% of the facilities nationwide.
4. Provide H% confidence that the exit levels accomplish the stated goals (while also minimizing any simulation uncertainty (I%) that arises as an artifact of the number of Monte Carlo iterations performed).

In order to develop exit levels meeting these criteria, the 3MRA implements a series of multimedia deterministic source and transport/fate modules and human/ecological exposure models, combined with a Monte Carlo sampling/simulation strategy that draws samples from distributions of input parameters used by the fate and risk modules. The input parameters modeled as random variables include those that describe the physical and operational characteristics of the WMU, local hydrogeology and habitat, human and ecological population characteristics affecting chemical intake and exposure, *etc.* The panel believes that the MCA as structured is capable of addressing the first three of the above-posed objectives (with reservations that many sources of variability/uncertainty are not characterized and setting aside issues relating to model validation), but the MCA is more limited in its ability to provide quantitative statements regarding the degree of confidence in the results (*i.e.*, the fourth objective above).

Given the complexity of the MCA, it is helpful for this discussion to render a simplified diagram of its basic components.³ Figure 2c-1-1 provides a depiction of the MCA in 3MRA using for illustration a single chemical for a single initial chemical concentration in the waste (C_w).⁴ Fundamentally, the MCA contains two sampling “loops” from which model parameters are drawn:

1. **Site-Based Parameters:** The site-based parameters are defined by a sample of 201 Subtitle D waste disposal facilities included in the 1985 Westat survey. In the case of the Landfill WMUs used in this illustration, the sample size is N=56 landfills. Input parameters describing site-specific WMU characteristics (*e.g.*, size of WMU, loading rates, *etc.*) are drawn from this site based database. Additional site-based information includes the population within 2-km, local watershed and habitat information, *etc.* At any particular site, these parameters are considered fixed or “constant,” whereas the “variability” across WMUs arises from the empirical differences in site conditions from one site to the next throughout the U.S.⁵

³ The Panel’s interpretation of the basic structure of the MCA was developed from reading Volume 4 and from discussions during several “fact-finding” calls with the Agency. The basic structure as depicted here was confirmed to be a correct interpretation of the MCA as implemented during the public meeting with the Agency that took place October 28 - 30. This figure is a modification/simplification of Figure 2-10 in Volume 4.

⁴ The full MCA in 3MRA simulates a range of five C_w values, spanning many orders of magnitude. From the MCA results for the five initial C_w values, an interpolation of the results allows the determination of the single exit level ($C_{w,EXIT}$) that meets the stated protection goals.

⁵ Examples of the site-based input parameters for the Landfill WMU are given in Volume 4, Table 8-9b and Table 8-9f where the site based “certain” parameters are those indicated as site based in the column “Site” and the corresponding distribution type is “constant,” indicating constant at a particular site but variable from site to site.

In this sense, the 56 Landfill WMUs in the 3MRA database represent a specific sub-sample from the “universe” of possible Landfill WMUs. Once sampled, certain parameters for a particular site are no longer random, but instead represent those particular combinations of site-specific parameters for the particular site in the database.

2. National/Regional Parameters: These include variables describing human exposure factors, ecological exposure factors, regional hydrogeology factors, *etc.* and are based on information that is not site-specific, but rather gathered from a variety of regional and national sources.⁶ Although discussions between the panel and the Agency indicate there is agreement that these distributions inherently represent a combination of variability and uncertainty in characterizing the underlying model parameter, in 3MRA these input distributions are assumed implicitly to reflect primarily parameter variability. The panel generally views the PDFs that contribute to the distribution of sites protected (*e.g.*, G%) to be a blend of uncertainty and variability. No analysis has been presented in the 3MRA to quantify the degree of uncertainty in these parameters.

The MCA process then requires running a sufficiently large number of simulations to generate a model result that is unaffected by the specific number of iterations performed (1,000 simulations for illustration here). It is important to recognize that the WMU database consists of 201 Subtitle D facilities surveyed by the EPA in 1985. For any specific WMU type, the number of WMUs for which site-specific data are available varies: Land Application Units (28), Landfills (56), Waste Piles (61), and Surface Impoundments (137). The Landfill WMU (with 56 sites modeled) is used for discussion purposes here.

⁶ Examples of these parameters are given in Vol. 4, Table 8-9q, and using particular examples for human exposure include factors such as soil ingestion rate, food intake rates, drinking water intake, *etc.*

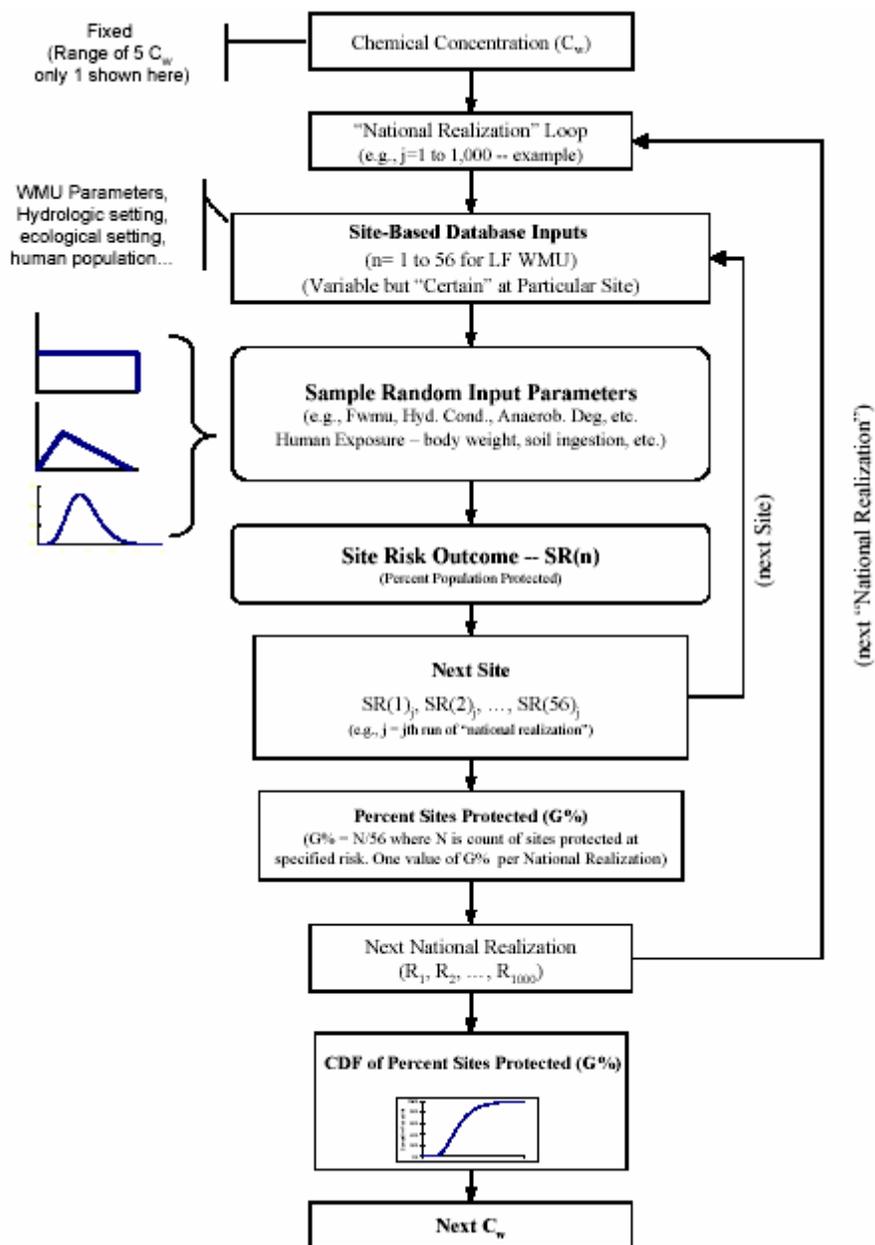


Figure A2c-1-1
3MRA Monte Carlo Schematic – Landfill WMU Example, Single C_w

According to the problem definition as posed by EPA, the “experimental unit” for developing exit levels consists of the set of WMU sites around the country (e.g., 56 for Landfills). Thus, a single outcome of the “national experiment,” or a single “national realization” in the parlance of 3MRA, is given by running a single MCA iteration across all sites (e.g., 56 Landfills) for a given value of C_w . This single iteration selects random samples from the national/regional distributions of input parameters and applies these

random samples to the site-specific input parameters for each of WMUs. Each such single iteration for the Landfill WMU example gives the following model outcomes:

56 site-specific (independent) values of the percent population above/below specified cancer risk and non-cancer hazard quotient benchmarks within 2-km of each site.

56 site-specific (independent) values the percent of the habitats which fall below/exceed ecological hazard quotients within 2-km of each site.

A single estimate of the percent of the sites (*e.g.*, percent of the 56 sites for Landfill WMUs) that are protected, or in other words a single value of “G%.”

Depending on how the results are tallied from these 56 simulation outcomes, it is possible to construct a cumulative distribution function (CDF) of the population risk, or percent sites protected. In 3MRA, the individual or the population risk results themselves are not stored to create a CDF of risk or non-cancer hazard indices. Instead, the risk results are first tallied in a series of “bins” associated with specified “risk ranges.” From these risk bins, the percent of the population at a particular site falling within the specified risk range bins is then tallied (the risk bins are described in Volume I, Section 14.2.2). For example, for a particular simulation if 94% of the population at a particular site falls within the risk range of 2.5×10^{-6} to 7.5×10^{-6} , then this result would be tallied in the “population protection bin” corresponding to the range “>90% to ≤95%”.

In order to determine the percent sites that achieve a specified level of population protection, it is a simple matter of tallying the results for particular population protection “bin” of interest (*e.g.*, >90% to ≤95%). In this fashion, the Landfill WMU simulation outcomes for a single national realization yield 56 “pass/fail” values for a particular level of protection simply by tallying the number of sites that fall within the specified protection bin of interest. Thus, G% is given by $N/56$ where “N” is the number of sites that fall within the population protection bin of interest. In this manner, 3MRA calculates a single estimate of the “percent sites protected,” or “G%,” corresponding to a specified population protection threshold for each “national realization.”

Clearly, for each “national realization” the single value of G% that is calculated has little significance by itself. It represents the modeled outcome for 56 sites that is but one particular combination (of essentially infinite combinations) of the set of hundreds of model input parameters treated as random variables. Thus, in order to generate a meaningful result, one that develops a distribution of the number of sites protected (a distribution of G%), the MCA must be performed a large number of iterations. The actual number of iterations should be sufficiently large such that model simulation errors are minimized. The “outer” loop in Figure 2c-1-1 shows this repeated iteration process, using for illustration 1,000 iterations.

When this MCA is completed for a single chemical concentration (C_w) and WMU type, the result is a CDF of G%. An illustrative example of the CDF for G% for a single

of C_w is provided in Figure 2c-1-2 (in this illustrative example it is noted that the presumptive percent population protected, or P%, is 99% at each site). Note that the x-axis for this example CDF is plotted in reverse order. This is because the probability of site protection decreases as the percentage of sites protected increases.⁷ In this example approximately 38% of the sites were “protected” in 90% of the modeled outcomes, whereas approximately 58% of the sites are protected in 50% of the modeled outcomes (e.g., the median outcome is that 58% of the sites are protected. Note that this example CDF of G% is hypothetical and was not generated using actual 3MRA model runs.

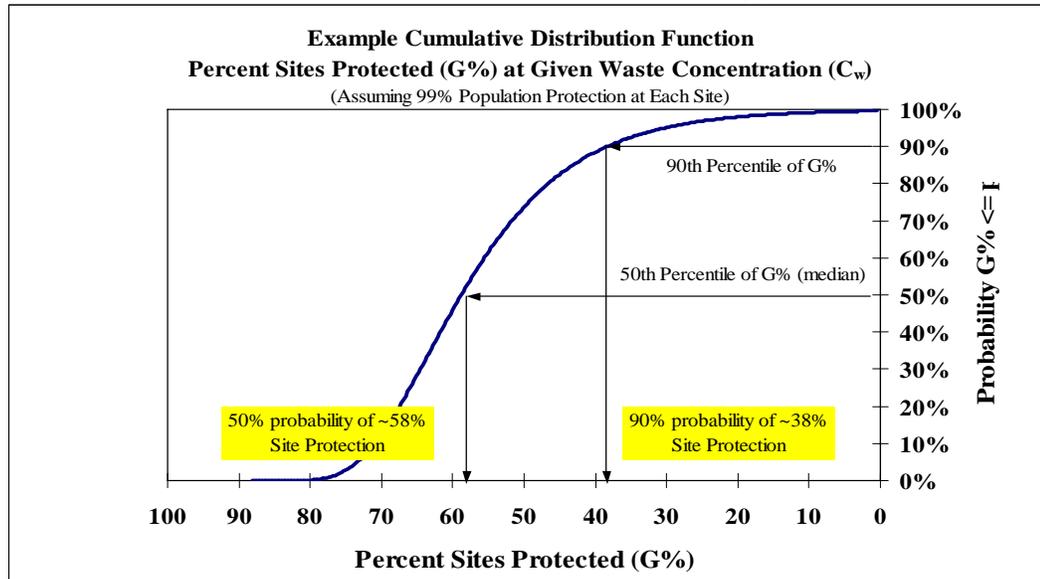


Figure A2c-1-2.
 Illustrative Example of 3MRA CDF of G%.

Evaluation of 3MRA MCA Results Provided to Panel

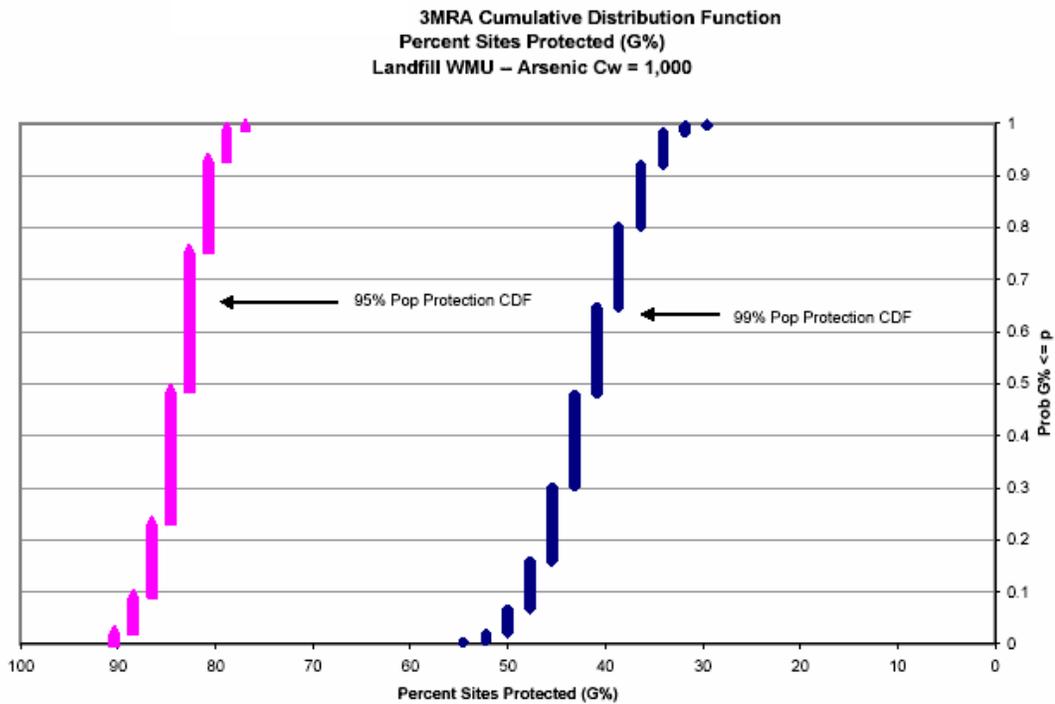
The panel was provided with actual MCA simulation results for several compounds (information provided 11/27/2003). In addition, a subset of the panel participated in an informational call with the Agency to review these materials on December 4, 2003. This discussion provides the panel’s observations and comments regarding the example results provided.

Results of percent sites protected (G%) were provided for two scenarios (for brevity, the discussion here addresses only human health protection, recognizing that ecological habitat protection measures were included in the results provided):

- 95% human population protection
- 99% human population protection

⁷ Alternatively, the CDF could be plotted as a “complementary CDF” as discussed in the 3MRA documentation.

As an example, Figure A2c-1-3 provides a plot of the MCA results of G% for a Landfill WMU for arsenic, for a particular waste concentration ($C_w = 1,000$ mg/kg). The figure plots the results for both 95% and 99% population protection. As these results show, for a given waste concentration, fewer sites meet the population protection criteria as the criteria increases from 95% to 99% protection (note the x-axis is plotted in reverse order). Several things are worth noting from these CDFs. The percent sites protected do not increase in a continuous fashion, but instead increase in discrete “bins.” This is a direct result of the fact that the WMU database constitutes only a discrete number of sites. In the Landfill WMU example there are 56 sites in the EPA database. Thus, if 1/56 of the sites meet the population protection criterion, then G% is 1.79%, if 2/56 sites meet the population protection criterion then G is 3.57%, if 55/56 sites meet the criterion then G% is 98.21%, and so forth.



