PEER REVIEW OF EPA'S HAZARDOUS WASTE IDENTIFICATION RULE RISK ASSESSMENT MODEL

The Vadose Zone and Saturated Zone Modules
Extracted From EPACMTP for HWIR99

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NOTE

This report was prepared by Eastern Research Group, Inc. (ERG), an EPA contractor, under Contract Number 68-W-99-001. The report presents comments provided by peer reviewers on the *Vadose Zone and Saturated Zone Modules Extracted From EPACMTP for HWIR99* document that is part of EPA's Hazardous Waste Identification Rule risk assessments.

The comments presented in this report have been compiled by topic and by individual peer reviewer. As EPA requested, this report provides the peer review comments exactly as they were submitted to ERG. Also attached are the original comments submitted by each individual reviewer.

PEER REVIEW - GROUNDWATER MODULES

A. INTRODUCTION AND BACKGROUND

The U.S. Environmental Protection Agency (EPA) identifies under Subtitle of C of the Resource Conservation and Recovery Act (RCRA) hazardous wastes that pose threat to human health and the environment. Wastes applicable under the Hazardous Waste Identification Rule (HWIR) were those designated as hazardous because they were listed, or had been mixed with, derived from, or contained the listed wastes. Under the HWIR proposal, waste generators of listed wastes that could meet the new exemption-level criteria defined by the HWIR methodology, would no longer be subject to the hazardous waste management system requirements specified under Subtitle C of RCRA for those wastes. Basically, this would establish a risk-based “floor” for low risk hazardous wastes that would encourage pollution prevention, waste minimization, and the development of innovative waste treatment technologies. The purpose of the rulemaking is to reduce possible over-regulation arising from the older “mixture” and “derived-from” rules promulgated earlier. The Office of Solid Waste of EPA, in cooperation with the Office of Research and Development of EPA, is working on a risk assessment approach for the identification of hazardous wastes. The Agency is developing a multimedia, mutipathway, and multireceptor risk assessment approach for identifying wastes based on constituent-specific exit levels for low risk hazardous wastes.

The “mixture” rule and the “derived-from” rule were promulgated as part of the first comprehensive regulatory program for the management of hazardous wastes under RCRA in May of 1980. The mixture rule defined as a hazardous waste any solid waste that is mixed with one or more listed hazardous wastes, and the derived-from rule labeled as hazardous waste any solid waste generated from the treatment, storage, or disposal of a listed hazardous waste. Both rules were are considered important definitions in regulating the disposal of hazardous wastes consistent with reducing risk to human health and the environment; however, since they apply regardless of the concentration or mobility of hazardous constituents associated with the solid wastes, the potential for over-regulation is a possibility. One of the primary purposes of HWIR is to provide a risk-based methodology for identifying possible instances of over-regulation, and to provide an avenue for safe relief from the Subtitle C disposal regulations as appropriate.

Some aspects of the HWIR methodology have been under development for a number of years. The Toxicity Characteristics (TC) Rule promulgated in 1990 focused on the ground water/drinking-water exposure route to humans. The Agency used EPA’s Composite Model for Landfills (EPACML), a subsurface fate and transport model, for the TC Rule. In 1995, the Agency proposed a multimedia risk analysis approach as part of HWIR. In this approach groundwater and the non-groundwater pathways were not fully integrated. However, The EPA’s Composite for Leachate Migration with transformation products (EPACMTP), an updated version of EPACML, was used for the groundwater analyses for HWIR95. The EPACMTP has undergone numerous reviews, including one by EPA’s Science Advisory Board (SAB). The overall HWIR95 approach, including the non-groundwater pathway analyses approach, were reviewed by the SAB. The Agency also received numerous comments from the public on the HWIR95.

The Agency has developed an integrated multimedia, multipathway, and multireceptor risk assessment (3MRA) approach. The 3MRA approach is based on the regional site-based Monte Carlo approach developed for EPACMTP. The approach is fairly comprehensive, is implemented on a nationwide basis and requires large computer simulation time. Therefore, the Agency had to make numerous simplifications for practical purposes. For the 3MRA model, the Agency has extracted the three-dimensional solution from the EPACMTP for the saturated zone and modified it so that we also have a pseudo-three-dimensional version for the purpose of enhancing the computational efficiency. The pseudo-three-dimensional version is based on a hybrid solution which consists of a one-dimensional numerical solution in the longitudinal dimension (x-direction) and analytical solutions in the other two dimensions. The Agency is particularly interested in the evaluation of these modules for use in HWIR99, given the limitations of both the court-ordered schedule and the state-of-the-science.

B. MATERIALS OFFERED FOR REVIEW

Materials to be Reviewed According to the Charge:

US EPA, 1999. The Vadose Zone and Saturated Zone Modules Extracted From EPACMTP for HWIR99.

Supporting Documents for information Purposes:

1. **EPA**'s **C**omposite **M**odel for Leachate Migration with **T**ransformation **P**roducts (EPACMTP):

a) US EPA, 1996. EPACMTP Background Document, Washington, DC 20460.
b) US EPA, 1997. EPACMTP User's Guide, Washington, DC 20460.
c) US EPA, 1996. EPACMTP Background Document for Finite Source Methodology for Chemicals with Transformation Products, Washington, DC 20460.
d) US EPA, 1996. EPACMTP Background Document for Metals, Washington, DC 20460.
e) US EPA, 1997. Test and Verification of EPACMTP, Washington, DC 20460.
f) SAB Report: Review of EPA's Composite Model for Leachate Migration with Transformation Products - EPACMTP. Prepared by the OSWER Exposure Model Subcommittee of the Environmental Engineering Committee, Science Advisory Board, Washington, D.C. EPA-SAB-EEC-95-010, August, 1995.
g) Response to the SAB Report: "Review of EPA's Composite Model for Leachate Migration with Transformation Products - EPACMTP. Prepared by the OSWER Exposure Model Subcommittee of the Environmental Engineering Committee, Science Advisory Board, Washington, D.C. EPA-SAB-EEC-95-010, August, 1995."
h) US EPA, 1998. A Study to Assess the Impact of Fractured Media in Monte-Carlo Simulations, Washington, D.C. 20460.
i) US EPA, 1999. Incorporation of Heterogeneity into Monte Carlo fate and transport simulations. Washington, D.C. 20460.
j) US EPA, 1997. Implementation of the Vapor-Phase Migration Simulation Module for the EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP). Washington, D.C. 20460.

C. CHARGE TO THE REVIEW PANEL

As stated earlier that the intended purpose of HWIR99 is to provide a generic national-level risk assessment tool to determine which wastes are most appropriately handled in Federal-regulated, hazardous waste management units (Subtitle C) and which wastes should be handled in State-regulated non-hazardous waste management units (Subtitle D). The review panelists should focus their efforts on providing informed answers to the questions posed below, with specific recommendations for improvements identified that are practical and implementable within about six months, if at all possible.

In so doing, it is asked that each panelist address the following component aspects of the general questions:

1) Are the vadose zone and saturated modules extracted from the EPACMTP reasonable for use in the HWIR Multimedia, Multipathway and Multireceptor model for nation-wide implementation? Is the mathematical formulation and the solution of the pseudo three-dimensional saturated zone module appropriate for use in the 3MRA model?

2) Is the pseudo-three dimensional module reasonably verified for practical purposes? Will the results derived using the pseudo three-dimensional version of the module be practically reasonable with the Monte Carlo framework for a nation-wide implementation of the model for the protection of human health and the environment?

3) The full version of EPACMTP can simulate the vapor transport of volatile chemical constituents. However, this feature is not included in the current version of the model to be used for HWIR. This simplification is based on results from the preliminary Monte Carlo simulation runs which indicate that the effects of volatilization on the concentrations of contaminants in ground water on a nation-wide basis are relatively negligible to small. This simplification helps in satisfying the computational efficiency requirements for thousands of simulations of the model needed for Monte Carlo runs. Is it reasonably justifiable to make this simplification in order to implement the model without utilizing the volatilization using the Monte Carlo analysis technique in the HWIR framework?