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FIGURE A2c-1-3
3MRA Cumulative Distribution Function
Percent Sites Protected (G%)

In Figure A2c-1-4, the 3MRA MCA results for nickel are plotted for a Landfill WMU for the 99% population protection scenario. Three values of C_w are shown, $C_w=10,000$ mg/kg, $C_w=1,000$ mg/kg, and $C_w=100$ mg/kg. One immediate observation from these results is that for $C_w=100$, for all values of H% up to approximately H% ~

90%, 100% of the sites achieve 99% population protection. At the other end of the scale, for $C_w=10,000$, none of the sites achieve 99% population protection. In order to calculate exit levels from the discrete ranges of C_w values modeled, the Agency interpolates between the results for particular values of C_w . Illustrative “exit levels” are shown on the figure corresponding to $H=95\%$ ($C_{\text{exit}} = 174$), $H=80\%$ ($C_{\text{exit}} = 355$), and $H=50\%$ site protection ($C_{\text{exit}} = 541$). These “exit levels” correspond to different percentiles of the $G\%$ distribution, namely the 95th, 80th, and 50th percentile of $G\%$.⁸ The exit levels are determined by interpolating between the CDF results for $C_w=1,000$ and $C_w=100$.

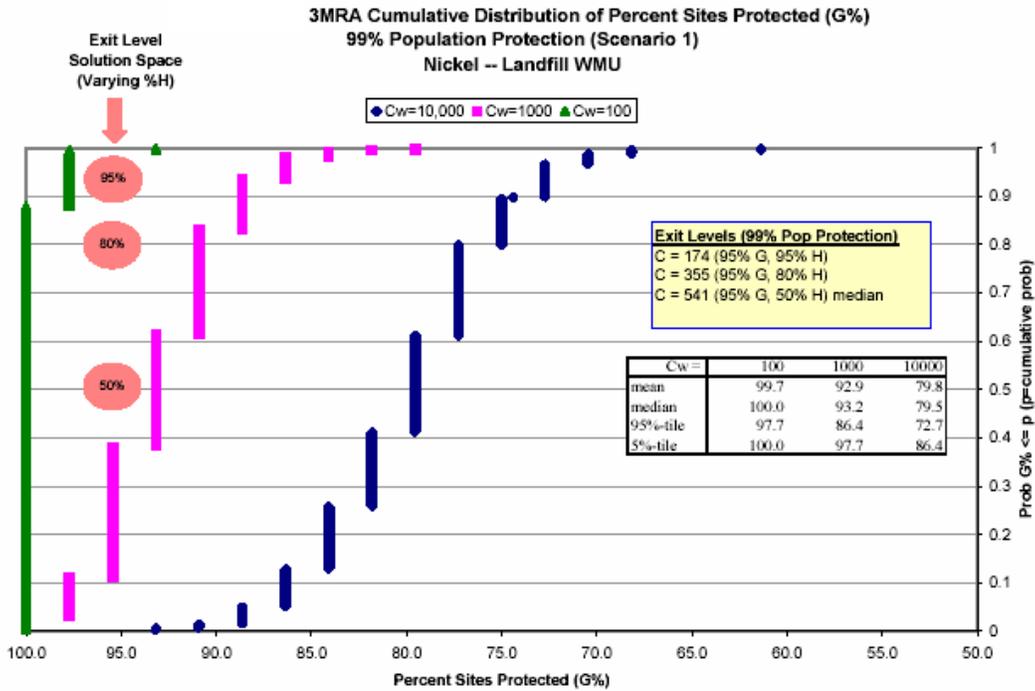


FIGURE A2c-1-4

One issue that revealed itself after being provided actual 3MRA simulation results is that the accuracy in the interpolation of the exit levels appears to be somewhat imprecise. As this example illustrates there is no difference in percent sites protected at the 50th and 80th percentiles of the $G\%$ distribution for $C_w=100$; all values up to approximately 88th percentile yield 100% site protection. Thus the lower limit for the interpolation for both the 50th and 80th percentile $G\%$ value is the same. Yet, logically, this cannot be so. If additional concentration values were modeled, it would be the case that a higher concentration is “acceptable” if the 50th percentile is the basis of site protection criterion, *versus* the case if the 80th percentile site protection is required. It

⁸ Note that one would actually select the 5th and 20th percentile of the $G\%$ distribution if the results were ordered from low to high (they are ordered from high to low on the figure).

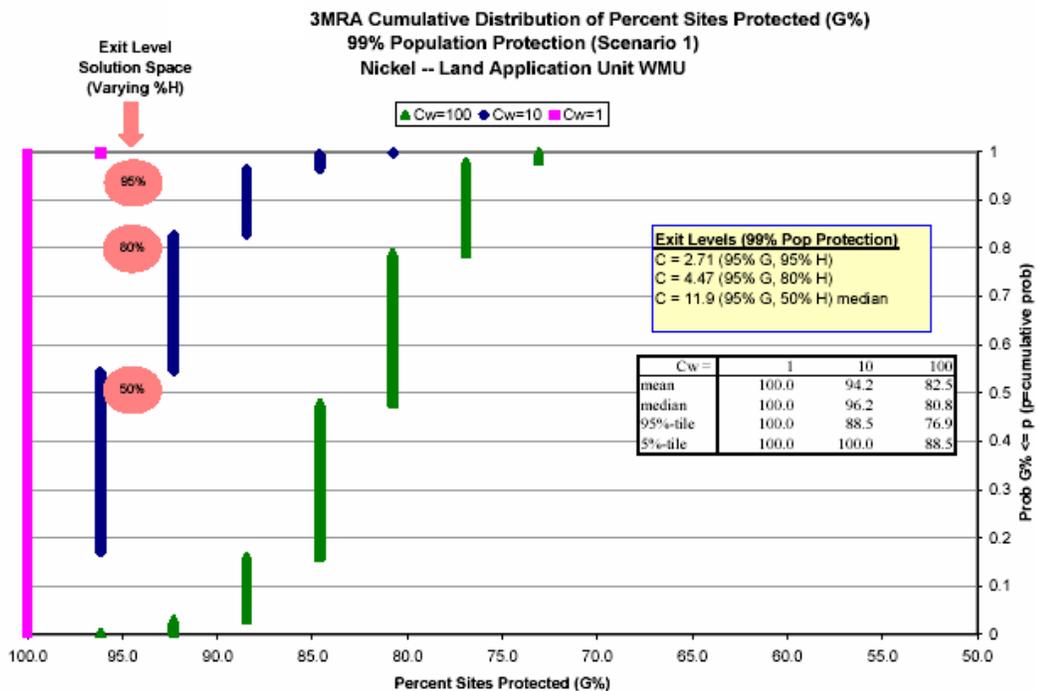
appears that the method adopted in 3MRA will tend to force the interpolation of the exit level to a lower concentration threshold than would be the case if a larger number of C_w values (*e.g.*, reduce the concentration range between C_w values) were modeled.

The panel's initial evaluation of the results also raises further questions regarding the interpretation of the 3MRA results that has been suggested in the 3MRA documentation and that has been presented to the panel during meetings and telephone conference calls with the Agency. The panel understands that the Agency will select an upper percentile from the G% distribution as the basis of setting exit levels (this upper percentile corresponds to H% in the 3MRA terminology). The panel agrees that selecting an "upper percentile" in this fashion is consistent with stated Agency risk assessment practice and policy relating to public health protection (*e.g.*, analogous to protecting the "reasonably maximally exposed" individual, or in this case population). However, the panel does not necessarily agree with the interpretation of the CDF of G% as representing exclusively the "uncertainty" of site protection resulting from the finite number of sites in the WMU database.

The G% distribution is derived as the iterative result of sampling from input parameter distributions that are "single dimensional." In the panel's view, these input distributions represent a hybrid distribution of natural variability and an unquantified component of uncertainty. Thus, for each simulation for a given WMU (*e.g.*, each iteration through a single site in Figure 2c-1-1), the value of population protection (P%) that is calculated reflects variability and uncertainty associated with the input parameters. As the simulation proceeds to the next site, this variability/uncertainty associated with input parameters gets applied at each site independently. The results in the P% at separate sites reflect different random combinations of site-specific/regional/national input parameters reflecting natural variability of population density, site characteristics, WMU characteristics, *etc.* from site to site. The differences in P% outcomes at each site inherently reflect the uncertainty imbedded within the "hybrid" distributions of variability/uncertainty that form the basis of the site-based/regional/national parameter base. Each estimate of percent sites protected (*e.g.*, each value of G%) thus reflects both parameter variability, parameter uncertainty, and differences based on different site conditions. The degree to which input parameter variability or uncertainty dominates the outcome cannot be determined (higher order ISE and/or SME dimensional uncertainty analysis will offer insights to this question). Regardless of whether the CDF of G% is interpreted as an expression solely of the uncertainty of sites protected, or a hybrid representing both variability and uncertainty, the Panel emphasizes its concurrence that selecting an upper percentile of the CDF of G% (*i.e.*, H% is this upper percentile) is appropriate. This approach is a reasonable means of meeting the Agency's stated goal of establishing national exit levels such that a specified percentage of the sites achieve the defined levels of population protection.

The panel recognizes that the number of sites in the WMU database influences the distribution of G%, but the influence appears to be simply the inevitable result of the particular number of sites modeled. That is, the fact that only 28 Land Application Units (LAUs) are modeled, constrains the G% "bins" to certain fixed percentages (*e.g.*, 3.57%,

7.14%, 10.71%, etc.) corresponding to 1/28, 2/28, 3/28, etc. sites protected. Likewise, for Landfill WMUs the G% bins are restricted to 1.79%, 3.57%, etc. simply because the number of landfills modeled is 56. A comparison of Figure 2c-1-4 (e.g., LF for nickel), with 2c-1-5 (LAU for nickel) illustrates the differences in the G% bins. Yet, these G% bins have no bearing on the statistical interpretation of the MCA results. Take for example the model simulations where 100% of the sites are protected. In such instances, the percentile of the G% distribution is 100% for the Landfill and LAU WMU regardless of the fact that N=28 for LAUs and N=56 for Landfills. Thus, the percentage of simulations (e.g., the probability axis on Figure 2c-1-4 and Figure 2c-1-5) that fall into a particular G% bin has no relationship to the number of WMU units simulated, but instead is a function of the random combination of particular input parameters/site parameters coupled with the particular waste concentration modeled.



MCA.xls Figure 2c-1-5 Ni LAU 3/5/2004

FIGURE A2c-1-5

Stated differently, there is one “true” (but unknown) distribution of G%, with only one “true mean” and “true variance.” It stands to reason then that as more sites are modeled, the ability to approximate this “true” distribution improves (ignoring other sources of error/uncertainty). Thus, when the 90th percentile of G% is selected from a distribution derived from a large number of modeled sites, there is greater confidence in this estimate of the 90th percentile than a situation where fewer sites are modeled. Yet, the number of sites modeled says nothing about the actual value of the 90th percentile itself. That is, modeling a larger number of sites does not translate into a reduction of the variance in G% (there is but one true value). Instead, including a larger number of sites

in the experiment reduces the uncertainty in estimating the true mean and true variance. The actual variance of G% is unrelated to the number of sites modeled (again there is only one fixed but unknown variance of G%).

Informational materials provided by the Agency to the panel on January 9, 2004 indicated that the Central Limit Theorem (CLT) offers an explanation for the underlying connection between the number of WMUs modeled, and the variance of G%. It is unclear to the panel how the CLT offers such an explanation. The CLT speaks to the distribution of means. The CLT states that for any arbitrary distribution type, the distribution of the means of these distributions tends to normality and that the variance of the mean reduces as a function of $1/N$ (e.g., σ^2/N , with N being the number of samples). Yet the distribution of G% in 3MRA is not a distribution of the means, it is the probability distribution of sites protected.

The panel notes that this statistical question (the connection between the number of WMUs modeled and the variance in G%), is not an issue that raises fundamental concerns about 3MRA. It is an issue of clarity and transparency in terms of describing the MCA methods in 3MRA. As noted in the panel's recommendations for the MCA (presented in the body of the panel report), the larger question is whether a sufficiently robust sample size of WMUs has been modeled to allow statements about the degree of protection offered by the exit levels when they are adopted on a national basis (e.g., extending to the thousands of waste management facilities across the country).

Monte Carlo Simulation Error/Precision (I%)

The panel would like to also comment on the issue of MCA precision, or output sampling error (OSE) is 3MRA terminology. The approach that is proposed in the 3MRA (e.g., Vol. IV, Section 2.5.3) is an appropriate and useful method for determining the number of MCA iterations need to bound OSE within acceptable limits. The approach outlined, and the results provided to the panel, provide reasonable assurance that the 3MRA results (e.g., selection of a particular percentile of the G% distribution to establish exit levels), will not be unduly affected by numerical simulation uncertainty. The panel does not see this as an issue that is a fundamental component of the decision framework for developing national exit levels. Instead, it represents good scientific practice and the algorithm for establishing the appropriate number of MCA samples to minimize OSE is reasonable. This algorithm could be easily used to establish the appropriate number of MCA samples under alternative MCA formulations, including the alternative approach to the MCA that the panel has offered.

Appendix 2c-2 Suggestions for Alternative MCA Data Synthesis

As described in the responses to Charge Question 2c, and illustrated previously in Figure 2c-1-1, the MCA in 3MRA consists of an iterative calculation process that contains two fundamental "looping" routines:

1. A site-based loop that holds site-specific parameters “constant” at a particular site, and
2. A national/regional loop that draws from probability distributions of model input parameters.

The “outer loop” in this MCA as proposed in 3MRA consists of sampling first from the national/regional/site-based input parameters, then applying these to each of the WMUs in succession (independent samples at each site). Thus, for the Landfill WMU example, the inner site-based loop results in 56 outcomes for each pass through the “outer loop.” The outcome that is stored in 3MRA is not the actual calculated risk, or percent population protected (weighted by population at each centroid) at the site, but rather a series of “pass/fail” results for each of a series of population protection bins (*e.g.*, 90-95%, 95%-98%, *etc.*) for a particular site and iteration. By storing the information in this fashion, the MCA in 3MRA is discarding valuable information, namely the value of the calculated population protection for each simulation. Currently there is no way to determine whether in meeting the goal, the majority of the sites achieve the percent population protection criteria by a wide margin, and a subset “just meet” the target. The actual degree of protection at any particular site is “concealed” by the current method of calculating (or summarizing) the percent sites protected.

To illustrate the panel’s suggestion of preserving the percent population protection on a site by site basis, we have presented an alternative MCA formulation that reverses the looping order in the 3MRA. That is the site-based loop is the “outer loop” and the national/regional loop is the inner loop. [The panel notes that the actual “order” of the loops is immaterial, and it is only a question of how the results are aggregated that is important. This suggested “re-ordering” of the looping structure is retained only for clarity and to distinguish it from the current method of aggregating the results.] If this approach is adopted, then a probability distribution of percent population protection can be constructed at each site. This process is straightforward and would require only a change in the way the results are processed, without modifying any fundamental model components. An illustration of how the site-based distribution of P% could be derived is shown in Figure 2c-2-1.

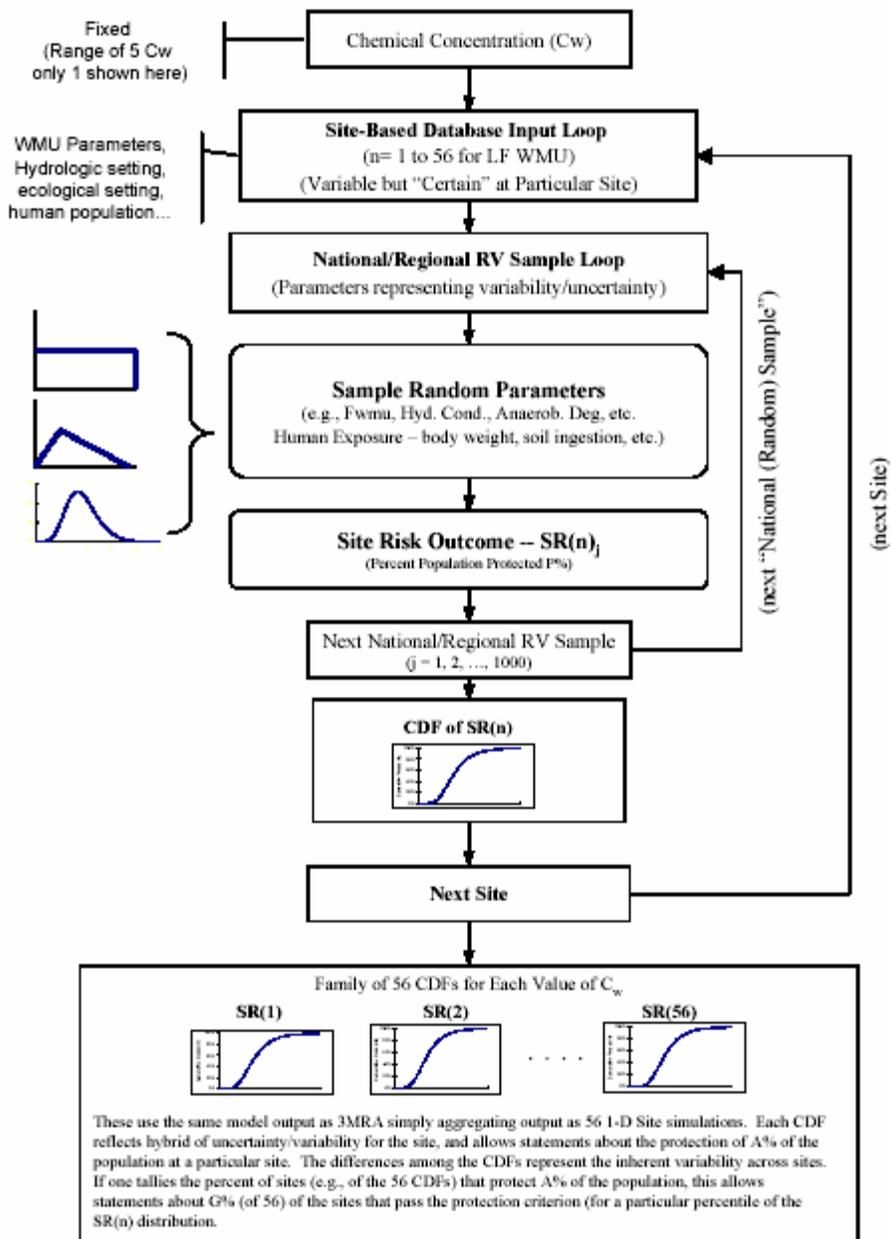


FIGURE A2c-2-1
3MRA Monte Carlo Schematic – Alternative Formulation by Site

It is the panel's view that a series of national iterations which retain and store the percent protected (P%) value from each site for each iteration and C_w could provide a more transparent and readily understandable approach. Thus, in the case of the LF WMUs, this approach would yield 56 independent probability distributions of P% for each C_w , or 5×56 total CDFs for the range of 5 concentration values modeled in 3MRA. These series of site-based PDFs would reveal at what concentration the degree of acceptable population protection (e.g., 95%, 99%, etc.) is achieved at a particular site.

Inspecting the results of all sites would then reveal the percent of sites (*e.g.*, G%) that achieve the defined level of P%. If the CDF of P% indicates 95% population protection (for a given C_w), that site “passes” the decision rule, otherwise it does not. The percentage of the sites meeting this goal is then calculated in a manner analogous to the approach in 3MRA (*e.g.*, $N/56$, where N is the number of sites meeting the protection criterion at a particular C_w and P% threshold).

The panel does not suggest that the moments or percentiles of the site-based P% distributions would be “added” or otherwise combined into a “derived” distribution of means. The panel believes this alternative approach does provide decision-makers the information to achieve G% site protection with a specified degree of confidence (*e.g.*, the confidence is derived from selecting the upper percentile of P% distribution). Also, the algorithms adopted to minimize OSE (*e.g.*, 1%), apply to this approach in the same manner in which they apply to the current 3MRA formulation.

If data storage requirement for such an approach would become unmanageable, it could be possible to store a subset of the percentiles of the P% distribution for each site, rather than the entire distribution.

Advantages of proposed approach:

The proposed method preserves data. This is useful to further characterize protectiveness. For example, a stakeholder may ask, “What is the P% for the 5th percentile (for example) of sites for which $P\% < 95\%$? Retaining the original P% values will allow that question to be answered.

P% incorporates both site-based spatial variability of exposure (*e.g.*, concentration term), and “standard” distributional approaches for input parameters as would be applied in a 1-D analysis.

The distribution of P% at individual sites is amenable to common distributional analyses, and does not imply a separation of uncertainty and variability.

This approach of considering each site as the basic “experimental unit” preserves the ability to evaluate inter-site variability and is more intuitive. Because the national analysis is nothing more than the “roll-up” of the site-based analyses, retaining the site as the basic unit for analysis does not hamper national decisions. The disadvantage of the current approach in 3MRA is that it does not allow an analysis of general site conditions that give rise to “high risk” scenarios, in essence completely removing any “site-based” inquiry from the results.

The approach recommended here is amenable to adding a 2nd order analysis, and is consistent with EPA’s stated intent of using the 3MRA modeling framework for both national and site-based analyses.

Appendix 2c-3 Probabilistic Analysis of Chemical Toxicity

Because of Agency policy decisions, the current version of 3MRA treats several parameters as fixed and certain when, in fact, they are variable and/or uncertain. Among these are the human toxicity criteria: cancer potency factors (CPF) and reference doses (RfD). Each of these parameters has several identified sources of variability and uncertainty, and each is related to the outcome in a linear 1:1 manner. Current values for these parameters are conservative estimates, intended to be reasonably certain of protecting most humans when combined with conservative exposure parameters in a deterministic risk assessment. However, using these deliberately biased estimates in a stochastic risk assessment violates a basic tenet of this practice, namely that distributions are unbiased.

The following discusses sources of variability and uncertainty (primarily uncertainty) and some suggested ways of incorporating the range of uncertainty into probability distribution functions (PDF)s for these parameters. Factors that contribute to variability inherent in how a heterogeneous human population responds to chemical exposure include pharmacokinetics, physiology, disease status, and age of exposure—some of which may be amenable to quantification. For instance, the Agency has begun to quantitatively address variability associated with age of exposure in its recent re-assessment of vinyl chloride (EPA, 2000). Numerous research groups are trying to develop ways to quantitatively account for the pharmacokinetic and physiological differences in which children handle toxicants (Ginsberg, 2003; Ginsberg *et al.*, 2004; Landrigan *et al.*, 2004.). However, for other factors such as disease status, nutritional status, age at exposure, and sensitive or susceptible populations where the variability is very large, it may prove much more difficult. A more complete discussion of this topic can be found in the references at the end of this section.

Cancer Potency Factors (CPF)

Most CPF are derived from rodent bioassays usually conducted for the majority of the animal's lifetime. A typical National Toxicology Program or similar protocol would involve rats and mice of both sexes exposed to two dosages and controls. The highest dosage is supposed to be a maximum tolerated dose, just below incipient overt toxicity, and the other dose usually one-half that amount. Several steps are involved in applying the results of these animal bioassays to estimate carcinogenic effects in humans, and each step involves uncertainty. In general, variability is reflected in the fact that some test animals in a given dose group develop cancer and some do not, and the same is presumably true of humans, although we seldom have good quantification of the human dose.

Selection of bioassay

If both species show positive results, a choice must be made which bioassay results to use in the calculation of CPF. Generally the species and gender that gives the highest CPF is used. If more than one satisfactory study is available for a given species

and gender, a median of the available results may be used. Study selection could be the basis for PDFs of rat and mouse potency by using the calculated potency from each satisfactory study to form a finite distribution.

Dose response modeling

If humans were typically exposed to dosages in the same range as the animal bioassays are conducted, there would be no need for extrapolation from high-dose observations to low dose predictions. That not being the case, curves are typically fit to the experimental data and extended through the origin. Although different types of curves make little difference in the observable range, they can make a very large difference at dosages a few orders of magnitude below the observable range, where the level of human exposures are often found. Although there are many approaches to curve-fitting, a common approach is the linearized multistage model, which generates curves described by a polynomial with various coefficients on the various exponents of dose. These coefficients are constrained only in that they cannot be negative. A family of curves is generated and they are ranked according to the magnitude of the coefficient on the linear term (Q). Typical Agency practice is to select the 95th percentile value of Q (Q*) as the CPF for the test species. A PDF for CPF could be generated by selecting all percentile estimates of Q and entering them into a finite distribution.

Dose scaling

Because of the large difference in body size between humans and laboratory rodents, dose scaling becomes an issue, *i.e.* what is the human equivalent of a 1 mg/kg/day rat or mouse dose? There are several factors that may affect this equivalency, the most important of which is kinetics of the compound. For example, if the test compound is the active carcinogen, and the compound is broken down to a non-carcinogenic metabolite in the liver, then the effective dose may scale according to liver function, which is generally related to body weight^{0.7}. In this case humans will be about 6 times as sensitive as rats on a mg/kg/day basis and about 12 times as sensitive as mice. On the other hand, if the test compound must be metabolized to the active form, rats and mice, with their higher metabolic rate, may be as sensitive as humans. In this case, effective dosage would be a function of body weight^{1.0}. Although compound-specific interspecies conversion factors would be ideal, development of these data would be a long-term project. In the interim, a uniform distribution for interspecies sensitivity ratio ranging from 1 to 12 for mice and 1 to 6 for rats could be used. For each iteration, the value selected from this PDF would be multiplied by the value selected from the PDF for rodent CPF and the result would be the human CPF. However this may substantially under-characterize the interspecies uncertainty in extrapolation, given the substantial qualitative species differences in pharmacokinetics and lack of site concordance that have been observed for some carcinogens.

Reference doses (RfD)

The majority of RfDs are derived from rodent bioassays usually conducted for the majority of the animals' lifetime, although many are based on subchronic studies or studies in dogs, humans or other primates. As with CPFs, several steps are involved in applying the results of these animal bioassays to estimate chronic toxicity in humans, and each step involves uncertainty. This uncertainty is compensated for using uncertainty factors (UF). If no-adverse-effect-levels (NOAEL) are based on adequate, long-term studies in sensitive humans, then UF would be unnecessary. For each step away from this ideal, the NOAEL is divided by a UF. Although uncertainty may be unidirectional or bidirectional, UF are unidirectional, *i.e.* they are only used to lower the RfD. Despite the fact that they are, by definition, uncertain, they are treated as certain in Agency risk assessments, including the current 3MRA analysis.

Inter-species extrapolation

Typically a UF of 10 is applied to compensate for uncertainty in extrapolation from laboratory animals to humans. This implies that humans are 10 times as sensitive to the effects of the chemical as the test species. However, humans may be more or less sensitive to the effects of the chemical than rodents are, depending on absorption, metabolism, excretion, whether the chemical has to be metabolized to the toxic form, the mechanism of toxic action, etc., *i.e.* the uncertainty is bidirectional. If the RfD is based on epidemiological data, this UF is not used. Although compound-specific interspecies conversion factors would be ideal, development of these data would be a long-term project. In the interim, published and unpublished data comparing similar endpoints in humans and laboratory species for various classes of chemicals could be used to develop a distribution for this parameter.

Intra-species extrapolation

Although the test animals exhibit variability (not all of the animals in a given dose group are adversely affected), it is thought that humans are likely to be genetically more heterogeneous than inbred laboratory animals. For that reason, a UF of 10 is typically included to ensure that the most sensitive human is protected. This implies that the most sensitive human is 10 times as sensitive to the effects of the chemical as the average human. The uncertainty is unidirectional, but the magnitude of the difference between average and sensitive humans may vary considerably. Epidemiological data may be helpful in estimating a range for this parameter.

LOAEL to NOAEL extrapolation

If an adverse effect was observed in every dose group tested in the definitive study, it is uncertain how much lower the dose would have to be to produce no adverse effect. The UF of 10 that is typically included to compensate for this uncertainty implies that the NOAEL is 1/10 of the LOAEL. This type of uncertainty is unidirectional. Other information such as the slope of the dose-response curve, data from other members of the

same class of chemicals, range-finding or shorter-term studies, or estimates based on the magnitude of the effect at the LOAEL could be used to establish a reasonable range for this UF.

Sub-chronic to chronic extrapolation

If only short-term (less than the majority of the lifetime of the animal) studies are available, it is uncertain how much lower the NOAEL would be in a full chronic study. A UF of 10 included to compensate for this uncertainty implies that the chronic NOAEL is 1/10 of the sub-chronic LOAEL. This type of uncertainty is unidirectional. Other information such as mechanistic information and a time-response curve for the class of chemicals could be used to establish a reasonable range for this UF.

UF for inadequate database

If the database for a particular chemical does not include the results of studies pertaining to a particular type of effect such as reproduction or immunotoxicology, an uncertainty factor may be incorporated to compensate for this uncertainty. This type of uncertainty is unidirectional. Information such as mechanistic information and a range of ratios between chronic NOAELs and NOAELs for the missing type of study for other members of the class of chemicals could be used to establish a reasonable range for this UF.

Publications Relating to Probabilistic Analysis of Chemical Toxicity

Baird, S.J.S., J.T. Cohen, J.D. Graham, A.I. Shlyakhter and J.S. Evans. 1996. Noncancer risk assessment: a probabilistic alternative to current practice. *Human and Ecological Risk Assessment* 2(1):79-102.

EPA, 2000. Integrated Risk Information System (IRIS) file for Vinyl Chloride (CASRN 75-01-4). Last updated 8/07/2000. <http://www.epa.gov/iris>.

Evans, J.S., G.M. Gray, R.L. Sielken Jr., A.E. Smith, C. Valdez-Flores, and J.D. Graham. 1994. Use of probabilistic expert judgment in uncertainty analysis of carcinogenic potency. *Regulatory Toxicology and Pharmacology* 20:15-36.

Evans, J.S., J.D. Graham, G.M. Gray, and R.L. Sielken, Jr. 1994. A distributional approach to characterizing low-dose cancer risk. *Risk Analysis* 14(1):25-34.

Evans, J.S., L.R. Rhomberg, P.L. Williams, A.M. Wilson, and S.J.S. Baird. 2001. Reproductive and developmental risks from ethylene oxide: A probabilistic characterization of possible regulatory thresholds. *Risk Analysis* 21(4):697-717.

Ginsberg, G. 2003. Assessing cancer risks from short-term exposures in children. *Risk Analysis*: 23(1): 19-34.

Ginsberg, G., W. Slikker, J. Bruckner, and B. Sonawane. Incorporating children's toxicokinetics into a risk framework. 2004. *Environmental Health Perspectives*: 112(2): 272-283.

Landrigan, P., Kimmel, C., Correa, A., and B. Eskenazi. 2004. Children's health and the environment: public health issues and challenges for risk assessment. *Environmental Health Perspectives*: 112(2): 257-265.

Swartout, J.C. P.S. Price, M.L. Dourson, H.L. Carlson-Lynch, and R.E. Keenan. 1998. A probabilistic framework for the reference dose (probabilistic RfD). *Risk Analysis* 18(3):271-282.

On March 17, 2004 the EPA Office of the Science Advisor published a staff paper, *An Examination of EPA Risk Assessment Principles & Practices* (EPA/100/B-04/001, March 2004). The 3MRA Panel's last meeting was March 18, 2004; therefore, the Panel did not consider this staff paper in its review. The staff paper, which will serve as a vehicle for opening up a broader dialog about the practice of risk assessment at EPA, does not represent official EPA policy. However it does address uncertainty and variability in risk assessment and may be of interest to the readers of this Appendix.

Appendix 3b

3MRA Panel Review of the Generic Soil Column Model With Recommendations for Improvement

Introduction

The 3MRA team developed the generic soil column model (GSCM) to describe the dynamics of constituent fate and transport within non-wastewater waste management units (WMUs) and surface soils in watershed areas. Because it was to be applied to all the WMUs and watersheds the term GSCM was used. It has undergone a previous EPA peer review process (Bartenfelder, 1999). Considering the fact that GSCM is not a legacy model, and the key role it plays in mobilizing chemicals and providing the mass inputs for all the "downstream" modules, the 3MRA panel considered elected to contribute a further review. Selected panelists conducted this review and participated in fact finding sessions with the EPA developers. In general this review examines aspects of GSCM not covered by the original EPA review, however a few key issues raised by the first panel are revisited. In addition the 3MRA panel review contains detailed recommendations for redeveloping the GSCM and its associated modules.

This review consists of three parts: a) GSCM theory and process description, b) status of module testing and validation and c) recommendations for GSCM and module redevelopment.

GSCM Theory and Process Development

The governing equations used for the GSCM are similar to those proposed by Jury *et al.* (1983, 1990) and Shan and Stevens (1995). These models were not truly

multi-phase, multi-transport soil column models; rather, they were developed primarily for pesticide evaporation from agricultural soils. Nevertheless the Jury *et al.* model has a history of EPA sponsorship and was used as the starting point for developing the GSCM. The 3MRA team fashioned an innovative solution technique that was computationally efficient and sufficiently flexible for the unique design and operational aspects of each WMU type. Details of GSCM theory and use are documented in Kroner and Cozzie (1996). The following is a brief description of key sections in the document followed by a critique.

In the Kroner and Cozzie document chemical fate in the soil column is controlled by the three processes of diffusion, pore-water advection and reactive decay. Molecular diffusion in the air-filled and the pore-water phases quantify the diffusion process. A single chemical species mass balance is performed which combines the air, water and soil phase to yield a second order partial differential equation (PDE) in terms of total concentration C_T in the soil mass. This dependent variable is a function of time (t) and position (z) in the soil layer. As noted in the 3MRA documentation, an explicit finite difference solution to the PDE exhibited high numerical diffusion; shorter time steps were needed for thinner sections to reduce this problem, resulting in long computation times. An analytical solution resulting from superimposing the three fate process was adopted to overcome these problems to yield an innovative quasi-analytical approach. Several versions of the GSCM with differing soil column physical structures were adopted to accommodate the specific needs of the various WMUs. However, the basic theory was consistent throughout.