4) Is the representation of flow and transport through fractured media by using the equivalent hydraulic conductivity approach justifiable for a model which is implemented on a nationwide basis using the Monte Carlo approach?

5) Is the technical approach planned to be used for factoring in the effects of heterogeneities in aquifers on the subsurface flow and transport of chemical constituents adequate using the Monte Carlo procedure?

Reviewer Comments Summary Report for the Vadose Zone and Saturated Zone Modules Extracted From EPACMTP for HWIR99

General Comments:

Dr. Mendoza: The above report, produced by HydroGeologic, Inc., for the U.S. EPA in August 1999, was reviewed with respect to a number of specific question put to the review panel. These questions are addressed individually below. A number of supporting documents were supplied for background information. They are listed in an appendix.

This review is offered from the perspective of a contaminant hydrogeologist who specializes in developing conceptual models and implementing numerical and analytical solution techniques to solve such models. The reviewer is not a toxicologist and does not have any specialized knowledge of nonlinear isotherms or decay models for metals. The review deals only with the concepts and reported implementation contained in the primary report. The actual code has been neither examined nor tested. Furthermore, the databases to be used for Monte Carlo simulations have not been examined.

EPACMTP refers to the EPA's Composite Model for Leachate Migration with Transformation Products. HWIR99 refers to the 1999 version of the Hazardous Waste Identification Rule. The significant differences between HWIR99 and earlier versions of the HWIR are not apparent from the material provided for review; however, it appears that the primary objectives of this work were to produce a subsurface transport model that is far more efficient and considers more processes than previous models (e.g., EPACML). The actual mode of application of the EPACMTP model is somewhat unclear from the supplied material; however, it has been assumed that the model will be used to evaluate a wide number of possible scenarios to determine the maximum source concentration that should be permitted for each of a large number of different contaminants.

The subject report is very well written and documented. There are very few glaring errors and most statements are justified with evidence. With a few exceptions, discussed below, this methodology should be applicable to the proposed usage for HWIR99.

Charge 1a: *Are the vadose zone and saturated modules extracted from the EPACMTP reasonable for use in the HWIR Multimedia, Multipathway and Multireceptor model for nation-wide implementation?*

Dr. Forster: Yes, both the vadose zone and saturated modules extracted from the EPACMTP 3MRA model seem reasonable for use in the HWIR model for nation-wide implementation.

Dr. Hossain: The vadose and saturated zone modules appear to be properly extracted from EPACMTP. This conclusion is based upon reviews of the mathematical formulations and the comparative study presented.

The modules extracted can be considered reasonable for use in HWIR multimedia, multipathway, and multireceptor model for nation-wide implementation. However, a discussion on HWIR99 leading to the need for the development of this new model is needed.

Dr. Mendoza: In general, yes. The apparent practical requirements for the subsurface flow and transport models are that they be computationally fast, yet conceptually rigorous. In many respects these two requirements are at odds with one another. That is, a conceptually rigorous model would normally be site-specific and explicitly include the effects of heterogeneities. Such models are not normally computationally fast because of the need to include a tremendous amount of detail. However, in this application, where a large number of generic sites are to be considered to provide insight into the gross, average behavior of contaminants under "typical" conditions, the overall conceptual approach is appropriate.

One-dimensional vertical flow is an appropriate representation for gross flow in the unsaturated zone. Problems that might be associated with the unsaturated zone model are that (a) it does not consider the impact of macropores or fractures and (b) it does not include the effects of molecular diffusion. Macropores might lead to focussing of higher concentration water reaching the watertable at a faster rate than the equivalent porous medium approach might predict. Such processes are also neglected in HELP model. However, for steady-state simulations where the source for saturated zone transport is areally distributed, the error associated with this approximation is probably not significant. The neglect of molecular diffusion as a transport mechanism might be more significant in some cases and could be easily implemented. If a landfill were located on low permeability media, molecular diffusion might enhance the flux of contaminants to the saturated zone compared to advection (and hydrodynamic dispersion). Because the molecular diffusion term can simply be added to the dispersion term, there appears to be no good reason to neglect it.

Dr. Schwartz: The modules extracted from EPACMTP are reasonable for use in the HWIR implementation. The modules capture many of the key processes involved with contaminant transport in saturated and unsaturated systems. The methods used in formulating and solving the equations appear robust, yet are sufficiently simple to minimize burdens in using these relatively sophisticated codes. The treatment of the processes and details of the mathematical approach are well documented in various reports. The EPACMTP family of codes has been around long enough to have a good history of verification checks and independent peer reviews. From a modeling perspective, the coupling of the vadose zone and saturated models appears to work well and certainly simplifies the modeling approach.

This review does not look in detail at the various data used in applying the model. The important question is whether the relatively sophisticated model treatment is adequately supported by data. In other words, an elegant model, which might only be supported by mediocre data, overall doesn't provide a net gain in the rigor of the overall analysis. Obviously, other reviewers were concerned about this point, especially in assessing whether the treatment of biodegradation of organic compounds is conservative and/or realistic.

The collection of reports alludes to some validation testing, where model assessments are compared with the known behavior of plumes at real sites. There appears to be some need for additional work to demonstrate that this overall modeling approach can capture the behavior of the differing settings to which it is being applied. Such check in essence validates the modeling approach and the supporting data, as a complete package. For example, it is not clear to me that the vadose zone/aquifer concept reasonably represents all settings in a generic manner.

***Charge 1b**: Is the mathematical formulation and the solution of the pseudo three-dimensional saturated zone module appropriate for use in the 3MRA model?*

Dr. Forster: Yes, for application to homogeneous and unfractured sites (see discussions below).

Dr. Mendoza: Almost. The overall approach of using a product solution is well recognized in the literature. For instance, Domenico [1987] takes a similar approach and the Domenico model is implemented in the U.S. EPA's BioScreen model. The biggest concern with this approach is the definition of the source term. The report goes to great lengths to specify the effective dimension of the source in the *x* (longitudinal) direction. In particular, the possibility of a groundwater divide, due to mounding, is considered. However, the same consideration does not appear to be given to the *y* (transverse) direction. On page D-8 of the report it is stated that a particle originating at the side of the source is *advected* within the horizontal plane using a two-dimensional analytical solution given in Appendix B of a 1996 EPACMTP Background Document. The supporting materials do not include such a solution, so this methodology could not be fully evaluated. Nonetheless, it seems reasonable that the transport mechanisms should include both advection and dispersion in the lateral direction. If the solution does include only advection, this approach should be more fully evaluated for cases where laterally extensive groundwater mounding below the source does occur. If both advection and dispersion are considered, and suitable scenarios are evaluated in the comparison simulations (see below), the approach should be better documented.

Dr. Schwartz: The HWIR99 report explains that the more rigorous treatment for flow and transport in the saturated zone was too computationally intensive for routine applications in Monte Carlo simulations, which prompted an effort to develop a simplified but more efficient approach. The report is vague on the need and justification of the simplifications in the first place. For example, since 1995 when EPACMTP became more commonly used, processor speeds and memories have expanded to the extent that most of us have junked the 1995-type equipment. Are Monte Carlo analyses still out of the question with the newest computers, and has there been a diligent effort to speed up or to optimize the original 3-D approach (e.g., different computers; different compilers; smaller grids; fewer realizations; eliminating some MC calculations by scaling approaches etc)? From a reviewer's point of view, justification for the decision to create a simplified but less accurate module has not been provided. Similarly, it would be useful to provide users with comparative numbers on the efficiency of the various approaches.

Indications are that the formulation of the pseudo three-dimensional model is appropriate for use in the package. If an optimized numerical approach for solving the flow and transport problems is really not practical then the analytical/numerical approach would seem to provide the only viable approach. It is not exactly clear how much speedup has been achieved through the simplifications.

The simplified approach has been successful in meeting the need to speed the code up, yet retain most of the key processes. There have been good ideas implemented here, which overcome the process limitations associated with pure analytical solutions.

Charge 2a: *Is the pseudo-three dimensional module reasonably verified for practical purposes?*

Dr. Forster: I am satisfied that the pseudo three-dimensional module has been reasonably verified for practical purposes.