In the simplest structural form the soil column is assumed to consist of one homogeneous zone whose properties (i.e.; density, porosity, chemical composition, water content, temperature, etc.) are initially uniform in space (z) and time (t). This column is divided into horizontal chemical layer sources each of a depth dz . A standard error-function analytical solution is used to solve the partial differential equation. Initially the concentration profile is assumed uniform in each layer and zero elsewhere. With application of the effective solute convective velocity, V_E , the center of diffusive mass is translated downward at a rate V_E . Chemical disappearance within the layer is by an assumed first order decay reaction.

Combined in a superposition fashion the three processes are quantified in the individual layers. The adjoining layers do not interact; each is treated separately for its diffusive, advective and reactive losses. The following two paragraphs describe how the quasi-analytical model is used to estimate the chemical masses movement across the upper and lower boundaries of the soil column.

Chemical mass is moved from both upper and lower ends of the soil column by accounting for the movement from each individual soil layer through these interface planes. In effect the upper ($z=0$) and lower soil column boundaries ($z=z_{sc}$) are planes located in these z positions which are imbedded in an imaginary homogeneous soil column that extends to infinity in each direction away from the interfaces. The process is illustrated in Figure A3b-1 for the top-most layer; it has one face at the air-soil interface.

The interface is at the $z' = 1$ position. Initially ($t=0$), the concentration profile in the top layer is the rectangle-shaped piece of highest C_T^0 and width $dz=2$ as shown. After time t for a diffusion-only process, a bell-shaped profile results. The fraction of the initial mass that is attributed to diffusion from the first layer to the air is calculated from the dark red shaded area. The adjacent layer deeper in the soil column, which operates independently,

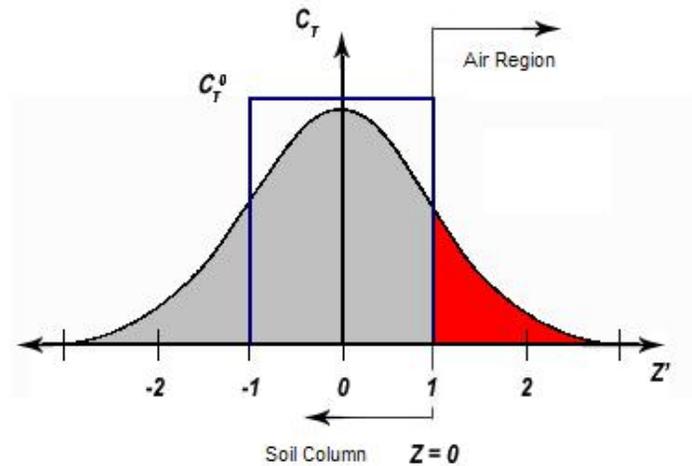


Figure A3b-1. GSCM Layer diffusion through the air-soil interface.

has a smaller diffusion tail that goes beyond the air-soil interface. The third layer has a smaller one still and on through the entire pile. However, this is not how the process of "evaporation" works, is not the one employed in the Jury *et al.* model, and has no credence in inter-phase mass-transport theory (Thibodeaux, 1996). The substitution of a solid phase on the atmospheric side of the interface slows down the natural transport processes that would otherwise operate here. Rather than depicting a turbulent eddy diffusion process, one of chemical molecular diffusion through a porous media is used. The concentration profile structure depicted in Figure A3b-1 on the air-side of the interface is not theoretically possible and the procedure used in the GSCM will likely result in underestimates of the mass transferred to the atmosphere by an unknown factor.

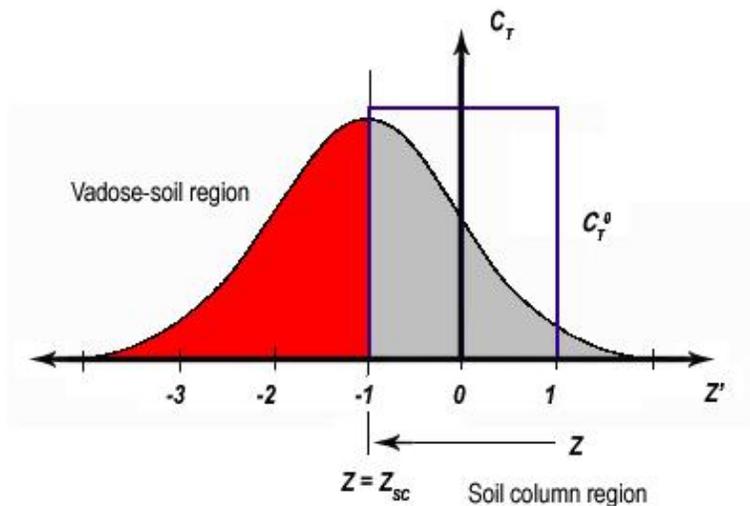


Figure A3b-2. GSCM Layer diffusion plus advection through to soil-vadose zone interface.

A slightly more complex process that combines water advection can be used to portray the wastepile-vadose interface. For advection with velocity V_E superimposed upon diffusion the concentration profile in the bottom most layer of the soil column moves down the soil column (i.e., water flux driven chemical transport) as illustrated in Figure A3b-2. The diffusion profile is not symmetrical about $z^1=0$ as in Figure A3b-1 but is translated whole symmetrically around $z^1 = -1$. The interface between the bottom of the waste pile at $z=z_{sc}$ that abuts the vadose zone beneath is located at the $z^1 = -1$ position. The fraction of the initial mass that is attributed to diffusion plus advection into the vadose is calculated from the dark or red shaded area shown in Figure A3b-2. According to the GSCM this mass moves into an imaginary, semi-infinite soil column with waste-pile physical and chemical characteristics located below the bottom interface, $z = z_{sc}$. The next waste-pile layer above the interface one contributes a smaller “leaching” tail that crosses the bottom plane. Each successive layer behaves similarly contributing “leached” fractions. Again, this is not how the chemical leaching process occurs from the waste-pile to the vadose zone. Chemical movement into the vadose zone does not reflect the physical or chemical properties and the reactive decay of the receiving zone.

To account for chemical decay, the concentration C_{TO} undergoes a first-order ($\exp(-kt)$) decay. The mass that crosses the interface boundaries is corrected using this decay loss fraction. Due to the changes in the soil column properties across the interface, going from waste to vadose, the profile structure depicted on the vadose side is theoretically impossible. The dark or red shaded area depicted in Figure A3b-2 that extends into the vadose zone is based on waste properties. The GSCM is theoretically challenged to correctly quantify the interphase chemical transport to the vadose. The following paragraph describes how the individual layer processes are combined to transport mass from the soil column; the above just focused on individual layers.

The soil column consist of a multi-layer stack, each layer dz in depth; the number of layers is $N=Z_{SC}/dz$. Figures A3b-1 and A3b-2 are for the top and bottom layers only. Each adjacent layer in the stack behaves identically to the two illustrated. However, because they are one layer thickness removed from the respective interfaces, less of their initial mass moves across the two imaginary interface boundaries. Chemical movement from below the layer into the surface layer at $z=0 + dz$ is similarly calculated. The N-layer summed dark shaded equivalent mass fractions protruding through the air-soil interface, corrected for the “water” out-diffusion, are used to obtain the volatilization from the WP or LAU. That N-layer summed dark shaded equivalent mass fractions protruding through the bottom interface is that used for computing the leachate from the WMU and the reactive decay summed over each of the N-layer decreased that available for movement from the soil column.

In Section 3.0 of the Kroner and Cozzie document, the GSCM is described as it is used in the local watershed/soil column module. The developers did a particularly good job including all the runoff processes and in connecting the GSCM to the runoff model. A compartment model was used for the runoff and it was positioned atop the first layer in the soil column. Positioned here the runoff compartment received chemical inputs from the soil column and therefore passes the chemical composition needed for quantifying resuspension/erosion losses in the hydraulic modeling component.

As described above the GSCM is used to commence chemical movement from the non-wastewater WMUs by all the release pathways. Although this is an innovative solution to a complex environmental chemodynamic, process it is theoretically incorrect. The faulty construct lies in assuming the soil column can be modeled by chemical release into two semi-infinite imaginary soil zones and that a molecular diffusion process simulates chemical mass movement across the top (air-soil) and bottom (soil-vadose) interfaces of the soil column. In reality a phase change occurs at the upper interface and a physical properties change occurs across the vadose zone interface. The concentration profiles at the respective ends of the soil column will assume significantly different shapes than those illustrated in Figures A3b-1 and A3b-2 because of the constraints imposed by the individual phase transport processes in the boundary layer adjoining these surfaces.

The second major theoretical error with the GSCM involves its governing equation (Equation 2-8 in Kroner and Cozzie, 1999). Generally three phases can exist within the soil column. If it is saturated with water the soil phase is present but the air (i.e., soil gas) phase is absent. In order to simplify the mathematics it is common to employ a local equilibrium assumption (LEA) for chemical distribution between the three places. This allows the expression of the concentrations in the individual phases to be expressed in terms of the total contaminant concentration C_T (see Equation 2-6 in the Kroner and Cozzie document). Such a tactic is common in ground water contaminant modeling such as is done in HYDRUS, however it is problematic for modeling a thin soil column. For the WMU applications the soil column is positioned within a relatively thin zone between an underlying vadose zone and an overlying air mass. Within these thin zones the boundary process becomes very significant since large fractions of the chemical

mass reside within and move across these planes. Typically in groundwater contaminant plume modeling only a very small fraction of the chemical mass is located near the boundaries.

A solution of Equation 2-8 at fixed time t is a quantitative relationship of total concentration, C_T , with distance z , with non-zero concentration gradients at both ends of the soil column. The GSCM computed concentration profiles within the three soil phases (i.e., pore-air, pore-water and solid particles) must have parallel, curvilinear shapes and finite concentration gradients everywhere. Since the phases are assumed to be in equilibrium the concentrations are related one to another by non-zero constants and all the gradients are likewise related. For example, since dC_T/dz is non-zero at the air-soil interface the liquid concentration gradient dC_L/dz must be non-zero as well. However, without liquid water on the air-side of the interface there can be no diffusion across through this phase. Without diffusion the dC_L/dz must be zero. But if it is zero, the equilibrium non-zero gradient requirement is violated. Thus, performing only a single mass balance that yields a solution giving the total chemical concentration and assuming the phases are always in equilibrium leads to theoretically inconsistent concentration patterns. In reality, due to the chemical depletion from and re-partitioning within the mobile phases (i.e., air and water) of the layers near the interfaces, they cannot and will not be so simply related implying that the GSCM computed concentration gradients and profiles of C_G , C_L , and C_S are incorrect. The individual concentrations in pore air, pore water and soil particles cannot be linearly related by constants as demanded by the LEA. The EPA developers realized some of these theoretical difficulties and fashioned ad hoc corrections (see p. 2-8, 2-9, 2-12 & 2-13 in Kroner and Cozzie, 1999).

In summary there are two theoretical problems with the GSCM. First, the quasi-analytical solution requires two imaginary semi-infinite soil sections located top and bottom the soil column to act as surrogate sinks to the air above and the vadose below for the diffusive and advective mass transport. Secondly, the application of the LEA in the relative short soil column forces the concentration profiles and chemical gradients in air, water and solid particles near the two interfaces to have parallel profile shapes. Both theoretical problems work together to fabricate a quantitative chemical release model that is at odds with the known scientific fate and transport processes operative at the interfaces and within this multi-phase system (Thibodeaux, 1996). The result is that the GSCM computations will likely give erroneous chemical concentration and flux predictions of unknown magnitudes.

Status of Module Testing

Prior to developing a new model it is common for the developer to give a thorough review of existing similar models in the published literature. Only two such literature citations were noted in this regard; they were Jury *et al.* (1990) and Shan and Stephens (1995). Presumably these were the ones most applicable to the needs of the 3MRA model. Requested technical input received from EPA and its own literature reviews revealed no appropriate model and this has convinced the panel that the Agency was correct in commissioning the GSCM.

Being a new model GSCM has a very brief history of use. Clearly it does not have the legacy status of the two wastewater modules that constitute the other chemical waste sources for the 3MRA model. Being innovative the model must pass a special testing protocol that assures its conformity with the simpler, less innovative and conventional ones presently in use. It is common practice to test a new model with numerical calculations against existing similar models and against laboratory and/or pilot scale experimental data. The 3MRA team responded to this comment and the panel received a brief report of a one-to-one comparison of the GSCM and MODFLOW-SURFACE (EPA, 2004).

The 3MRA team concluded that the GSCM performed well, producing comparable infiltration results, performing very well for certain chemicals under defined conditions and less well for others. This outcome is not unexpected since Table 1 in the document shows that both models have basically the same theoretical key attributes. The main difference is in the PDE solution technique. MODFLOW-SURFACE uses a numerical Eulerian approach while that for the GSCM uses a semi-analytical Lagrangian approach.

The numerical testing should include some level of heuristic sensitivity analysis (SA) to test the realism of its computational response to obvious inputs. This approach verifies some generally expected behavioral input versus output responses. For example, an increase in infiltration rate should result in an increase in the leached chemical flux from the bottom of the soil column and a decreased evaporation flux out the top. One such test was performed and reported, but it was very simplistic and involved only the single layer within the soil column (see Kroner and Cozzie, 1996 pages 2-6 and 2-7). Nevertheless this demonstrates the type of numerical SA that should be performed on the GSCM using several chemicals that reflect the full range of waste substance properties. The GSCM should be extensively tested using laboratory and/or pilot scale data. Numerous sets of experimental data involving both vapor (alone) and aqueous (alone) chemical breakthrough time profiles exist in the literature. These cover a wide range of both chemical properties and soil types that provide real simulation challenges for the GSCM. A more robust test that included the LAU module with both leachate and vapor was performed with mixed results (Schmelling and Jewett, EPA 2002; Schmelling, Wang and Liu, AWMA 2003). Although the results were encouraging, such continued evaluation using only the GSCM is highly recommended by the 3MRA panel in order to gain more confidence for its use in 3MRA. As it is presently doing, the EPA should continue to publish the results in the peer review literature.

Five key model assumptions are made in the operation of the GSCM. They are as follows and are contained in the Kroner and Cozzie document for which the specific citation locations are referenced:

- 1) The volatilization loss is assumed proportional to the total mass loss by the ratio of gas-phase diffusivity to the total effective diffusivity (see Equation 2-23). Is there experimental evidence for this assumption in a chemical three-phase system at equilibrium?

- 2) The developers assume that mass is not lost across the top boundary due to diffusion in the aqueous phase in the soil. In making this assumption the developers are tacitly acknowledging that the governing equation (Equation 2-8) is theoretically incorrect. While it is true that no aqueous diffusion occurs, this assumption is in effect a correction imposed on the computational algorithms. In fairness to the developers, they do acknowledge that a more rigorous treatment would be desirable.
- 3) An implied assumption is made that numerical diffusion can be avoided completely by using Equation 2-26 for computing the integration time step. No supportive arguments are offered to justify this assumption.
- 4) The model developers assume that a “reflective” soil column source below the actual soil column is an appropriate procedure for transforming the zero concentration boundary condition to a zero flux boundary condition (BC). The parameter used to accomplish this is defined as “bcm”; the model user must specify it over the range is 0 to 1. The “reflective” source concept is widely used and accepted in simple air dispersion models for plumes that contact the ground surface and when a zero flux BC is desired. By doing this, the developers are introducing another correction into the chemical transport computational algorithm. Based on the solution to the governing equation (see Equation 2-16) a zero boundary is already applied to each layer in the soil column. It is not clear how the modelers justify arbitrarily imposing a non-zero B.C. on the stack of layers that form the waste/soil column. This bcm parameter plays a major role in controlling the chemical diffusive rates emerging from the bottom of the column. Based on what information does the user select a value of bcm to specify in the algorithm? (see page 2-10). To the 3MRA reviewers it appears to be an adjustable parameter. It is unclear to the reviewers whether the bottom layer concentration, C_{T0} , (see the sentence below Equation 2-26) which quantifies the chemical mass convected out the lower boundary (i.e., leachate) is in anyway adjusted by the choice of the bcm. It seems that it should. All these factors (both diffusive and advective), taken together, affect the mass of chemical delivered to the vadose zone below the waste soil column. This mass enters the ground water pathway module, which in turn delivers a concentration to receptors using water wells or surface waters for their water supplies.
- 5) In the solution to the governing equation the superposition solution requires a sequential approach. The developers prioritize the processes with diffusion first, followed by decay and then advection. They acknowledge that systemic error could result from this choice and that the size of the error would be dependent on the relative loss rates associated with the three processes. The ordering of processes needs to be investigated numerically to resolve the issue of the assumed ordering. This GSCM limitation appears on page 2-12.

Validation

In the previously section the specific issue of validating the GSCM as a separate unit was covered. What follows is an evaluation of the validations performed on the Land-Based Source Modular and Watershed Module of the 3MRA Modeling System; all these modules contain the GSCM. The following comments are based on the two plus pages in the section entitled “Summary of Validation” (4.2.4) in Volume 3 of the 3MRA documentation. It is not clear what criteria are used to accept or reject the “data” versus model predictions of a particular validation test. Examples of the “moving target” criteria follow as each of the four validation activities are presented and discussed. The panel agrees that using verified software components based on empirical data is an excellent approach. However, the Land-based Source Modules and the Watershed Modules each contain several of these empirical software components. The components are connected by mass balances in the hydrology model, in the soil erosion model, and in the constituent fate and transport model to produce the Local Watershed Model algorithm, for example. In addition, performing the mass balances requires some assumptions to be made about process structure, etc. The final result of this algorithm development procedure includes the empirical data as imbedded elements. To claim that the final modules are implicitly validated because they contain the imbedded empirical data is not factual. In the opinion of the panel validation of the final overall module construct is needed.

HELP model vs. LAU module. This was a model versus model comparison of run-off and infiltration at six sites. Under the circumstances such model-to-model “bench marking” is an appropriate validation activity. The following end-point comparisons were listed: “...on EPA expected long-term averages to be in reasonable agreement. The comparative results were mixed.” “...predictions were quite similar...showed relative large differences”. “With regard to differences in infiltration...there was no bias in the 3MRA.” However for runoff the 3MRA predicted more at all sites. No numerical values were given to quantify differences. In summary the bench marking results were ruled adequate for the 3MRA national screening-level purposes.

Dioxin LAU half-life comparison. Soil half-lives in sewage sludge were compared. Remaining concentrations at equivalent human health risks were calculated for the LAU in order to estimate the half-lives. “The range of half-lives over the selected percentiles was 20 to 48 years, which is in reasonable agreement with the observed half-lives at several monitored sites.” At a face-to-face panel meeting EPA provided data on the observed half-lives to support the reasonable agreement assertion. EPA concluded that the data vs. model was corroborated, at least in a broad sense.

Soil-column study data. The LAU Module is again compared to experimental data obtained on organic chemicals during application of municipal wastewater onto soil. Four elements of evaluation were tested: volatilization, first order chemical decay, appropriateness of the quasi-analytical solution and whether LAU thickness and temperature play significant roles in volatilization. The volatilization rate was reported to be in the “right order of magnitude” for all categories of compounds, however for the

highly volatiles the model was consistently lower than observed. The SA for layer thickness showed none however the SA with temperature “showed certain sensitivity” on volatilization. Although not specifically designed for 3MRA testing, the 1981 soil-column study was the nearest thing to a pilot-scale validation performed on the GSCM. At a face-to-face panel meeting EPA provided two manuscripts authored by Schmelling, *et al.* (2002 and 2003) that detailed the soil-column experiment plus data and how it was used in the LAU validation study. Based on the results, the combined LAU plus VZ modules appear to be functioning properly as to leachate generation concentration and quantity (the reader should appreciate that only the top 7.5cm of the 150 cm column was the LAU portion). The other 142 cm section was the VZ. Data from three identical columns was used in the validation study. The experiment design and the data generated were more applicable to testing the VZ than testing the LAU module. In the opinion of the 3MRA panel, based on this single experiment the LAU module (aka GSCM), the validation is incomplete.

General observations on the validation of GSCM in comparison to the legacy models. Although it is a key piece in the 3MRA model and has been incorporated into several modules, the GSCM has in comparison undergone much less validation testing. EXAMS, the surface water module, is compared to 8 data sets; EPACMPT, the vadose zone and aquifer module, is compared to 4 data sets and ISCST, the air module, has been validated extensively. The validation studies performed on these three modules suggest that they are in substantial agreement with the available data. The EXAMS, EPACMPT and ISCST are dependent on the LAU/Watershed modules for their inputs. Understandably because they are new the GSCM and the Land-based Source/Watershed modules have received more limited validation studies in comparison.

The panel recognizes the difficult challenges the 3MRA developers faced with the absence of an appropriate chemical fate and transport legacy model for the waste-pile source term and the watershed soil column characterization. The level-of-effort activities at quickly developing an appropriate model and validating it are understandable and consistent with the resource constraints of the 3MRA project. However, the GSCM is hamstrung by some serious theoretical flaws that may frustrate the best intended efforts at validation. The Agency may want to consider an alternative approach that is more realistic from a chemical process perspective.

Recommendations for redevelopment of the GSCM and LAU Module

Based on its review the 3MRA panel finds that the GSCM to a high degree contains features inconsistent with the science and practice in chemical fate and transport processes for such multiphase systems. Most significantly the use of a single total species mass balance based and the linear chemical equilibrium between phases assumption limits the ability to incorporate mechanism-based boundary conditions at either end of the modeled soil column. Mechanistically correct boundary fluxes are key to launching the appropriate chemical masses to the air, surface water and groundwater pathways from these non-wastewater WMUs. In the spirit of constructive criticism the 3MRA panel offers the following concepts and ideas for redeveloping the GSCM and its

associated modules. The recommendations focus on correctly formulating the chemical, physical and biological processes in order to realistically represent chemical behavior in the soil column. The panel is well aware that there may be significant mathematical constraints in the computational algorithms as to time and numerical error propagation to contend with in affecting a solution of the redeveloped model. However, it seems logical to commence the redevelopment task using the most realistic description possible.

The next section contains an overview of general concepts for developing an alternative to the current GSCM. The proposed alternative retains the general approach and many specific features of the original GSCM while adding some and changing other features that will overcome its shortcomings. The overview contains the following subsections: 1) soil column chemical processes, 2) column layer structure, 3) mass balances and 4) boundary conditions.

Soil column chemical processes. Table A3b-1 contains a list of all the processes proposed for the alternative modeling approach. The original GSCM contained molecular diffusion, water advection, and reactive decay. Recent advances in chemical transport processes have focused on particle movement by biological macro-fauna and similar particle movement mechanism in both surface soils (McLachlan *et al.*, 2002) and surficial bed sediments (Thibodeaux and Bierman, 2003). These so called “vertical direction sorbed phase” transport processes contribute significantly or dominate all other diffusive ones for highly sorbed chemicals. McLachlan *et al.* report the volatilization rate from the surface soil was up by a factor of 65 for chemicals with log K_{OA} range > 2 to <6. This has been added in Table A3b-1 as bioturbation. The original EPA peer review (Bartenfelder, 1999) noted that rain-event driven rapid infiltration and vertical hydraulic dispersion are very significant transport processes and should be included in the GSCM. These are both related to water movement downward in the column. The air-side resistance in soil columns becomes significant during short exposure times and for rapid particle transport within the soil column surface layer. These three are also listed in the table.

Table A3b-1. Soil Column Processes vs. Unit Type

Process	WMUs			Watersheds	
	LAU	WP	LF	Local	AOI
molecular diffusion*	–	–	–	–	–
water advection	–	–	?	–	–
reactive decay	–	–	–	–	–
dispersion	–	–	?	–	–
bioturbation ⁺	?	?	X	?	–
rapid infiltration	?	?	X	?	–
air-side resistance	–	–	X	–	–

* Includes air and water. ⁺ Also includes cryoturbation and surface cracking/erosion.

- Denotes process is active. ? Denotes process may be controlled.

X Denotes process is absent

In Table A3b-1 processes, the WMU modules and the watersheds modules that utilize the GSCM are listed as well. Not all processes are active across all unit types. For example, bioturbation is absent in the soil column of a landfill because of the daily cover provided and the short duration the waste remains at the surface. In soils it may take many months to years before the surface layer is colonized by the macro-fauna. Depending on the way the WMU surfaces are managed, bioturbation may or may not be present at LAUs, WPs and in the surface layers of the local watershed. Cultivation, mowing and other grounds maintenance activities may hamper the development of significant populations of macro invertebrates that contribute to the bioturbation of particles. Rapid water infiltration is similarly affected by these maintenance operations. Unlike molecular diffusion in air and water, which is ubiquitous, bioturbation and rapid infiltration are site specific and highly seasonally variable. For the Monte Carlo simulation these can be estimated by PDFs that capture their magnitudes and frequencies of occurrence using a random number generator coupled to the seasons through Julian Day realizations. Provisions should be made to include these process advancements into the GSCM as they “come into practice” with increased knowledge and availability of data.

Structure of the soil column layers. This structure should be consistent with the processes to be modeled and the composition of the soil column. The WMUs are formed of waste material “soil” and the watershed soil as a native, natural soil. Figure A3b-3 illustrates some general features of the layer structure of the soil column. Much here is similar to that in the original GSCM. From the top down three stacks of layers are shown. The top-column stack contains layers that are used within the upper region of the soil column where bioturbation, cracking, rapid infiltration, etc. predominantly occur. The first layer in this stack is the surface layer, which connects the soil column to the atmosphere above. The mid-column stack contains layers where molecular diffusion, water advection, and dispersion are the active processes. The bottom-column stack is shown as a single layer. Its processes are identical to those in the mid-column stack but its use is to connect the soil column to the vadose zone below.

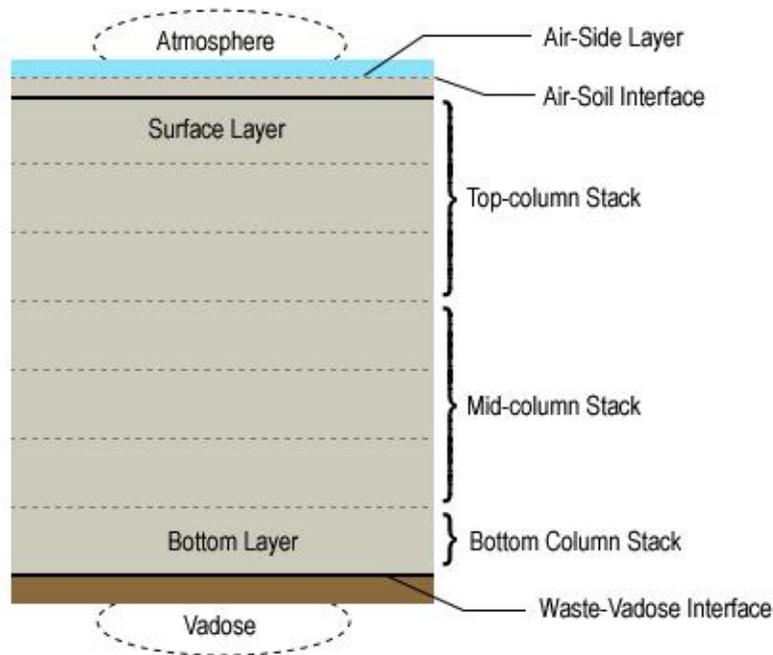


Figure A3b-3. Generic Soil Column Structure

The number of layers in the individual stacks is variable. Likely at a minimum number, the top and middle stacks consist of three layers each and the bottom stack is one layer. Using a larger numbers of layers may increased run time without any real enhancement in computation accuracy. As will be presented in the next subsection, the individual layers are compartments of uniform composition. In contrast, the soil column layers in the original GSCM have concentration gradients within. Compartment model constructs with uniform concentrations within appear elsewhere in the 3MRA model system and its use here is appropriate as well.

Compartment mass balances. In this section the mathematical description that incorporates the processes and the soil column structure will be presented. Due to the similarities in process variables, the nomenclature used here is that of Kroner and Cozzie (1999). The alternative governing mass balance equation in terms of the chemical concentration in the water, C_L , is presented in a similar layout as that of the original GSCM which is Equation 2-8 and is as follows:

$$\frac{dC_L(j)}{dt} = \frac{D_{EL}}{dz} \left[\frac{C_L(j+1) - C_L(j)}{dz} \right] - \frac{D_{LE}}{dz} \left[\frac{C_L(j) - C_L(j-1)}{dz} \right] - I \left[\frac{C_L(j+1) - C_L(j)}{dz} \right] - k_L C_L(j) \quad \text{Eq. A3b-1}$$

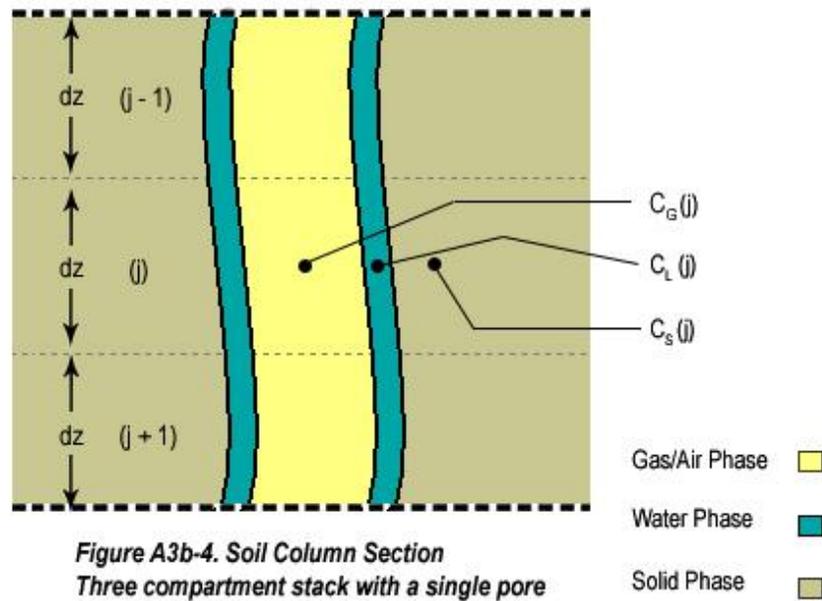
$$+k_{23} a_v [C_s(j) / K_d - C_L(j)] - k_{12} a_v [C_L(j)H^1 - C_G(j)]$$

The dz variable is the height of the compartment and does not denote a differential. However dt is a differential. The term to the left of the equal sign is the chemical accumulation in the water phase (i.e., pore water). The first term on the RHS of the equality is the net molecular diffusion of the chemical in the water from and two adjacent compartments. Linear rate equations and finite differences in concentration quantify the flux between compartments. The next line contains the net water advection chemical infiltration from the jth compartment and the reactive decay disappearance of the chemical in the water phase. The last line on the RHS of the equality is the input rate from the adjoining solid phase and the output rate to the adjoining air/gas phase in the porous structure. This line obviates using the LEA. The resulting governing equation is a first order ordinary differential equation whereas that in the GSCM is a second order partial differential equation. Inherently numerical solutions involving integration of ordinary differential equations are simpler and involve more stable mathematical procedures than PDEs.

However with these possible advantages are some disadvantages. Two additional governing mass balances are required for each layer. These are for the air and soil phases and are structured similar to Equation A3b-1. Thus for each soil layer/compartment there are three governing equations. Three concentrations, C_L, C_G, and C_S appear in Equation A3b-1; these represent the phase/compartment averages as illustrated in Figure A3b-4. For the seven layer soil column structure shown in Figure A3b-4 a total of twenty one (3x7) equations will be required. Procedures for integrating sets of linear, coupled ODES are well developed.

The compartmental model approach proposed places greater emphasis on process realism and less on mathematical exactness. For example, in the original GSCM the use of Fick's first law for the diffusive fluxes results in the mathematically correct second order PDE. The proposed alternative approach uses an integrated form of Fick's first law that yields a first order ODE. The result is simpler mathematically without loss of process rigor. Such constructs with their lesser mathematical burdens have been found to make very good predictions and are used extensively in the environmental compartmental modeling and this includes some 3MRA modules (see Appendix 2a-1 for a description of the types of models used in 3MRA).

Boundary conditions. The three equations for the surface layer and the three for the bottom layer contain inter-phase transfer coefficients. These will result in flux equations for the transfer of chemical mass to the air and vadose. Assumed zero concentrations in the air and the vadose will uphold the feed-forward feature of the original GSCM. Similarly to the original, the chemical concentrations in the surface layer will provide the means for quantifying the concentrations needed for particulate resuspension quantities



for both the air and surface water runoff pathways. Equation A3b-1 contains only one of the many processes listed in Table A3b-1. This was done as a simplification; obviously some of the others listed will need to be included in the appropriate layer mass balances. The upper and lower layer mass balances will need to include transport terms for chemical movement to the air and vadose, respectively. The incorporation of inter-phase transfer coefficient boundary conditions that capture the volatile, soluble, and particulate phase chemical forms departing the upper surface add a dimension of realism not possible with the original GSCM.

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Appendix 4-1

Comments Regarding 3MRA Documentation

Comments Not Specific to Particular 3MRA Volumes

The documentation indicates in numerous places that the earlier problems of mass balance violations in the 1995 predecessor models have been corrected. The panel recommends that the Agency should demonstrate using example 3MRA results where mass balance is attained, and conversely, where a numerical verification is not possible due to the nature of the model domain (this verification could perhaps be placed in Volume III). Specifically, the 3MRA output files (and analysis tools such as the Site Visualization Tool) should provide for the tabulation or visual plots of sufficient model outputs (source terms, mass fluxes, concentration in environmental compartments, and, where possible, chemical mass in environmental compartments) to allow an independent user the ability track mass (and/or concentration) through the modules in a more readily transparent manner. During panel and Agency public meetings, the Agency presented several additional “visualization” summaries of the chemical mass and mass fluxes in those environmental compartments where mass is readily tracked. The panel recommends that the Agency complete the development of these “analysis” tools as a component of the SVT to allow for a more transparent examination of model predictions.