Dr. Hossain: The three-dimensional transport model can be considered reasonably verified for the simpler test cases presented in Figures A.8-A.17. However, one must not assume that it will be true for all other flow regimes. Further, the document must also explain the underestimation of the peak concentrations by SZM-3D1 in Figures A.8 and A.9, and apparent discontinuities in EPACMTP PCE, TCE, and VC results in Figures A.14, A.15, and A.17, respectively. A verification of the saturated zone flow model for other flow geometry is also needed.

Dr. Mendoza: No. The verification tests for the saturated zone module appear to focus on how well the pseudo-three dimensional solution represents a variety of transport scenarios under simple flow conditions with a constant source size. On the whole, the solution simulates these scenarios reasonably well, although the agreement is not "excellent" (as stated on page 52). It is not clear from the report how well the pseudo-three dimensional module represents cases where significant groundwater mounding occurs below the source. Additional comparisons need to be performed for scenarios where the source landfill is laterally extensive and groundwater mounding is significant. That is, the impact of flow on the transport solution needs to be more fully evaluated.

Dr. Schwartz: The report shows that for a few test cases the module can reproduce results of a more rigorous model with fair to good accuracy. The report probably overstates the quality of the fits obtained in the cross-verification trials.

I think that the verification testing shows the potential of the simplified approach. However, more convincing results are required because in a Monte Carlo framework extreme parameter associations may be created. The main problem is that the cause of the "errors" has not been elucidated in detail. For example, assuming mass to come out of a downstream patch produces an error that affects the timing and perhaps the concentration. One could surmise that larger sources than the one analyzed would have a greater error, while smaller sources might be subject to smaller errors. These conceivably could be worse fits generated for problems that had more of a three-dimensional flow configuration (perhaps higher recharge cases).

I think that more work has to be done in understanding what simplifications create what errors. This knowledge would provide a basis for evaluating the likely performance of the code as it is applied in Monte Carlo situations and to different geographic regions.

***Charge 2b**:* *Will the results derived using the pseudo three-dimensional version of the module be practically reasonable with the Monte Carlo framework for a nation-wide implementation of the model for the protection of human health and the environment?*

Dr. Forster: The results derived using the pseudo three-dimensional version of the module should be practically reasonable for *homogeneous, unfractured sites* if suitable guidance and post-processing environments are provided to the software users. Because enhancements for aquifer heterogeneity and fractured media were developed for the fully 3-dimensional version, additional work is required to finalize the details of their implementation within the pseudo three-dimensional version of the module.

Dr. Hossain: Figure A.18 provides a comparison of the Monte-Carlo results obtained by EPACMTP and pseudo 3-D SZM. An inspection of the figure leads to the conclusion that the application of the pseudo 3-D model approximates the results obtained by the EPACMTP very closely. Therefore, it can be concluded that results obtained by using pseudo 3-D SZM can be considered reasonable with the Monte-Carlo framework. A discussion on Monte-Carlo simulation and how to use model results in the Monte-Carlo simulations is, however, needed.

Dr. Mendoza: If the above concerns with respect to source representation and verification are properly addressed, the proposed pseudo-three dimensional model should adequately represent the gross, average behaviour of a contaminant plume emanating from a landfill. The overall conceptual model is suitable for a screening model and the solution technique is sound for such a model. The question of whether the implementation of the solution technique is *practical*, depends upon the efficiency of the code, the speed or number of the computers it is run on, the number of Monte Carlo simulations necessary, the patience of the personnel involved, etc. It is, however, hard to imagine many more efficient algorithms: the solution needs to represent transport in three-dimensions. Thus, appreciable savings in computational time could only be realized by neglecting daughter products which would allow the use of a very simple analytical solution [c.f., Domenico, 1987]. Such a simplified approach does not seem possible if it is indeed necessary to consider toxic daughter byproducts.

Dr. Schwartz: As stated above, there are positive indications that results using the simplified module would be appropriate. The simplified approach is not always conservative vis-à-vis predictions, but the discrepancies appear to be relatively small. The biggest problem, in my opinion, is that without a clear understanding of the origin of the discrepancies, it is unreasonable to extrapolate from just a few verification trials.

***Charge 3**: The full version of EPACMTP can simulate the vapor transport of volatile chemical constituents. However, this feature is not included in the current version of the model to be used for HWIR. This simplification is based on results from the preliminary Monte Carlo simulation runs which indicate that the effects of volatilization on the concentrations of contaminants in ground water on a nation-wide basis are relatively negligible to small. This simplification helps in satisfying the computational efficiency requirements for thousands of simulations of the model needed for Monte Carlo runs. Is it reasonably justifiable to make this simplification in order to implement the model without utilizing the volatilization using the Monte Carlo analysis technique in the HWIR framework?*

Dr. Forster: At first glance it seems reasonable to neglect the volatilization aspect of EPACMTP when using the Monte Carlo analysis technique in the HWIR framework. In the absence of supporting documentation that describes the input to the simulation runs, however, I am unable to confirm my initial response.

Dr. Hossain: When volatilization is ignored model prediction can be considered conservative and some degree of conservatism is always desired in subsurface transport modeling.

Dr. Mendoza: Yes, for the conceptual model under consideration. Vapour transport may have two, opposing, impacts on subsurface transport: lateral diffusive transport may spread low-levels of contamination over a larger area and volatilization may lead to mass losses to the atmosphere. The conceptual model under consideration is that of contaminant migration from a landfill. For this scenario it is usually appropriate to picture the source as being vertically and laterally confined with respect to vapour transport. That is, a low-permeability cap should prevent significant losses to the atmosphere and limit lateral migration. Neglect of atmospheric losses will be conservative, but not overly so if source concentrations are based on measured values within the landfill. Neglect of diffusive vapour transport may lead to a slight underestimation of concentrations in the lateral direction; however, over long periods of time, such concentrations are likely to be orders of magnitude less than those due to groundwater transport.

Dr. Schwartz: Volatilization has the ability to expedite transport away from the source and effectively increase the footprint of the source. Indications from the 1997 report are that the effects of volatilization are relatively unimportant on a nationwide basis. This finding is reasonable and probably valid as a general conclusion.

I would note, however, that in the modeling approach, transport associated with volatilization is modeled primarily as a diffusion process. The few field studies on this topic suggest that at DNAPL sites there is a component of density-driven flow that significantly overwhelms diffusive-type transport. Migration laterally can be much larger and migration to the water table is more rapid than is the case with dispersion. It still would not likely make a big difference. The overall mass flux in the vapor phase into the saturated zone would likely be small irrespective of the vapor transport mechanism. The main point here is that one analysis probably can't form the basis for doing away with volatile transport. However, my feeling is that the process can be dismissed.

***Charge 4**:* *Is the representation of flow and transport through fractured media by using the equivalent hydraulic conductivity approach justifiable for a model which is implemented on a nationwide basis using the Monte Carlo approach?*

Dr. Forster: The porous media approach proposed for representing flow and transport through fractured media might be justifiable if certain issues are addressed in greater detail than currently found in the documents provided (US EPA, 1999a and 1999b). The EPACMTP code was enhanced to incorporate the presence of fractures at some sites in the Subtitle-D landfill database by developing and assigning hydraulic conductivity multipliers within three classes of fractured rock sites. The absence of the report by Dynamac (1997a, 1997b, 1998), however, leaves me unable to assess the soundness of their approach for defining either the fracture media classes or the multiplicative factors.

Preliminary numerical experiments performed to assess the impact of sites with fractured media (US EPA, 1999b) show the following:

- the software implementation appears to work correctly
- the impact of the multipliers, *as defined*, show negligible impact of increased hydraulic conductivity on peak receptor well concentration

What the numerical experiments fail to show, however, is whether or not the consequences of flow and transport through fractured rock are adequately represented using the porous media approach. This is best accomplished by comparing the results of simulated flow and transport through fractured media to simulations through unfractured, equivalent porous media.