The Agency presented the panel with very helpful information relating to earlier Panel concerns about the possibility of mass “imbalance” when chemical burdens in certain environmental compartments are based on simple biotransfer coefficients (*e.g.*, plant uptake as one example). The panel agrees that this information addresses such concerns and recommends that this information be included as an appendix to the 3MRA documentation.

Table 4-1 in Volume IV provides a very nice summary of the 3MRA components. The panel recommends using this table earlier (in Volume I) in its discussion of the many interrelated components of 3MRA .

A glossary should be included. Many words in the documentation are not in common use or are defined in this context differently from their everyday use. Perhaps

EPA could consider creating a searchable electronic index of the entire documentation where a modeling practitioner could query a topic and the “help” module would identify a list of choices within the documentation from which an individual could find details on that topic.

Specific Comments -- Volume I

Volume I provides a useful overview of the purpose and structure of 3MRA, and prepares the reader for the information provided in the subsequent volumes. The repetition of fundamental information is generally summarized adequately in each subsequent volume so that generally each volume can be read independently of the other volumes. There remains a need to develop a more “digestible” summary, aimed at a non-technical audience.

Although Volume I goes part of the way toward fulfilling this need, it needs an expanded executive summary written in layman’s terms. EPA could consider developing a more graphical summary as one means of more effectively conveying the complex topics addressed in 3MRA. Lacking a more understandable expanded summary, the only people who are likely to understand the system truly will be the developers. If that is the outcome, the decision-makers will not relegate their power to the creators of the model, and the technical tools will sit on the shelf and collect dust.

Competing with the need for a more widely understandable summary, is the need to add to the summary in Volume I to provide sufficient detail for the more technically oriented reader. Thus, Volume I would benefit from the addition of some the additional technical information in Volume II and Volume IV in order to provide sufficient information on the intended strategy of application and the interpretation of modeling results, especially the uncertainties.

A clearer description of what the exit concentrations refer to is required. Based on discussions with the Agency during public meetings, the Panel understands that the national exit level represents the concentration in the waste stream as it would enter a WMU, and not the concentration of the contaminant within the WMU. A clearer description of the distinction between the “exit concentration” and the concentration of chemical as applied to a WMU is required in the document. In particular, Volume 1 should include explicit equations that indicate how the land-based source terms (*e.g.*, Section 5) are calculated, including how the fraction waste (f_{wmu}) term impacts the source concentration. As noted in comments on Question 1, the Panel recommends that the Agency include an analysis of the distribution of f_{WMU} associated with national exit levels in the final 3MRA documentation.

The document should be clear as to whether the national exit levels are being calculated based on the percent population protected for a “site” as a whole (*e.g.*, potentially accounting for multiple WMUs at a site), for specific WMU types, or for specific waste types (*e.g.* liquid or solid. For example, on page 3-4 in Volume IV it is suggested that EPA is considering developing WMU-specific exit levels (which the Panel

believes has merit). Yet in Volume I, and elsewhere, the exit levels appear to be defined only as the result of the sum total of all combined WMUs at a particular site. The document should be clear on this point one way or another.

Another area where additional explanation of exit levels would help the reader, is reiterating the fact that the exit concentrations are chemical-specific. Even though the Agency is developing exit levels for 40+ chemicals, chemical interactions are not considered.

The concept of risk bins (intervals) is a new one and one that needs further explanation. In addition, the notion of “percent of population protected” requires further clarification. In particular, the documentation should provide more tangible examples of how the spatial variation in modeled chemical concentration in environmental media are combined with population density (census centroids) in order to calculate “population risk” or “population protection” at a given site. Clear, specific examples, should be provided.

The equation notation is oriented toward a modeler who specializes in one topic area to see the clear linkage to related topic areas and algorithms, however there are instances where different notation is used for the same equations depending on specific sub-model considerations. These sometimes differing formulations of the same general equation does create the possibility of injection confusion and ambiguity. One example of this is the difference between Equation (5-6) used for the GSCM and Equation (5-16) which describes the soil surface layer for the Watershed module. The later equation contains a source/sink term not shown in the equation for the GSCM. It would appear that the equation for the GSCM model should include a chemical source term added to the soil column with waste applications. On a related note, it is potentially confusing to the reader to use lower case symbols for the concentration terms (*e.g.*, “ c_1 ”, c_2 , *etc.*) for Equation (5-14) then use upper case symbols in (5-16). Finally, using “ c_1 ” and “ c_2 ” in this context to represent the “total” concentration in runoff and soil, respectively, perhaps unnecessarily introduces confusion between the definition of “ c_2 ” and “ C_T ” where that later notation is used in the GSCM to define “total concentration.”

Volume 1 (and elsewhere) could provide more context (in summary fashion) to the reader on the nature of the 201 sites in the database (by region, size, industry, WMU and waste types, *etc.*). Although there are indeed 201 sites in the database, exit levels for many solid wastes will be set based on specific land application units (LAU), of which there are only 28, landfills (only 56 in the database), *etc.* Likewise, only 137 sites managed liquid wastes, so exit levels for liquids will be based on only 137 sites. This should be clarified in the documentation. As it stands, the indication that the database included data for 201 Subtitle D sites can be erroneously interpreted to imply that the site database is more robust than is in fact the case for specific WMU types. In addition, Volume I should provide more details on what steps the Agency undertook to determine that the 201 sites selected are representative of the universe of possible waste management sites (including whether they are representative of current sites, given the age of the WMU data in the database).

According to Vol. 1, page 5-6 bullet 2: “concentration can be adjusted for other wastes which do not contain the constituent.” Again on page 9-7 of Volume 1 there is a reference to incorporating a “fracture multiplier” for the aquifer module. It would be helpful to add a table to the documentation showing all the options and ad hoc adjustments such as these that are contained within the 3MRA model and which option(s) are selected for the purpose of setting national exit criteria.

Inclusion of a bio-uptake factor in the human and ecological exposure modules would enhance the versatility of the model. Any transfer factor or bio-uptake factor that is omitted has an implicit value of unity, but the omission of this implied value is not apparent to the reader. Explicitly including such a factor improves transparency even if the default value is one (1.0) in some cases where there is no evidence to support another value. However, the inclusion of such a parameter would facilitate the use of chemical-specific values when available and would also facilitate inclusion waste-specific bio-uptake data in the future to support de-listing petitions.

The panel notes that Volume I generally uses graphics effectively to orient the reader as to model structure and function, although improvements are needed. Some example figures/graphics that the Panel found to be most in need of clarification are identified below, although this list is not intended to be all inclusive. [Note that for some of these, they appear in multiple places in the document and the Panel recommends that the modifications would be consistent throughout the document.]

Vol. 1, Fig. 1-2. This figure (which also appears elsewhere) is very busy with a multitude of interconnected compartments such that its value to the reader becomes lost. Figure 2-3, which has similar elements, is much more intuitive. In addition, Figure 2-3 could possibly be enhanced with the addition of the model(s) that are associated with each module (where appropriate and without adding undue clutter to the figure).

Vol. 1, Fig. 1-4. Both the Y-axis, and X-axis of this plot require better labeling to clarify them (this applies to many of the plots depicting the risk outcomes in the form of probability curves). The figure appears to imply that there is an increasing probability of protecting a larger percentage of the population, whereas intuitively, the probability of population protection should decrease as the percentage of the population protected increases. (If “complimentary” cumulative distribution functions are to be used to illustrate the results, then the graphs require better labeling, and the text should provide a description of the reason a complimentary CDF is used in simple terms.)

Vol. 1, Fig. 1-5 isn’t clearly labeled and also seems counterintuitive. What do the individual curves labeled with different percentages depict? Also, for a given waste concentration these percentages should move inversely, *i.e.* a high percentage of the population might achieve 50% protection but a smaller percentage would achieve 95% protection. Rather than attempt to fit all plots (5 C_w values) on a single figure (the notation on the X-axis is quite confusing), the Panel recommends simplifying these figures to show perhaps two values of C_w on a plot such as Figure 1-4.

Figure 2-9 is not clearly labeled and could be improved. This figure is used to illustrate the notion of “risk binning” of the MCA results and seems counterintuitive, suggesting that an increasingly large number of people are subject to increasing risk.

Specific Comments -- Volume II

Although the data sets used are generally identified, it would be helpful to provide a concise summary (perhaps by module) of the date, size and scope of the data set, and other important contextual information that identify the major data sets used to support the models. While this information may exist in the voluminous documentation, a concise summary in one location would be helpful.

There are many data distributions that are indicated as being selected using “best professional judgment.” Again, it would be useful to summarize in a more “global” manner, the types of important model parameters that are based on empirical data, and those that are based on professional judgment. As suggested earlier, a global matrix of data inputs categorized by “empirical/site,” “empirical/national or regional,” “professional judgment,” and “operational” would be helpful.

Specific Comments -- Volume III

Volume III provides a reasonably straightforward indication of the verification/validation efforts conducted to date by the Agency. However, as noted in responses to Question 3, the Panel has concerns about the completeness and extent of model validation and important components of the validation have yet to be completed. The ongoing validation efforts and results will require updating the documentation.

Specific Comments -- Volume IV

To characterize and bound the uncertainties for the policy maker it is essential for them to understand the potential impact that their decision will have. It is equally important for them to understand how to delineate that uncertainty and comprehend how sensitive the 3MRA system is in its yielding exit concentrations. Therefore, it is important that the material in Volume 4, Uncertainty and Sensitivity Analysis, be either re-written at a more understandable level or take the majority of the material and place it in an appendix for the reader/user to pursue at a his or her leisure. The chapter is dense, even for those whose vocation is risk assessment and those familiar with probabilistic methods used for risk characterization. Eliminating redundant information could in many instances condense the material in Volume IV.

Section 2 in particular reads like a textbook in some places. The panel suggests that the discussion be more focused on the actual methods used in the 3MRA and how the results thereof should be interpreted for decision-makers and stakeholders. There simply is too much tutorial information that gets in the way of learning what uncertainty, variability and sensitivity analysis is all about in 3MRA. The need for clarity and

simplicity of explaining how 3MRA addresses uncertainty *versus* variability (if indeed it does this explicitly) takes precedence over completeness in describing the “taxonomy” of sensitivity, uncertainty, and the like. The document should target the model user as the principal reader, not the academic scholar or statistician. As it stands, the document is guilty of swamping the reader in a “sea of linguistic ambiguity,” (e.g., p. 2-13) rather than providing clarity. In particular, the document relies on 3MRA jargon such as ELPI, ELPII, RSOF, *etc.* which are perhaps useful shorthand for describing some of the mechanics of how 3MRA stores and processes information, but this type of information is more geared toward modelers, rather than describing the conceptual model formulation.

There is a rich and often confusing lexicon of terms describing uncertainty, variability, and sensitivity in the literature, and the report devotes considerable space to reviewing this literature. However, it is not the Agency’s primary job to sort all that out for the benefit of the 3MRA user. Rather their responsibility is to define clearly and unambiguously how the terms uncertainty, variability, and sensitivity (and their derivatives) are used and addressed in the 3MRA context. Specific examples should be provided, rather than speaking in vague generalities using statistical jargon. How are they estimated, examined, analyzed, and interpreted in 3MRA? Only then should the authors elaborate on how the use of these terms/concepts/analyses, *etc.* as implemented in 3MRA relate to others in the literature, and only as is necessary to clarify for the reader/user what 3MRA is doing. Furthermore these elaborations can be relegated to an appendix.

The documentation must be consistent in its treatment of variability and uncertainty. Although the documentation (e.g. Section 2.6) spells out the various kinds of uncertainty and identifies those that the model addresses and those that it does not address, other places might give the impression that variability and uncertainty are separately quantified. Volume 1, Section 1.2.1 states, “Quantifying variability and uncertainty in exposure and risk estimates is an important capability of any modeling system. The 3MRA modeling system was designed with a two-stage Monte Carlo analysis capability, which enables users to distinguish between variability and uncertainty in input variables”. Section 2.1.1 (page 2-4, paragraph 1,) states “the distilled output prediction can, for example, be represented as predicting 90% receptor population protection at 95% of sites with a 98% probability (or confidence or belief) of meeting this ‘dual criteria’ population protection level.” The panel does not believe that 3MRA presents a quantitative separation of variability and uncertainty in the “traditional” sense of evaluating input parameter uncertainty/variability (and the documentation recognizes this also, albeit the ambiguity in the documentation gives rise to confusion on this issue), nor does the panel believe that a more rigorous 2-Stage Monte Carlo analysis that would separate and quantify uncertainty is realistic in the near future. The documentation should be clear and consistent on this point, and the panel recommends that the “pseudo 2-D” terminology be avoided. Although the panel believes that a true 2-D uncertainty analysis may not be possible with current data and computing resources, as noted in Question 2c, we recommend that a second dimensional “input uncertainty” analysis be included in the uncertainty/sensitivity analysis for 3MRA.

Statements in Volume 4 mention that the reader might get conflicting impressions as to whether 3MRA version 1.0 actually distinguishes between uncertainty and variability. As noted above, the Panel agrees that discrepancies between statements in Volume IV and Volume I do indeed confuse this issue, and these discrepancies should be resolved.

In addition, the document creates confusion in the reader regarding the various versions of 3MRA (*e.g.*, ver. 1.0, ver. 1.X, and ver. 2.0). The additional functional capabilities of 1.X and 2.0 over 1.0 are outlined in the report, but what about problem solving? What kinds of problems can be investigated with the PC version 1.0? On the one hand it appears that the Monte Carlo Analysis requires the SuperMUSE, yet the reason(s) for this remain unclear in the current documentation. The document should be very clear on the distinctions between the versions, and which version is being used to develop exit levels.

Software issues/Initial Conditions. Some concentration ranges need to be expanded to spread out the probabilities. It does little good to have 100% protection at all concentrations. The ongoing plans for further Monte Carlo model sensitivity and verification testing could be improved or clarified. The discussion as it stands is described in abstract terms. The panel recommends that the documentation provide specific examples (using real 3MRA parameters) of just how the uncertainty/sensitivity analysis results will be presented in tabular and graphical form. As it stands, the document discusses some of the mechanics of the proposed analysis using 3MRA “jargon,” but does not provide the reader with a clear understanding of the kinds of output uncertainty/sensitivity analysis will generate, and how this analysis might enlighten the regulators who formulate the exit levels, and the public who must interpret the results. Furthermore, the discussion in the document included many development program details, such as budget estimates and schedule timing that, while they may be of interest to some readers, seemed peripheral to the mission of the main document. They may just be an indication of a “work in progress”, but those facts relevant to the more permanent readership could be included as an Appendix or Addendum.

The summary of model parameters in tables in Section 8 (*e.g.*, Tables 8-9a, b, *etc.*) should include the 2nd moment (*e.g.*, variance or standard deviation) where appropriate when describing probably distributions. Currently, only the first moment is provided, with a range. The text and tables in Section 8 should offer more details and clarification to the reader in order to interpret the distinction between the site-specific “empirical” data/distributions used in the modeling *versus* the regional/national distributions. Only after several discussions with the Agency was it clear how the “constant” distribution types for the site data actually was not meant to imply a constant value across all sites, but instead an empirical sample from the Westat Subtitle D survey database, that was “constant” at a given site but varied from site to site as a site-specific value.

For some WMU types, the number of disposal sites in the Agency database are relatively small (*e.g.*, Landfills = 56, LAU = 28, Waste Pile = 61). The documentation should discuss the implications this small number of sites has on the level of confidence that can be placed on statements about the “percent of sites protected.”

The sequence of Tables 8-9a-t and Tables 8-10a-n (“dictionary files” for SSF and GRF files) are quite useful, but do not provide sufficient information to allow a user to interpret the results in the SSF and GRF files. The Panel recommends that the Agency provide further documentation regarding the information found in the SSF and GRF files.

Figures illustrating the MCA iteration/looping scheme could be simplified to illustrate the approach for a single chemical and single WMU.

Specific Comments -- Volume V

While the 3MRA model may be intended primarily as a tool for establishing regulatory exit levels, the Agency has indicated it may have other uses as well. In addition, the Public must be provided sufficient and transparent documentation to be able to run and evaluate the 3MRA model results. With this in mind, the Panel feels that the existing user’s guide elements of the documentation could and should be improved.

In attempting to run the model and its initial example cases, some Panel members found that information from both Volumes IV and V contained needed model summary material and descriptions of application methods before the model could be run, but the information could be improved by including it in a single volume. A set of several sections seemed to contain sufficient information for someone with a general knowledge of the purpose of the model and its constituent elements, but who wanted to run the model with minimum time devoted to “refresher” reading. A candidate outline of the material that would go into such a 3MRA User’s Manual is found in Appendix 4-2. The outline draws information from Volumes IV and V, and leaves Volumes I, II and III for a separate reading exercise.

A diagram showing stepwise requirements for installing, and running the model would be helpful. Such a figure could include necessary steps to initialize any header files, run “cleanup” routines between runs, and provide information on model input/output file locations.