In developing an enhancement to EPACMTP that accounts for heterogeneity the US EPA (1999c) used finely-gridded flow and transport simulations in heterogeneous domains as a testing ground for establishing the validity of their approach. Adopting a similar approach, but using a simulator that accommodates discrete fractures in porous media, would provide an improved basis for justifying the porous media approach and for estimating the range in hydraulic conductivity multipliers that should be considered when dealing with fractured media. The discrete fracture models should be constructed to represent generic fracture systems found in the 126 fractured media sites in the landfill database.

When considering porous media equivalents to fractured media it seems important to distinguish between fractured, low-permeability rock (e.g. crystalline rocks) and fractured, high-permeability rock (e.g. sandstone). If we assume a hypothetical situation where a unit volume of each rock type is cut by exactly the same fracture network (fracture geometry, spacing, orientation, aperture, area, etc. are indistinguishable) then two different hydraulic conductivity multipliers would be anticipated in the equivalent porous media. The multiplier applied to the fractured crystalline rock should be much greater than the multiplier applied to the sandstone. This distinction between generic rock types does not seem to be incorporated in the approach to defining hydraulic multipliers outlined by the US EPA (1999b).

The fractured media enhancement was developed for the fully 3-dimensional version of EPACMTP. Once the multipliers are fully justified, it seems appropriate to use this approach to populate a 3-D gridded model domain with a heterogeneous distribution of hydraulic conductivity values. Yet, the US EPA's strong interest in maximizing computational efficiency has led them to develop a heterogeneity enhancement (US EPA 1999c) that, at present, doesn't seem intended to incorporate the heterogeneous hydraulic conductivity structures that might best represent fractured media. Ultimately, it seems appropriate to integrate the two enhancements.

The fractured media enhancement was developed for the fully 3-dimensional version of EPACMTP, rather than the one-dimensional flow and pseudo 3-dimensional transport version developed for HWIR99. No methodology is proposed for implementing the fractured media enhancement within the pseudo 3-dimensional version. I cannot support the concept of using a porous media equivalent for fractured sites within the pseudo 3-dimensional version of HWIR99 without a clearly defined methodology and the results of supporting numerical experiments.

Dr. Hossain: Flow and contaminant transport modeling, in general, are always challenging. The accuracy of model predictions depends to a large extent on the conceptual model developed by employing field data. Our ability to collect enough field data to develop an accurate conceptual model is always limited. The conceptual model can, at best, be considered an educated guess.

Simulation of flow and transport in fractured media is even more challenging. Equivalent hydraulic conductivity approach is frequently employed for convenience. It can be considered justifiable, if the results of modeling are interpreted in the light of data quality and uncertainty in the model parameter estimation.

Dr. Mendoza: Over long timeframes fractured media should behave in a manner that is similar to “heterogeneous” media, but the effect may be accentuated. Thus, the following discussion on the incorporation of heterogeneities is relevant to this question.

Dr. Schwartz: The approach to simulating fractured rocks involves considering sites of one of three types and adjusting the hydraulic conductivity within the Monte Carlo simulation. The results are more or less obvious namely that there is no change in peak concentration as compared to media without fractures. The plume would move somewhat faster with more or less the same plume shape – giving rise to similar concentrations at the receptor well. The fracturing fundamentally doesn’t do much to alter the transport. This model of fracturing would show important effects when the contaminant parent/daughter degraded with a relatively short half-life.

This simple fracture model likely does not capture the important interaction between the character of the fracturing and the transport. The dispersivity would depend on the geometry of fracturing, along with the retardation factor. Fracture zones might exist that essential channelize flow to the receptor well in worst cases or cause the plume to miss the well under more favorable conditions. I think that considerably more effort will be required if it is essential to add fractures to the analysis. The present analysis is not particularly convincing of its simplicity and lack of realism.

***Charge 5**:* *Is the technical approach planned to be used for factoring in the effects of heterogeneities in aquifers on the subsurface flow and transport of chemical constituents adequate using the Monte Carlo procedure?*

Dr. Forster: Overall, the approach to dealing with heterogeneous aquifers seems reasonable when applied within the fully 3-D version of HWIR99. The proposed approach involves defining a CDF for var*(ln K)* that is ultimately translated into computed variability in receptor well concentration. This seems an elegant solution for maximizing computational efficiency while still attempting to recognize the impact of heterogeneity. I find it disconcerting, however, to discover that only a single-layer (10 m thick) flow and transport model was used as the basis for defining CDFs of var*(ln K)* . From my geologist's perspective it would seem that variability imposed by vertical layering should also be incorporated in the CDFs. Using a single-layer model provides insight only into the variability that might result solely from horizontal flow around lower permeability grid blocks. Repeating the numerical experiments with a multi-layer model, however, would enable the US EPA to assess the potential impact of vertical components of flow around lower permeability grid blocks. Because vertical correlation lengths are likely much smaller than lateral correlation lengths, I suspect that different results might be obtained by incorporating vertical layering. This effort might not be necessary If it can be shown that geological conditions at the landfill sites do not yield thin (less than 1 m thick), discontinuous layers of lower hydraulic conductivity within thin layers of higher conductivity.

Subject to the concerns expressed above, the technical approach seems adequate for factoring in the effects of heterogeneity within the pseudo three-dimensional version of the HWIR99 saturated transport module. Additional numerical experiments are likely required, however, to redefine appropriate CDFs for var*(ln K)* as applied in a 1-dimensional flow context.

Dr. Mendoza: Based on the results of simulations presented in the background documents, the increased dispersion that is attributed to heterogeneities does not appear to have a large impact on the gross results of Monte Carlo simulations. Such increased dispersivities must, of course, increase the uncertainty in the Monte Carlo results. This makes mathematical and physical sense because increased dispersivities, used in this way, simply imply greater uncertainty as to where the plume is located.

The net result of enhancing dispersivities to account for gross heterogeneities is that plumes become more dispersed. This approach is appropriate if the objective is to determine whether or not a particular plume might intersect a well. However, if the objective is to determine the maximum concentration that a well might be subjected to, this approach is not suitable. If this latter scenario is applicable from a toxicological viewpoint, it would be more appropriate to use smaller (i.e., unmodified) dispersivity values and bias the well locations such that they are more likely to intersect the plume. That is, an alternative approach, that would better represent the maximum concentrations that might be found in a well, would be to preferentially locate wells directly downgradient of the source.

Dr. Schwartz: The approach used for representing the effects of heterogeneities needs rethinking and more development work. The theory for this correction-factor approach comes from a July 1999 report on "Incorporation of Heterogeneity into Monte-Carlo Fate and Transport Simulations". This report explains an analysis approach that provides theory to develop a correction-based approach for Monte-Carlo simulations. I have concerns about the analyses presented in that report, the most serious of which I outline as follows.

Dispersion at the macroscopic scale is created by heterogeneity in hydraulic conductivity. There is theory that lets one estimate dispersivity values from the heterogeneous structure of the porous medium – variance in log K and correlation length scale. If you build a heterogeneous field, then macroscale dispersivity is automatically created in the transport. Given that the heterogeneity accounts for macroscale dispersion, the dispersivity value that needs to be defined in the model is the local-scale value, which will be small e.g., 0.1 m. In the 1999 report, both large dispersivity values and heterogeneous medium coexist, which is an important conceptual error. The existence of a dispersivity of say 100 m implies that there is heterogeneity with a correlation length scale of 10s to 100s of meters (depending upon the variance in log K) that is not considered. If in fact big dispersion exists at sites, then big-scale heterogeneity will exist as well; this heterogeneity is not represented in the analysis.

The report does not consider correlation in the hydraulic conductivity field, as is normally represented by a correlation length scale. This treatment implies that the correlation length scale is much smaller than the size of the grid blocks, or 10 m. Thus, the heterogeneity that is being modeled is of small scale, which as expected produced very little impact on the transport. The simulation results with large dispersivity are simply saying that there is a large scale heterogeneity present, which swamps the smaller effects. It makes little sense to effectively include the small-scale heterogeneity and not explicitly consider the more important larger scale.

The analysis that is presented in this report needs to be redone with an appropriate consideration of the role of heterogeneities in dispersion. If it is decided to run simulations with large dispersion (<u>see my note, additional comments</u>), then it will be necessary to include the largest scale heterogeneity and account for the correlation structure in the field. For example, large dispersivity values imply the existence of direct high permeability pathways from a source to a receptor well 100 m away from the site (see e.g., HWIR99). Similarly, high permeability pathways that miss the well will route mass in another direction. Thus the variation in concentrations observed at the receptor well could be huge when these high-permeability pathways exist.

Additional Comments:

Dr. Forster: It is important to note that providing answers to the above questions was complicated by the fact that little information was available to show how the HWIR99 modules are intended to be used in practice. For example, who will actually apply the software? I can imagine that consultants, or in-house staff, working for corporations responsible for cleaning up waste might have a different application approach than staff of federal or state agencies. In any case, the US EPA will ultimately need to provide guidelines for using the HWIR99 modules so that the software user can make intelligent decisions regarding whether or not to use the pseudo 3-dimensional module, what receptor well concentrations would mark the threshold for deciding whether the waste is hazardous or non-hazardous and how to apply the results of heterogeneity and fractured rock modules. A sense of the possible guidelines are inferred from the EPACMTP User's Guide (US EPA, 1997), however, this document was produced before approaches for dealing with heterogeneity and fractured rock were developed.

Dr. Hossain:

Page 4, Paragraph 1, 3rd line:

"This approach is reasonable as long as the height of the mound is ***small relative*** *to the thickness of the saturated zone."*

Comment: The term "small" should be defined.

Page 4, Paragraph 2, 1st line:

"The unsaturated zone is assumed to be initially contaminant-free and contaminants are assumed to migrate vertically downward from the disposal facility."

Comment: Will the unsaturated zone always be free of contaminants initially? If not, the model should be flexible enough to account for any existing contaminants in the unsaturated zone. When the transport equation is solved numerically, such contaminants can be accounted for as initial condition to the model.

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"The aquifer is assumed to be initially contaminant free."

Comment: Will the saturated zone always be free of contaminants initially? If not, the model should be flexible enough to account for any existing contaminants.

Page 4, Paragraph 6, 2nd line:

"For the simulation of metals with non-linear adsorption, both modules utilize sorption isotherms generated by ***MINTEQA2****."*

Comment: The limitations of using MINTEQA2, if there is any, should also be discussed.

Page 6, Unsaturated flow submodule

Comments:

1. Equation 2.1 and the associated boundary conditions are appropriate. Utilization of Mualem-van Genuchten model, to simulate permeability-water content relation, is also appropriate.

   However, a discussion on the parameter estimation for the van Genuchten model would be of help to the users.

2. The non-linear flow equation was solved by combined Newton-Raphson and bi-section method.

   The combined Newton-Raphson and bisection method should guarantee convergence. A discussion on convergence of the solution method, however, may be needed to educate the users.

<u>*Page 7, Unsaturated Transport submodule*</u>

Comments:

1. Equation 2.6 and the associated boundary conditions should simulate the 1-D transport adequately. However, the inability of the model to account for initial condition remains to be a concern. Furthermore, a discussion on the ability of MINTEQA2 speciation model to provide metal isotherm data may be considered necessary.

2. Transport equation has been solved by the method of upwind finite elements. It is essential to discuss the effect of upwinding on model predictions. Artificial dispersion associated with upwinding can be significant under certain conditions. The user must be helped to understand the effect of upwinding on model predictions.

3. The effect of varying time step on model predictions should also be discussed.

<u>*Page 9, Infiltration and contaminant mass fluxes:*</u>

Comment: Annual average may not be a conservative approach.

<u>*Page 11, Organic constituents*</u>

Comment: Limitation of utilizing organic carbon distribution coefficient in defining adsorption characteristics should be discussed.

<u>Page 17, Paragraph 2, 2nd line</u>
"The initial contaminant concentration is set to zero."

Comment: It may not always be the case.

<u>Page 18, Figure 3.1</u>

Comment: The origin of the co-ordinate axes should lie on the lower bounding plane of the aquifer.

<u>Page 18, Paragraph 2, 5th line</u>
"Nodal spacing in the latter case are automatically assigned based on Peclet number criteria…….."

Comment: The Peclet number criteria should be explained.

Dr. Mendoza: (Editing Oversights)

HWIR99 is not defined.

Figure 3.1 does not include definitions of x_u and x_d.

In several places the text claims that the saturated zone model can consider both linear and nonlinear sorption processes (e.g., implied last paragraph page 4; stated twice on page 17). From the reviewer's understanding of the numerical method, along with contrary claims elsewhere in the text (e.g., pages 4 and 25), this is not true. The model only considers a linear sorption model in the saturated zone.

It would appear that the source for the saturated zone can only be square. This should be documented.

The termination criterion discussed under Section 3.2.3 implies that the source concentration can only decrease. Is this true?

NTSCRW and NTSFST are not defined in Table 3.3.

The domain discretization is not described in the model validation sections (pages 41 and onward). It is relevant to both the model and independent testing.

The third equation on page D-7 should indicate a range of validity of $x > x_d$, rather than $u > u_d$.

Overall, references to the scientific literature are somewhat sparse.

A reference for equation 2.22 and the evidence that supports its use should be supplied.

A reference or further explanation should be provided for equation D.23 on page D-8.

There a small formatting problems with references in a number of places.

Dr. Schwartz: In the regulatory problem that is being addressed by this modeling effort, there are two processes that make a great difference to dose at the receptor well – dispersion and chemical destruction of contaminants. This conclusion assumes that the well is always hit by the plume. (Not the same assumption as EPACMTP.) Dispersion can thin the mass before it reaches the well and the chemical processes break it down. Because dispersion is operative for all contaminants, it will be a key process in determining the dose from wells. In reading all the documents, it is not clear that there is a consistent and appropriate treatment of dispersion. I'll discuss points in the following section.

Detailed field tracer tests over 100-300 m show that dispersion is a relatively insignificant process. Dispersivity values are often small in sand aquifers (less than 1 m). Larger values obtained in many tests are generally discounted by Gelhar as being overestimates due to errors. Vertical transverse dispersivity is usually small with diffusion-scale numbers. Thus, overall plumes from relatively large sources should not be impacted by dispersion.

Many of the test cases in the present reports are based on appropriate dispersion values (e.g., HWIR99). There are other documents where the dispersivity approach is of concern. The EPACMTP document (1997) (Table 7.5) probably overestimates dispersivity values for travel distances of 150 m. For greater distances, dispersivity values are scaled as a function of travel distance. According to Equation 7.9 (which contains a serious typo) at a distance of 2000 m the longitudinal dispersivity would be about 70 m and the vertical transverse dispersivity would be 0.4 m. These are large values, along with the values used in the Heterogeneity report (July, 1999).

The problem as I see it comes to the distance scaling of dispersivity values. I think if one believes the geostatistical origins of dispersivity, one also ought to believe in a single constant asymptotic dispersivity value that applies to the aquifer. It may take some travel distance (e.g., 10-100 correlation lengths) to reach this dispersivity but eventually it will be attained. For dispersivities to increase constantly along a unit, the correlation structure of the unit would need to keep changing. This might occur but has never been documented. Similarly, there should be no reason to scale vertical transverse dispersivity values. A plume cannot magically assume some capability to spread vertically once it has moved away from the source. In summary, I think that the EPA's thinking on dispersion as applied in this work and elsewhere is wrong.

The Yucca Mountain project looked at far-field modeling for 20 to 30 km away from the repository. Simulations involving modestly large longitudinal values, 100s of meters over the travel distance were scrapped in favor of a stream-tube model that severely minimized the effects of dispersion. My recollection is a factor of 2x or 3x reduction in the source concentration over 20-30 km due to dispersion.

***Recommendations*:**

Dr. Forster:

1. Prepare a brief report outlining the input parameters for, and results of, comparisons between

EPACMTP simulations of plausible landfill sites both with and without accounting for the vapor phase. Submitting this report for review will provide a sound foundation for neglecting vapor transport in the HWIR99 approach.