Because one of the major requirements of the system is to implement on IBM-compatible personal computers (thereby making it an accessible PC-based system), it would be useful to present the minimum requirements up front -- not only in the User’s Manual, but also in the very beginning (maybe as a separate stand alone box). This would be especially useful for those who either are not technically adept, or lack up-to-date systems. Furthermore, the minimum requirements as stated (64 megabytes of RAM) appear to be incorrect. Some panel members systems could run a portion of the program and then simply could not continue because it didn’t have enough “horsepower.”

The documentation in Volume V, Section 4.3, devoted to Post Simulation Analysis is a candidate for further improvement. The authors may have assumed that the typical reader of Section 3, particularly Section 3.3.9 would have a reliable memory of how the model output was organized and how all of the postprocessors use those files. The current documentation was a bit abbreviated and could lead to new model-user frustration, but with modest user training, could not be greatly faulted. Although with user training, it might not be unreasonable to have Agency personnel continue to use the present documentation, the potential for frustration of new users due to the abbreviation of several key topics in Volume V, especially that section devoted to post-processing analysis.

The topics under the sub-heading of “Consolidation of Risk Time Output Data” in Section 2.0 (p. 2-11) are sufficiently important that it deserves its own sub-section (*e.g.*, Section 2.1.4). Furthermore, this section would really be enhanced with a graphic displaying how consolidation of data occurs, using an example of how the risk bins get filled as the simulations proceed.

Special emphasis should be given to the “clean-up” procedure. Several panelists have been puzzled by results that do not make sense, only to learn later that the processor was analyzing results of an earlier run.

The discussion of 3MRA Monte Carlo Scheme (Section 2.3) again introduces confusion regarding whether input parameter uncertainty is included in the 3MRA analysis. While the matrix provided in Figure 2.3 is a useful means to illustrate a traditional “2-D” analysis, it does not reflect the actual analysis conducted in 3MRA. In addition, the examples in Figure 2.3 require improved annotation and labeling. They are unclear and use non-standard abbreviations/shorthand that is not explained in the text.

Additional examples and model scenarios. The panel suggests that additional simulation exercises (some example problems) be included in Volume 5. These examples would provide more context for the types of different questions that can be addressed by 3MRA, and also provide an independent user of the model “benchmark” examples of model output (to provide “confirmation” that the user can correctly run the model under different conditions). This model-use training exercise should include multiple runs to allow the user to be sure that he or she has used the clean-up procedure correctly.

Appendix 4-2

Candidate Outline for Improved “3MRA User’s Manual”

- 1.0 INTRODUCTION [Combination of present IV (I.0) and V (1.0)]
- 2.0 OVERVIEW OF SCIENCE [Current IV (3)]
- 3.0 OVERVIEW OF 3MRA VERSION 1.0 [Current IV (4)]
- 4.0 MODEL METHODOLOGY SUMMARY [Current V (2)]
- 5.0 INSTALLATION AND USE OF 3MRA [Current V (4)]
- 6.0 CASE EXAMPLES
 - 6.1 Single Site, Single Realization [Current IV (3.2)]
 - 6.2 Example Benzene Case [Current IV (7)]
 - 6.3 Example Mercury Case [New Example from model validation experience]
- 7.0 INTERPRETATION OF RESULTS AND UNCERTAINTIES [Current IV (1.3, 7.2)]
- 8.0 REFERENCES
- 9.0 TECHNICAL SUPPORT FOR CURRENT AND FUTURE 3MRA APPLICATIONS

Appendix A – 3MRA Technology [Current V (3)]

Appendix B – 3MRA Inputs & Outputs [Current IV (8)]

Appendix C – Probability Models and UASA Applications for 3MRA [current IV (2)]

Appendix D – 3MRA Version 1.X Enhancements [Current IV (6)]

Appendix E – The SuperMUSE System for Testing 3MRA [Current IV (5)]

Appendix F – UASA Plan [Current IV (9)]

Much of the inspiration for this approach came from trying to run the model the first two times. Because the initial attempt immediately followed a reading of all of Vol. IV, including Section 3, as well as Volume V, the logic seemed relatively clear. However on subsequent return, it seemed difficult to remember where some of the key instruction material was located: Volume IV or Volume V?.

Appendix 4-3

3MRA Editorial Comments

Throughout the document, reference is made to “soil concentration,” “air concentration,” *etc.* While it may seem cumbersome, it is more appropriate and correct to refer to “chemical concentration in soil,” and “chemical concentration in air,” *etc.*

The word “data” is plural. There is not a consistent treatment of the verb form that follows “data.”

There were occasions when tables and figures referenced in the text were either not present, or incorrectly referenced (see Volume V, p. 2-3 and p. 2-15 as examples).

There are occasions where the notation used in figures differs from the notation used for variables in the text (capitalization, acronyms, *etc.*). In addition, there are occasions where the figures introduce acronyms that are not explained in the text. The document has a tendency to introduce many acronyms that are in some cases not needed, and detract from the readability. This is particularly so in the discussion of uncertainty and variability and the discussion of the “mechanics” of the “exit level processors.” A more judicious use of acronyms would enhance the documentation from a readability standpoint.

Vol. 1, p. 5-14. The boundary condition in the second bullet appears to be inconsistent with the statement in the bullet on the bottom of p. 5-24.

Each volume is a stand-alone document; therefore it would be helpful for either a header or footer that contains a reference to what volume it is.

A more judicious use of commas would enhance the overall reading, especially for those chapters whose writers prefer to use long sentences.

**Biosketches for SAB
Multimedia, Multipathway, and Multireceptor Risk Assessment Modeling System
Review Panel Members**

(in alphabetical order)

Andrea Boissevain

Ms. Andrea Boissevain is the Principal and Senior Scientist with Health Risk Consultants, Inc., a woman-owned environmental consulting firm in Fairfield, CT. Ms. Boissevain has extensive experience as a risk assessor with skills that range from designing exposure models to managing multi-media quantitative human health assessments for state and federal Superfund sites across the nation. After receiving her Masters in Public Health (Environmental Health Concentration) from Yale University Department of Epidemiology and Public Health in 1984, she worked with a large environmental engineering concern before starting her own firm in 1989.

Ms. Boissevain is currently developing exposure assessment methodologies to evaluate individual exposures to a variety of indoor pollutants, including volatile organic compounds. Several of the sites she is working on are grappling with exposure to soil gas vapors associated with impacted groundwater. Knowing the science, assessing the health risks, and developing outreach strategies to inform the public are daily challenges she addresses. Risk communication and making science understandable to myriad audiences now comprise a large component of her work. Her basic science background (A.B. Vassar College, Biology) and her pursuit of toxicology (graduate school and beyond) coupled with her love of writing has shaped her firms commitment to communicating with people (clients and the public alike) about the health implications of exposures (both acute and chronic) to hazardous substances.

With respect to funding sources and contract support, HRC serves a variety of private (Fortune 100 firms, engineering and law firms) and public sector clients, most notably the Department of the Navy, U.S. Environmental Protection Agency, the Connecticut Department of Public Health and the Town of Stratford. Ms. Boissevain is a long standing member of the Society for Risk Analysis, American Public Health Association, and the New England Society for Risk Analysis. She also served on panel of experts that employed risk-based principles to screen and prioritize over 2000 state-classified abandoned hazardous waste sites for the Virginia Department of Environmental Quality (VDEQ). A subset of sites were sampled, information collected, and a hazardous ranking scheme developed. The expert panel assembled provided professional judgment in the final priority assignments of the sites to enable VDEQ to assess state [financial] liability for cleaning up abandoned sites.

Linfield Brown

Linfield C. Brown is Professor and former Chairman of the Civil and Environmental Engineering Department at Tufts. Professor Brown earned his BSCE and MS from Tufts and his Ph.D. in Sanitary Engineering at the University of Wisconsin-Madison. His research has covered a broad range of topics in sampling strategies, flow

equalization, oxygen transfer, and most recently, uncertainty analysis in water quality modeling, multi-response parameter estimation, and the use of genetic algorithms for model calibration.

Dr. Brown has served as consultant to both industry and government. As a research engineer with the National Council for Air and Stream Improvement (NCASI), he developed their national program in mathematical water quality modeling. While on sabbatical leave at the USEPA Center for Exposure Assessment Modeling (CEAM), he designed and implemented a computational framework for incorporating uncertainty analysis into the water quality model, QUAL2E. He is the author of over 50 technical papers and reports covering the fields of environmental engineering and statistics and has offered over two dozen workshops in the U.S., Spain, Poland, England, and Hungary on water quality modeling and control. He is co-author of the book *Statistics for Environmental Engineers*, which describes the practical application of statistics to a variety of environmental engineering problems. He founded and was academic director of an innovative multi-disciplinary Masters program in Hazardous Materials Management, and initiated a similar program in Environmental Science and Management for mid-career professionals, targeted specifically for women and minorities. He received from Tufts, the prestigious Lillian Liebner Award for excellence in teaching and advising. Dr. Brown currently serves as consultant to the Environmental Models Subcommittee of the U.S. EPA Science Advisory Board and is director of the Tufts ABET accredited BSEvE program. In addition to his university support, Dr. Brown receives funding from the New England Water Pollution Control Commission, which, in turn receives that funding from EPA Region I.

John P. Carbone

Dr. Carbone is currently a senior scientist within the Toxicology Department of the Rohm and Haas Co., one of the world's largest manufacturers of specialty chemicals. Dr. Carbone received his Ph.D. in endocrine physiology in 1982, his graduate research focused on PCB and PBB effects on thyroid and adrenal function. After a postdoctoral fellowship at Thomas Jefferson University Hospital, Dr. Carbone joined the faculty of Thomas Jefferson University Medical school where he participated in teaching, research and grant writing. In 1991, Dr. Carbone joined the Toxicology Department at the Rohm and Haas Co. His initial responsibilities included sub-chronic study director. Dr. Carbone migrated toward environmental risk assessment where during the past 11 years he has developed expertise in environmental exposure analysis, specifically fate and transport modeling of chemicals in the environment.

Dr. Carbone participated in the FIFRA Environmental Modeling Task Force as chair of the statistics subcommittee. In that committee, Dr. Carbone led the development and implementation of an uncertainty analysis approach for a multiparametric fate and transport model, PRZM. PRZM models chemical movement via runoff and movement through the vadose zone. In the approach that was developed, uncertainty associated with model parameterization was accounted for by using a sensitivity analysis coupled with a Monte Carlo approach to account for the variability associated with these inputs.

In addition, Dr. Carbone has extensive experience with a variety of both U.S. and European fate and transport models. He also closely monitors endocrine disrupter issues and is a key advisor for the Rohm and Haas Co. regarding the European Chemicals Policy and the Water Framework Directive. Dr. Carbone is a member of the Society for Environmental Toxicology and Chemistry and also serves on the editorial board of Environmental Toxicology and Chemistry where his expertise is in fate and transport modeling and environmental risk assessment. Dr. Carbone also works with the Alkylphenol Ethoxylates Research Council where he is an active member of the environmental subcommittee. Dr. Carbone's work is fully supported by the Rohm and Haas Co.

James Carlisle

Dr. Carlisle is Senior Toxicologist, Office of Environmental Health Hazard Assessment, California Environmental Protection Agency. He also holds the following degrees: Doctor of Veterinary Medicine, University of California, Davis, and Master of Science in Aquatic Pathobiology, University of Stirling, Scotland.

His professional responsibilities include oversight of the Emerging Environmental Challenges Program; the Environmental Indicators Program; the OEHHA California/Baja California Border Environmental Program; the Development of Guidelines and Health Criteria for the Cal EPA; the Schools Risk Assessment Program; Oversight of contract research to develop transfer factors for contaminants at school sites; and Risk Assessment review and oversight for the State Water Resources Control Board, the Integrated Waste Management Board, and local agencies in California.

He previously served on the Governor's Panel of Experts in Carcinogen Identification. His professional activities and responsibilities do not involve external grant or contract support.

Peter L. deFur

Dr. Peter L. deFur is president of Environmental Stewardship Concepts, an independent private consultant, serving as a technical advisor to citizen organizations and government agencies. He is an Affiliate Associate Professor in the Center for Environmental Studies at Virginia Commonwealth University where he conducts research on environmental health and ecological risk assessment. Dr. deFur is President of the Association for Science in the Public Interest (ASIP) and on the board of the Science and Environmental Health Network (SEHN). Dr. deFur was previously a senior scientist at the Environmental Defense Fund (now ED) in Washington, DC and held faculty positions at two universities before that. He has extensive experience in risk assessment and ecological risk assessment regulations, guidance and policy. He served on the NAS/NRC various study committees, including the Risk Characterization Committee that released its report entitled, "Understanding Risk," in June 1996. Dr. deFur has served on numerous scientific reviews of EPA ecological and human health risk assessments, including the assessment for the WTI incinerator in Ohio and EPA's

Ecological Risk Assessment Guidelines. Dr. deFur also served on EPA's Endocrine Disruptor Screening and Testing Advisory Committee and is now on EDMVS.

Dr. deFur received B.S. and M.A. degrees in Biology from the College of William and Mary, in Virginia and a Ph.D. in Biology from the University of Calgary, Alberta. He was a postdoctoral fellow in neurophysiology in the Department of Medicine at the University of Calgary. Dr. deFur conducts research on the identification of and effects of endocrine disrupting chemicals, particularly in aquatic crustaceans. He is also interested in the effects of low oxygen conditions on aquatic animals and systems in estuaries and coastal environments. He also conducts research on precautionary approaches to environmental regulations and on citizen involvement in environmental programs, policies and regulations.

Dr. deFur was appointed to BEST of the National Academy of Sciences/National Research Council in 1996. He is on the Advisory Committee to the Board of the Coalition to Restore Coastal Louisiana, and a peer reviewer for professional journals. He has published numerous peer reviewed articles, invited perspectives and review articles for the public on subjects ranging from habitat quality to wetlands, toxic chemical and risk assessment. During the past ten years, Dr. deFur has been extensively involved in scientific research, regulation and policy concerning the generation, release and discharge of dioxin and related compounds. He has published a number of papers on regulation and policy aspects of these compounds, considered in many ways prototype endocrine disruptors. Dr. deFur has been extensively involved in the EPA reassessment of dioxin since 1991. He was a technical advisor to the EPA Superfund Ombudsman office, and is presently technical advisor for the Port Angeles cleanup of the Rayonier mill site, the water quality program in the state of Indiana, and to citizens groups for the Rocky Mountain Arsenal superfund site. Dr. deFur serves as a technical consultant to citizen organizations that are involved in cleanup actions at contaminated sites around the country.

Joseph DePinto

Dr. DePinto is currently a Senior Scientist at Limno-Tech, Inc. (LTI) an environmental consulting company specializing in the development and application of water quality and ecosystem models for addressing a myriad of problems in aquatic ecosystems. He joined LTI in June, 2000 after spending 27 years in academia, including 10 years as Director of the Great Lakes Program at the University at Buffalo. During that time, Dr. DePinto was an active part of the Great Lakes research community and he is continuing in that role at LTI. During his professional career, Dr. DePinto has directed projects on such topics as nutrient-eutrophication, toxic chemical exposure analysis, contaminated sediment analysis and remediation, aquatic ecosystem trophic structure and functioning, and watershed, river, and lake modeling. Dr. DePinto received his Ph.D. in Environmental Engineering in 1975 from the University of Notre Dame. His studies have led to over 100 publications and the direction of more than 45 Master's theses and 12 Ph.D. dissertations.

Recent projects, both prior to and subsequent to joining LTI, that are relevant to the subject SAB panel include (funding source in parentheses): development and application of an integrated exposure model for PCBs in Green Bay, Lake Michigan (EPA-ORD); development and application of sediment and contaminant fate and transport models to assess and evaluate remediation of contaminated sediments in several river systems, including the Buffalo River (EPA-Great Lakes National Program Office (GLNPO)), St. Clair River (Ontario Ministry of Environment), Lower Fox River (Fox River Group), Kalamazoo River (Kalamazoo River Study Group), Niagara River, and Hudson River (EPA-Reg 2 through TAMS); assisted the Delaware River Basin Commission in development of a PCB fate and transport model for application to a TMDL analysis for the Delaware River/Estuary (DRBC); led a team of scientists and engineers at the University at Buffalo in the development of a Geographically-based Watershed Analysis and Modeling System (GEO-WAMS), a Modeling Support System that coupled a Geographic Information System (ARC-INFO) with existing and newly developed watershed and water quality models (EPA-ORD); development and application of a contaminant fate, transport and bioaccumulation model for Lake Ontario in support of the development of a lakewide management plan (LaMP) and TMDL for that system (EPA-Region 2); and development of an aquatic ecosystem model for Saginaw Bay, Lake Huron to investigate the ecological impacts of zebra mussels on nutrient cycling and primary production and on PCB cycling and bioaccumulation (EPA, ORD and GLNPO).

Three relevant ongoing projects being conducted by LTI with Dr. DePinto as the Principal Investigator are: “Developing a Model Framework for Assessing Ecological Impacts of Water Withdrawals in the Great Lakes Basin” (Great Lakes Protection Fund); “Development of an integrated ecological response model for the International Joint Commission Lake Ontario – St. Lawrence River water levels/flows study” (USACE-IWR); and “Linking a fine scale hydrodynamic model (POM) for Lake Ontario with a course grid toxic chemical exposure model (LOTOX2)” (EPA-GLNPO through University at Buffalo).