2. Developers should assess the possible significance of neglecting layered permeability structures when defining CDFs for var*(ln K).* in approximating the impact of aquifer heterogeneity on receptor well concentrations.

3. The proposed enhancement for representing fractured media enhancement requires a comparison of discrete fracture model simulation results to those of equivalent porous media. This effort would help to properly define and justify the hydraulic conductivity multipliers that might be appropriate in different rock types.

4. Heterogeneity imposed by fractured rock should be accounted for in the fully three-dimensional EPACMTP software using an approach that defines CDFs for var*(ln K)* in fractured media.

5. Enhancements for heterogeneity and fractured rock within the pseudo three-dimensional saturated flow module of HWIR99 should not be implemented until new numerical experiments are carried out to show how well the enhancements might work in this context. Although the approach is hopeful, a big step is being made when in reducing the problem from 3-D to 1-D.

Dr. Schwartz:

(a) I think it would be important to revisit the basic concepts of dispersion (see 6.) with a view to producing a more defensible agency stance on this important issue.

(b) The pseudo three-dimensional approaches are promising to make the Monte Carlo analyses more tractable. I would recommend work to optimize the original 3-D code to see whether limitations of 1995 have perhaps gone away with more powerful compilers and computers. It is not clear that the compiler being used is by any means the fastest one around.

If the pseudo three-dimensional approach is followed, it will be necessary to know more precisely where the deviations are being produced. Knowing more about the error will enable one to evaluate the extent of errors produced in a Monte Carlo analysis. The work on this topic so far has been necessary but not sufficient.

(c) The analyses of heterogeneities and fractures are wrong and simplistic, respectively. If it is felt that these features need to be considered in the complete evaluation, then more work will be necessary. I think the progress in dispersion [recommendation (a)] will contribute to the understanding of the impact of heterogeneities. If one needs to choose between the two, I would suggest work on heterogeneities.

References:

Dr. Forster:
Dynamac, 1997a. Interim Report on the ORD-OSW HWIR Science Plan. July 6, 1997.

Dynamac, 1997b. faxed Correspondence from Dr. Sam Lee of Dynamac Forp. to Dr. Zubair Saleem, US EPA-OSW. June 24, 1997.

Dynamac, 1998. Impact of Fracture and Heterogeneity on the Hazardous Waste Identification Rule, Draft version. Prepared for NRMRL/SPRD by Dynamac Corp. Ada, OK. March 30, 1998.
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US EPA, 1999b, A Study to Assess the Impacts of Fractured Media in Monte-Carlo Simulations. U.S. Environmental Protection Agency, Office of Solid Waste, Washington, D.C.

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US EPA, 1996, EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP), Background Document. U.S. Environmental Protection Agency, Office of Solid Waste, Washington, D.C.

Dr. Mendoza:
Domenico, 1987. An analytical model for multidimensional transport of a decaying contaminant species. Journal of Hydrology, 91(1987), 49-58.

ATTACHMENT A

Peer Review of "Vadose Zone and Saturated Zone Modules Extracted From EPACMTP for HWIR99" by:

Craig Forster
University of Utah

ERG Task No. 17
Contract No. 68-W-99-001
Peer Review of EPA's HWIR Risk Assessment Methodology

November 22, 1999

Craig B. Forster
University of Utah

INTRODUCTION

As requested, I have reviewed the document "The Vadose and Saturated Zone Modules Extracted from EPACMTP for HWIR99" prepared for the US EPA by HydroGeologic, Inc. (US EPA, 1999a). In performing this review I also found it necessary to work extensively with additional documents provided in the review packet (US EPA, 1996, 1999a, 1999b and 1999c). Other documents in the packet were also used, but to much lesser degree.

The "Charge to the Review Panel" states that the intended purpose of HWIR99 is to provide a generic national-level risk assessment tool to determine which wastes are most appropriately handled in Federal-regulated, hazardous waste management units (Subtitle C) and which wastes should be handled in State-regulated non-hazardous waste management units (Subtitle D). My review is presented primarily as a set of answers to the questions posed in the "Charge to the Review Panel" and outlined in the following sections.

QUESTION 1

Are the vadose zone and saturated modules extracted from the EPACMTP reasonable for use in the HWIR Multimedia, Multipathway and Multireceptor model for nation-wide implementation?

Yes, both the vadose zone and saturated modules extracted from the EPACMTP 3MRA model seem reasonable for use in the HWIR model for nation-wide implementation.

Is the mathematical formulation and the solution of the pseudo three-dimensional saturated zone module appropriate for use in the 3MRA model?

Yes, for application to homogeneous and unfractured sites (see discussions below).

QUESTION 2

Is the pseudo three-dimensional module reasonably verified for practical purposes?

I am satisfied that the pseudo three-dimensional module has been reasonably verified for practical purposes.

Will the results derived using the pseudo three-dimensional version of the module be practically reasonable with the Monte Carlo framework for a nation-wide implementation of the model for the protection of human health and the environment?

The results derived using the pseudo three-dimensional version of the module should be practically reasonable for *homogeneous, unfractured sites* if suitable guidance and post-processing environments are provided to the software users. Because enhancements for aquifer heterogeneity and fractured media were developed for the fully 3-dimensional version, additional work is required to finalize the details of their implementation within the pseudo three-dimensional version of the module.

QUESTION 3

The full version of EPACMTP can simulate the vapor transport of volatile chemical constituents. However, this feature is not included in the current version of the model to be used for HWIR. This simplification is based on results from the preliminary Monte Carlo simulation runs which indicate that the effects of volatilization on the concentrations of contaminants in ground water on a nation-wide base are relatively negligible to small. This simplification helps in satisfying the computational efficiency requirements for thousands of simulations of the model needed for Monte Carlo runs. Is it reasonably justifiable to make this simplification in order to implement the model without utilizing the volatilization using the Monte Carlo analysis technique in the HWIR framework?

At first glance it seems reasonable to neglect the volatilization aspect of EPACMTP when using the Monte Carlo analysis technique in the HWIR framework. In the absence of supporting documentation that describes the input to the simulation runs, however, I am unable to confirm my initial response.

QUESTION 4

Is the representation of flow and transport through fractured media by using the equivalent hydraulic conductivity approach justifiable for a model which is implemented on a nationwide basis using the Monte Carlo approach?

The porous media approach proposed for representing flow and transport through fractured media might be justifiable if certain issues are addressed in greater detail than currently found in the documents provided (US EPA, 1999a and 1999b). The EPACMTP code was enhanced to incorporate the presence of fractures at some sites in the Subtitle-D landfill database by developing and assigning hydraulic conductivity multipliers within three classes of fractured rock sites. The absence of the report by Dynamac (1997a, 1997b, 1998), however, leaves me unable to assess the soundness of their approach for defining either the fracture media classes or the multiplicative factors.

Preliminary numerical experiments performed to assess the impact of sites with fractured media (US EPA, 1999b) show the following:

- the software implementation appears to work correctly
- the impact of the multipliers, *as defined*, show negligible impact of increased hydraulic conductivity on peak receptor well concentration

What the numerical experiments fail to show, however, is whether or not the consequences of flow and transport through fractured rock are adequately represented using the porous media approach. This is best accomplished by comparing the results of simulated flow and transport through fractured media to simulations through unfractured, equivalent porous media.

In developing an enhancement to EPACMTP that accounts for heterogeneity the US EPA (1999c) used finely-gridded flow and transport simulations in heterogeneous domains as a testing ground for establishing the validity of their approach. Adopting a similar approach, but using a simulator that accommodates discrete fractures in porous media, would provide an improved basis for justifying the porous media approach and for estimating the range in hydraulic conductivity multipliers that should be considered when dealing with fractured media. The discrete fracture models should be constructed to represent generic fracture systems found in the 126 fractured media sites in the landfill database.

When considering porous media equivalents to fractured media it seems important to distinguish between fractured, low-permeability rock (e.g. crystalline rocks) and fractured, high-permeability rock (e.g. sandstone). If we assume a hypothetical situation where a unit volume of each rock type is cut by exactly the same fracture network (fracture geometry, spacing, orientation, aperture, area, etc. are indistinguishable) then two different hydraulic conductivity multipliers would be anticipated in the equivalent porous media. The multiplier applied to the fractured crystalline rock should be much greater than the multiplier applied to the sandstone. This distinction between generic rock types does not seem to be incorporated in the approach to defining hydraulic multipliers outlined by the US EPA (1999b).

The fractured media enhancement was developed for the fully 3-dimensional version of EPACMTP. Once the multipliers are fully justified, it seems appropriate to use this approach to populate a 3-D gridded model domain with a heterogeneous distribution of hydraulic conductivity values. Yet, the US EPA's strong interest in maximizing computational efficiency has led them to develop a heterogeneity enhancement (US EPA 1999c) that, at present, doesn't seem intended to incorporate the heterogeneous hydraulic conductivity structures that might best represent fractured media. Ultimately, it seems appropriate to integrate the two enhancements.

The fractured media enhancement was developed for the fully 3-dimensional version of EPACMTP, rather than the one-dimensional flow and pseudo 3-dimensional transport version developed for HWIR99. No methodology is proposed for implementing the fractured media enhancement within the pseudo 3-dimensional version. I cannot support the concept of using a porous media equivalent for fractured sites within the pseudo 3-dimensional version of HWIR99 without a clearly defined methodology and the results of supporting numerical experiments.

QUESTION 5

Is the technical approach planned to be used for factoring in the effects of heterogeneities in aquifers on the subsurface flow and transport of chemical constituents adequate using the Monte Carlo procedure?

Overall, the approach to dealing with heterogeneous aquifers seems reasonable when applied within the fully 3-D version of HWIR99. The proposed approach involves defining a CDF for var*(ln K)* that is ultimately translated into computed variability in receptor well concentration. This seems an elegant solution for maximizing computational efficiency while still attempting to recognize the impact of heterogeneity. I find it disconcerting, however, to discover that only a single-layer (10 m thick) flow and transport model was used as the basis for defining CDFs of var*(ln K)* . From my geologist's perspective it would seem that variability imposed by vertical layering should also be incorporated in the CDFs. Using a single-layer model provides insight only into the variability that might result solely from horizontal flow around lower permeability grid blocks. Repeating the numerical experiments with a multi-layer model, however, would enable the US EPA to assess the potential impact of vertical components of flow around lower permeability grid blocks. Because vertical correlation lengths are likely much smaller than lateral correlation lengths, I suspect that different results might be obtained by incorporating vertical layering. This effort might not be necessary If it can be shown that geological conditions at the landfill sites do not yield thin (less than 1 m thick), discontinuous layers of lower hydraulic conductivity within thin layers of higher conductivity.

Subject to the concerns expressed above, the technical approach seems adequate for factoring in the effects of heterogeneity within the pseudo three-dimensional version of the HWIR99 saturated transport module. Additional numerical experiments are likely required, however, to redefine appropriate CDFs for var*(ln K)* as applied in a 1-dimensional flow context.

ADDITIONAL COMMENTS

It is important to note that providing answers to the above questions was complicated by the fact that little information was available to show how the HWIR99 modules are intended to be used in practice. For example, who will actually apply the software? I can imagine that consultants, or in-house staff, working for corporations responsible for cleaning up waste might have a different application approach than staff of federal or state agencies. In any case, the US EPA will ultimately need to provide guidelines for using the HWIR99 modules so that the software user can make intelligent decisions regarding whether or not to use the pseudo 3-dimensional module, what receptor well concentrations would mark the threshold for deciding whether the waste is hazardous or non-hazardous and how to apply the results of heterogeneity and fractured rock modules. A sense of the possible guidelines are inferred from the EPACMTP User's Guide (US EPA, 1997), however, this document was produced before approaches for dealing with heterogeneity and fractured rock were developed.

RECOMMENDATIONS

1. Prepare a brief report outlining the input parameters for, and results of, comparisons between EPACMTP simulations of plausible landfill sites both with and without accounting for the vapor phase. Submitting this report for review will provide a sound foundation for neglecting vapor transport in the HWIR99 approach.

2. Developers should assess the possible significance of neglecting layered permeability structures when defining CDFs for var*(ln K).* in approximating the impact of aquifer heterogeneity on receptor well concentrations.

3. The proposed enhancement for representing fractured media enhancement requires a comparison of discrete fracture model simulation results to those of equivalent porous media. This effort would help to properly define and justify the hydraulic conductivity multipliers that might be appropriate in different rock types.

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5. Enhancements for heterogeneity and fractured rock within the pseudo three-dimensional saturated flow module of HWIR99 should not be implemented until new numerical experiments are carried out to show how well the enhancements might work in this context. Although the approach is hopeful, a big step is being made when in reducing the problem from 3-D to 1-D.

REFERENCES

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ATTACHMENT B

Peer Review of "Vadose Zone and Saturated Zone Modules Extracted From EPACMTP for HWIR99" by:

Akram Hossain
Washington State University

Review
Of
The Vadose and Saturated Zone Modules Extracted from EPACMTP for HWIR99

By
Md. Akram Hossain
Assistant Professor
Civil and Environmental Engineering
Washington State University
2710 University Drive
Richland, WA 99352

COMMENTS ON APPLICABILITY AND UTILITY OF THE MODEL

1. The vadose and saturated zone modules appear to be properly extracted from EPACMTP. This conclusion is based upon reviews of the mathematical formulations and the comparative study presented.

   The modules extracted can be considered reasonable for use in HWIR multimedia, multipathway, and multireceptor model for nation-wide implementation. However, a discussion on HWIR99 leading to the need for the development of this new model is needed.

2. The three-dimensional transport model can be considered reasonably verified for the simpler test cases presented in Figures A.8-A.17. However, one must not assume that it will be true for all other flow regimes. Further, the document must also explain the underestimation of the peak concentrations by SZM-3D1 in Figures A.8 and A.9, and apparent discontinuities in EPACMTP PCE, TCE, and VC results in Figures A.14, A.15, and A.17, respectively. A verification of the saturated zone flow model for other flow geometry is also needed.

   Figure A.18 provides a comparison of the Monte-Carlo results obtained by EPACMTP and pseudo 3-D SZM. An inspection of the figure leads to the conclusion that the application of the pseudo 3-D model approximates the results obtained by the EPACMTP very closely. Therefore, it can be concluded that results obtained by using pseudo 3-D SZM can be considered reasonable with the Monte-Carlo framework. A discussion on Monte-Carlo simulation and how to use model results in the Monte-Carlo simulations is, however, needed.

3. When volatilization is ignored model prediction can be considered conservative and some degree of conservatism is always desired in subsurface transport modeling.

4. Flow and contaminant transport modeling, in general, are always challenging. The accuracy of model predictions depends to a large extent on the conceptual model developed by employing field data. Our ability to collect enough field data to develop an accurate conceptual model is always limited. The conceptual model can, at best, be considered an educated guess.
   Simulation of flow and transport in fractured media is even more challenging.

Equivalent hydraulic conductivity approach is frequently employed for convenience. It can be considered justifiable, if the results of modeling are interpreted in the light of data quality and uncertainty in the model parameter estimation.

GENERAL COMMENTS

Page 4, Paragraph 1, 3rd line:
"This approach is reasonable as long as the height of the mound is ***small relative*** *to the thickness of the saturated zone."*

Comment: The term "small" should be defined.

Page 4, Paragraph 2, 1st line:
"The unsaturated zone is assumed to be initially contaminant-free and contaminants are assumed to migrate vertically downward from the disposal facility."

Comment: Will the unsaturated zone always be free of contaminants initially? If not, the model should be flexible enough to account for any existing contaminants in the unsaturated zone. When the transport equation is solved numerically, such contaminants can be accounted for as initial condition to the model.

Page 4, Paragraph 3, 1st line:
"The aquifer is assumed to be initially contaminant free."

Comment: Will the saturated zone always be free of contaminants initially? If not, the model should be flexible enough to account for any existing contaminants.