Dr. DePinto has also participated in several workshops and advisory panels relevant to the topic. He participated in the SETAC Pellston Conference on “Criteria for Persistence and Long-Range Transport of Chemicals in the Environment,” in 1998; was a Peer Reviewer for EPA, ERL-Duluth, on the Dioxin Aquatic Risk Assessment Report, (July 1993 - October, 1993); invited expert review panel member, “Workshop on Application of 2,3,7,8-TCDD Toxicity Equivalence Factors to Fish and Wildlife,” EPA-sponsored workshop, Chicago, IL (January 20-22, 1998); invited member of Model Evaluation Group (MEG) for the Contamination Assessment and Reduction Project (CARP) of the New York/New Jersey Harbor Estuary Program (Oct. 2000 – present); commissioned reviewer, “Florida Pilot Mercury Total Maximum Daily Load (TMDL) Study” report prepared by Tetra Tech, Inc. for Florida Dept. of Environmental Protection documenting modeling work with E-MCM (April, 2000); is a member of the International Joint Commission, Council of Great Lakes Research Managers; and is an Associate Editor of the Journal of Great Lakes Research and Chair of the Publications Committee of IAGLR.

Alan Eschenroeder

Dr. Eschenroeder serves on the faculty of Harvard School of Public Health and operates an independent consulting firm. He received both his BME and PhD degrees in engineering at Cornell University. He has performed numerous risk assessments and has developed novel multimedia modeling techniques both for health and climate change investigations. His current area of research focuses on exposure analyses for contaminants emitted during military actions in the Middle East conflicts. In addition to serving EPA as a peer reviewer over recent decades, he has served and chaired various National Academy of Science special committees and subcommittees. His most recent grant support has come from the U.S. Agency for International Development, the China Project at Harvard, and the United Nations fund for reparations. Current support for consulting work derives from the law firm of Broiles and Timms, LLP on behalf of a private industrial client involved in litigation.

During the decade following his education and military service, he implemented computer-based tools in the field of hypersonic fluid dynamics to provide design inputs for space and defense applications. Using some of these same techniques he began the development of simulation models tracing the evolution of photochemical smog. This modeling work subsequently evolved into multimedia descriptions of contaminant fate and transport in air, water, soil and biota, as applied to exposure and health risk assessment. Examples of his recent research interests include: greenhouse gas tradeoffs in waste management, comparative health risks of rural burning versus controlled combustion of domestic waste in Slovakia, health impacts of mobile sources in China and the addition of socioeconomic influences to health risk assessments and life cycle analyses.

Jeffrey Foran

Dr. Foran is a broadly trained environmental scientist with expertise in toxicology, human and ecological risk assessment, and science-policy. He holds a Ph.D. in Environmental Sciences from the University of Florida, an M.S. in Biology from Central Michigan University, and a B.S. in Biology from the University of Michigan. Dr. Foran has served as a Scientist with the National Wildlife Federation, as Associate Professor at the George Washington University School of Medicine and Health Sciences, as Executive Director of the ILSI Risk Science Institute in Washington, D.C., and as Director of the UW-Milwaukee WATER Institute. Currently, he is President of Citizens for a Better Environment (CBE), is a private consultant for foundations and non-profit NGOs, and provides litigation support. He also holds an adjunct faculty position at the University of Michigan School of Natural Resources and Environment.

Dr. Foran is a member of both Tau Beta Pi (Engineering Honorary) and Sigma Xi (Scientific Research Honorary), he is a member of the Board of Directors of the Einstein Institute for Science, Health, and the Courts, and is President of the World Council of the Society of Environmental Toxicology and Chemistry (SETAC). He has served as an

advisor and consultant to numerous organizations including the U.S./Canadian International Joint Commission, the Organization for Economic Cooperation and Development (OECD), the World Health Organization, the International Program on Chemical Safety (IPCS), the U.S. Environmental Protection Agency, Centers for Disease Control and Prevention, the U.S. General Accounting Office, and the U.S. Department of Defense.

Randy Maddalena

Randy Maddalena, Ph.D., is a Scientist in the Exposure and Risk Analysis Group within the Environmental Energy Technologies Division at Lawrence Berkeley National Laboratory. He received his BS in Environmental Toxicology (1992) and his Ph.D. in Agricultural and Environmental Chemistry (1998) from the University of California, Davis.

The primary focus of his research is development, evaluation and application of models that predict chemical fate in multiple environmental media (air, water, soil, vegetation, sediment) and chemical exposures through multiple pathways (drinking water, food, feed, indoor air) for both human and ecological receptors. He also develops tools and methods for performing probabilistic risk assessment and sensitivity analysis applied to complex regulatory models. His most recent work combines the use of models and experimental data to investigate how vegetation influences the environmental fate and transport of semivolatile organic pollutants and how the uptake of these pollutants into ecological or agricultural food chains might contribute to dietary exposures.

Dr. Maddalena is a Co-chair of the Society of Environmental Toxicology and Chemistry (SETAC) Advisory Group on Fate and Exposure Modeling where he serves as an Editor of the Fate and Exposure Modeling column in the SETAC Globe. He is also a member of the International Society of Exposure Analysis and a member of the SAB's Integrated Human Exposure Committee. He receives funding from the EPA's National Exposure Research Lab for research on fate and exposure models; the DOE's Fossil Energy Program for experimental work on plant uptake of petroleum related hydrocarbons; and from the EPA's Office of Air Quality Planning and Standards for his work on the TRIM.FaTE model. Dr. Maddalena also recently completed a project funded by the EPA's Office of Emergency and Remedial Response where he developed a standardized approach for constructing inputs to probabilistic risk assessment models.

David Merrill

Mr. Merrill, a Principal at Gradient Corporation, has 15 years of experience in negotiating technically sound and cost effective solutions to environmental contamination problems. His expertise includes directing large-scale, multi-disciplinary risk assessments, multimedia chemical fate and transport modeling, complex data analysis, and database design for systems such as landfills, lagoons, chemical plants, MGPs, river systems, and groundwater contaminant plumes. With his extensive risk assessment experience and strong engineering background, he has negotiated risk-based cleanup levels and remedial strategies, interpreted complex site investigation data into effective conceptual site models, and evaluated many types of contaminant transport conditions,

including multimedia transport in water, sediments, and air. He has worked extensively with PCBs, solvents, metals and NAPLs and has served as an expert on cases involving PRP cost allocation disputes. Mr. Merrill has prepared technical comments on behalf of industry and trade organizations on Agency regulations including the PCB Megarule and multimedia modeling and risk assessment aspects of the LDR and the HWIR Rules.

All of Mr. Merrill's professional work is performed for Gradient. Gradient's client base includes Fortune 500 companies, law firms, trade associations, and to a lesser extent state and local municipalities and regulatory agencies. Over the last two years Mr. Merrill's clients have included law firms representing individual companies and PRP groups, trade associations, chemical companies, natural gas pipeline and oil companies, energy generation companies, and the U.S. EPA. Mr. Merrill received his B.S. in Soil and Water Science from the University of California at Davis, and his M.S. in Agricultural Engineering (Civil/Environmental Engineering focus) from Cornell University where he also completed the coursework and qualifying exams toward a doctorate degree.

Ishwar Murarka

Dr. Murarka is Chief Scientist and President of Ish Inc., a minority owned environmental consulting business. He also serves as visiting research associate at the University of Illinois in Chicago. Dr. Murarka holds a Ph.D. in Soil Science and Statistics (1971), and an MBA of Management Science (1974).

His areas of expertise include: Environmental Science and Technology topics pertaining to: management of solid and liquid wastes; characterization and assessment of contaminated sites; in-situ treatment technologies (e.g. chemical oxidation); and remediation/restoration of impacted land, groundwater, and sediments. His research activities cover transport, transformation, and fate of metals and organic compounds in the land and water environments.

Dr. Murarka has served on the External Advisory Committee of the Institute for Environmental Science & Policy for University of Illinois in Chicago; served as Peer Reviewer on Mercury Studies for EPA; served as a consultant for the EPA Science Advisory Board. He is involved in U.S. Experts Panel for an USAID project in India

He receives research grants/funding from USDOE/CBRC, EPRI, GTI, and NYGAS, as well as contract support on projects involving characterization and remediation of contaminated sites from various utility companies (e.g., Duke Energy, NYSEG, RG&E, Consumers Energy, Georgia Power, We Energy, First Energy, NISOURCE, SCANA, etc.

Douglas G. Smith

Douglas G. Smith, Sc.D. is a Principal Scientist in ENSR's Risk Assessment group with degrees in Environmental Health Sciences (specializing in Air Pollution and Industrial Hygiene) and Physics. He has 28 years of experience in risk assessment of toxic airborne materials, including atmospheric transport and diffusion modeling, with applications to environmental siting and permitting.

Most recently, Dr. Smith has led more than a dozen multi-pathway risk assessment projects in support of RCRA permitting and strategic planning for chemical industry members who use incinerators, or boilers and industrial furnaces (BIFs) for waste disposal and energy recovery. These projects are active in U.S. EPA Regions 2, 3, 4, 5, and 6 and have included supporting applications or updates for permits in New York, New Jersey, Ohio, Pennsylvania, Illinois, Georgia, Kentucky, Tennessee, W. Virginia, Louisiana, and Texas. In early 2000, Dr. Smith presented ENSR's team findings in response to an EPA request for an independent external peer review of their "Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities." Dr. Smith has also provided expert testimony on several other occasions for chemical industry clients in toxic tort proceedings and has authored more than 25 publications and technical presentations on hazardous air pollutants, modeling issues and accidental releases. His Sc.D. and M.S. degrees in Environmental Health Sciences are from Harvard University School of Public Health, and his A.B. in Physics is from Franklin and Marshall College.

Dr. Smith has also provided expert advice and support to clients in the chemical and pharmaceutical industries on exposure and risk analysis, as well as emergency response planning, preparedness and communication requirements for effective risk management programs. This support has included overall program design, as well as training and auditing for OSHA's Process Safety Management (PSM) rule, and U.S. EPA's Risk Management Planning (RMP) rule.

William Stubblefield

Dr. William Stubblefield is a senior environmental toxicologist with Parametrix, Inc. in Corvallis, Oregon. He also holds a courtesy faculty appointment in the Department Molecular and Environmental Toxicology at Oregon State University. Dr. Stubblefield has a Ph.D. in Environmental Toxicology from the University of Wyoming, a M.S. degree in Toxicology/Toxicodynamics from the University of Kentucky, and a B.S. in Biology from Eastern Kentucky University.

Dr. Stubblefield has more than 15 years of experience in environmental toxicology, ecological risk assessment, water quality criteria derivation, and aquatic and wildlife toxicology studies. He has authored more than 50 peer-reviewed publications and technical presentations in the areas of aquatic and wildlife toxicology and environmental risk assessment. He is a co-editor of a recently published book entitled, "Re-evaluation of the State of the Science for Water Quality Criteria," that specifically examines the issues and approaches to be used in the evaluation of environmental impacts associated with contaminants in multiple media. Dr. Stubblefield's research efforts have looked at the fate and effects of metal and hydrocarbon contaminants in the environment and the relationships between these contaminants in the water/sediment/soil compartments.

He has also investigated food chain concerns through research efforts such as the investigation of metals transfer in resident aquatic and terrestrial organisms on Alaska's North Slope. His most recent research uses a combination of laboratory and field

methods to investigate the effects of storm water-associated short-term pulse exposures of metals to aquatic organisms and examines the fate and disposition of storm water-associated metals in natural systems.

About 70% of Parametrix projects are funded by municipal and other government agencies the remainder are industrial clients. Funding for the majority of Dr. Stubblefield's metal related work comes from industrial trade associations or not-for-profit research organizations working in cooperation with U.S. EPA. Dr. Stubblefield is an active member of the Society of Environmental Toxicology and Chemistry, where he serves as the Society's vice-president, member of the Board of Directors, chairman of the Publications Advisory Council, chairman of the Metals Advisory Group, past member of the Editorial Board for Environmental Toxicology and Chemistry, and 2002 annual meeting co-chair. He has been an invited participant at a number of scientific and regulatory conferences, served on U.S. EPA peer-review panels, and frequently acts as a technical reviewer for a number of scientific publications.

Thomas L. Theis

Professor Theis is Professor of Civil and Materials Engineering and Director of the Institute for Environmental Science and Policy at University of Illinois at Chicago, a center that focuses on the development of new cross-disciplinary research initiatives in the environmental area. He was most recently at Clarkson University, where he was the Bayard D. Clarkson Professor and Director of the Center for Environmental Management.

Professor Theis received his doctoral degree in environmental engineering, with a specialization in environmental chemistry, from the University of Notre Dame. His areas of expertise include the mathematical modeling and systems analysis of environmental processes, the environmental chemistry of trace organic and inorganic substances, interfacial reactions, subsurface contaminant transport, hazardous waste management, industrial pollution prevention, and industrial ecology. He has been principal or co-principal investigator on over forty funded research projects totaling in excess of eight million dollars, and has authored or co-authored over one hundred papers in peer reviewed research journals, books, and reports.

He is a member of the U.S. EPA Science Advisory Board (Environmental Engineering Committee), is past editor of the Journal of Environmental Engineering, and serves on the editorial boards of The Journal of Contaminant Transport, and Issues in Environmental Science and Technology. From 1980-1985 he was the co-director of the Industrial Waste Elimination Research Center (a collaboration of Illinois Institute of Technology and University of Notre Dame), one of the first Centers of Excellence established by the U.S. EPA. In 1989 he was an invited participant on the United Nations' Scientific Committee on Problems in the Environment (SCOPE) Workshop on Groundwater Contamination, and in 1998 he was invited to by the World Bank to assist in the development of the first environmental engineering program in Argentina. Among his current projects is the Environmental Manufacturing Management Program, one of

the Integrative Graduate Education Research and Training (IGERT) grants of the National Science Foundation, which involves research on industrial pollution prevention problems emphasizing a systems approach.

Louis Thibodeaux

Louis Joseph Thibodeaux is currently the Jesse Coates Professor in the Gordon A. and Mary Cain Department of Chemical Engineering, College of Engineering, Louisiana State University, Baton Rouge, LA. His terminal degree is a Ph.D. in chemical engineering and presently his teaching, research and service is dominated by the field of environmental chemodynamics, or chemical fate and transport in multimedia compartments of the natural environment. Current areas of research expertise include chemical release processes to water from sediment beds and to air from soil-like dredged materials as well as chemical releases to water and air from environmental dredging activities. The key area of educational expertise is the textbook entitled: ENVIRONMENTAL CHEMODYNAMICS in its 2nd Edition, published by J. Wiley(NY) in 1996. It is used by practitioners worldwide and by numerous universities in engineering, environmental chemistry, geosciences and other environment oriented academic departments. He is the Emeritus Director of the U.S. EPA funded South and Southwest Hazardous Substance Research Center, headquartered at LSU and Directed by Danny D. Reible.

Professor Thibodeaux has served on advisory committees for the U.S. EPA, U.S. ACE, DOD, DOE, NRC and the private sector; all being related to environmental chemodynamic issues. He is a member of the Environmental Division of the American Chemical Society, the Society of Environmental Toxicology and Chemistry, and the Environmental Division of the American Institute of Chemical Engineers.

Professor Thibodeaux is fully employed by LSU doing research and teaching both graduate and undergraduate students. He also serves on the editorial board of several environmental journals and is presently receiving grant and/or contract support on four research projects from the U.S. EPA and the U.S. ACE. He receives research project funds through the cooperative agreement U.S. EPA/LSU in the S/SW Haz. Res. Ctr., ORD, Wash, DC. He also receives research funds from the U.S. Army Corps of Engineers for the ERDC or Waterway Experiment Station, Vicksburg, MS.

Curtis Travis

Dr. Curtis Travis has more than 25 years experience in the energy and environmental business sector and has published widely in the areas of environmental policy, molecular biology, and risk analysis. He holds a B.S. and M.S. in Mathematics from California State University (Fresno) and earned a Ph.D. in Applied Mathematics from the University of California (Davis). He is an internationally recognized expert in the field of risk analysis, and was the founding Director of the Center for Risk Management at Oak Ridge National Laboratory, where he was employed for 18 years.

He has worked in many areas of risk analysis including multimedia modeling, food chain uptake, pharmacokinetics, interspecies extrapolation, dose-response, and risk policy. Recently, he has worked on the cleanup of DOE hazardous waste sites, risk assessment for antimicrobial drug use in animals, and security issues related to food infrastructure in the United States.

Dr. Travis has authored over 270 publications, 8 books, and is on the editorial board of seven international journals. He has served on numerous National Academy of Science panels and governmental and private advisory boards. He is a past President and Fellow of the International Society of Risk Analysis and served as Editor-in-Chief of *Risk Analysis: An International Journal* for 17 years. Dr. Travis is a private consultant with his own firm, Quest Technologies. Almost all his work is for government agencies: the Department of Energy, the Food and Drug Administration, and the Department of Agriculture. He has received no financial support from EPA in the past 10 years, other than in a review capacity.

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