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"For the simulation of metals with non-linear adsorption, both modules utilize sorption isotherms generated by ***MINTEQA2****."*

Comment: The limitations of using MINTEQA2, if there is any, should also be discussed.

Page 6, Unsaturated flow submodule

Comments:

1. Equation 2.1 and the associated boundary conditions are appropriate. Utilization of Mualem-van Genuchten model, to simulate permeability-water content relation, is also appropriate.

   However, a discussion on the parameter estimation for the van Genuchten model would be of help to the users.

2. The non-linear flow equation was solved by combined Newton-Raphson and bi-section method.

   The combined Newton-Raphson and bisection method should guarantee convergence.

A discussion on convergence of the solution method, however, may be needed to educate the users.

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Comments:

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Comment: Annual average may not be a conservative approach.

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Comment: Limitation of utilizing organic carbon distribution coefficient in defining adsorption characteristics should be discussed.

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"The initial contaminant concentration is set to zero."

Comment: It may not always be the case.

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Comment: The origin of the co-ordinate axes should lie on the lower bounding plane of the aquifer.

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Comment: The Peclet number criteria should be explained.

ATTACHMENT C

Peer Review of "Vadose Zone and Saturated Zone Modules Extracted From EPACMTP for HWIR99" by:

Carl Mendoza
University of Alberta

Technical Review

The Vadose Zone and Saturated Zone Modules Extracted From EPACMTP for HWIR99

Review by:
Carl Mendoza
Earth and Atmospheric Sciences
University of Alberta
Edmonton, Alberta, Canada

December, 1999

Preface

The above report, produced by HydroGeologic, Inc., for the U.S. EPA in August 1999, was reviewed with respect to a number of specific question put to the review panel. These questions are addressed individually below. A number of supporting documents were supplied for background information. They are listed in an appendix.

This review is offered from the perspective of a contaminant hydrogeologist who specializes in developing conceptual models and implementing numerical and analytical solution techniques to solve such models. The reviewer is not a toxicologist and does not have any specialized knowledge of nonlinear isotherms or decay models for metals. The review deals only with the concepts and reported implementation contained in the primary report. The actual code has been neither examined nor tested. Furthermore, the databases to be used for Monte Carlo simulations have not been examined.

EPACMTP refers to the EPA's Composite Model for Leachate Migration with Transformation Products. HWIR99 refers to the 1999 version of the Hazardous Waste Identification Rule. The significant differences between HWIR99 and earlier versions of the HWIR are not apparent from the material provided for review; however, it appears that the primary objectives of this work were to produce a subsurface transport model that is far more efficient and considers more processes than previous models (e.g., EPACML). The actual mode of application of the EPACMTP model is somewhat unclear from the supplied material; however, it has been assumed that the model will be used to evaluate a wide number of possible scenarios to determine the maximum source concentration that should be permitted for each of a large number of different contaminants.

General Comments

The subject report is very well written and documented. There are very few glaring errors and most statements are justified with evidence. With a few exceptions, discussed below, this methodology should be applicable to the proposed usage for HWIR99.

Specific Comments

Each of the specific questions posed to the reviewers, shown in italics, is addressed below.

1a). *Are the vadose zone and saturated modules extracted from the EPACMTP reasonable for use in the HWIR Multimedia, Multipathway and Multireceptor model for nation-wide implementation?*

In general, yes. The apparent practical requirements for the subsurface flow and transport models are that they be computationally fast, yet conceptually rigorous. In many respects these two requirements are at odds with one another. That is, a conceptually rigorous model would normally be site-specific and explicitly include the effects of heterogeneities. Such models are not normally computationally fast because of the need to include a tremendous amount of detail. However, in this application, where a large number of generic sites are to be considered to provide insight into the gross, average behavior of contaminants under "typical" conditions, the overall conceptual approach is appropriate.

One-dimensional vertical flow is an appropriate representation for gross flow in the unsaturated zone. Problems that might be associated with the unsaturated zone model are that (a) it does not consider the impact of macropores or fractures and (b) it does not include the effects of molecular diffusion. Macropores might lead to focussing of higher concentration water reaching the watertable at a faster rate than the equivalent porous medium approach might predict. Such processes are also neglected in HELP model. However, for steady-state simulations where the source for saturated zone transport is areally distributed, the error associated with this approximation is probably not significant. The neglect of molecular diffusion as a transport mechanism might be more significant in some cases and could be easily implemented. If a landfill were located on low permeability media, molecular diffusion might enhance the flux of contaminants to the saturated zone compared to advection (and hydrodynamic dispersion). Because the molecular diffusion term can simply be added to the dispersion term, there appears to be no good reason to neglect it.

1b). *Is the mathematical formulation and the solution of the pseudo three-dimensional saturated zone module appropriate for use in the 3MRA model?*

Almost. The overall approach of using a product solution is well recognized in the literature. For instance, Domenico [1987] takes a similar approach and the Domenico model is implemented in the U.S. EPA's BioScreen model. The biggest concern with this approach is the definition of the source term. The report goes to great lengths to specify the effective dimension of the source in the x (longitudinal) direction. In particular, the possibility of a groundwater divide, due to mounding, is considered. However, the same consideration does not appear to be given to the y (transverse) direction. On page D-8 of the report it is stated that a particle originating at the side of the source is *advected* within the horizontal plane using a two-dimensional analytical solution given in Appendix B of a 1996 EPACMTP Background Document. The supporting materials do not include such a solution, so this methodology could not be fully evaluated. Nonetheless, it seems reasonable that the transport mechanisms should include both advection and dispersion in the lateral direction. If the solution does include only advection, this approach should be more fully evaluated for cases where laterally extensive groundwater mounding below the source does occur. If both advection and dispersion are considered, and suitable scenarios are evaluated in the comparison simulations (see below), the approach should be better documented.

2a). *Is the pseudo-three dimensional module reasonably verified for practical purposes?*

No. The verification tests for the saturated zone module appear to focus on how well the pseudo-three dimensional solution represents a variety of transport scenarios under simple flow conditions with a constant source size. On the whole, the solution simulates these scenarios reasonably well, although the agreement is not "excellent" (as stated on page 52). It is not clear from the report how well the pseudo-three dimensional module represents cases where significant groundwater mounding occurs below the source. Additional comparisons need to be performed for scenarios where the source landfill is laterally extensive and groundwater mounding is significant. That is, the impact of flow on the transport solution needs to be more fully evaluated.

2b). *Will the results derived using the pseudo three-dimensional version of the module be practically reasonable with the Monte Carlo framework for a nation-wide implementation of the model for the protection of human health and the environment?*

If the above concerns with respect to source representation and verification are properly addressed, the proposed pseudo-three dimensional model should adequately represent the gross, average behavior of a contaminant plume emanating from a landfill. The overall conceptual model is suitable for a screening model and the solution technique is sound for such a model. The question of whether the implementation of the solution technique is *practical*, depends upon the efficiency of the code, the speed or number of the computers it is run on, the number of Monte Carlo simulations necessary, the patience of the personnel involved, etc. It is, however, hard to imagine many more efficient algorithms: the solution needs to represent transport in three-dimensions. Thus, appreciable savings in computational time could only be realized by neglecting daughter products which would allow the use of a very simple analytical solution [c.f., Domenico, 1987]. Such a simplified approach does not seem possible if it is indeed necessary to consider toxic daughter byproducts.

3). *The full version of EPACMTP can simulate the vapor transport of volatile chemical constituents. However, this feature is not included in the current version of the model to be used for HWIR. This simplification is based on results from the preliminary Monte Carlo simulation runs which indicate that the effects of volatilization on the concentrations of contaminants in ground water on a nation-wide basis are relatively negligible to small. This simplification helps in satisfying the computational efficiency requirements for thousands of simulations of the model needed for Monte Carlo runs. Is it reasonably justifiable to make this simplification in order to implement the model without utilizing the volatilization using the Monte Carlo analysis technique in the HWIR framework?*

Yes, for the conceptual model under consideration. Vapour transport may have two, opposing, impacts on subsurface transport: lateral diffusive transport may spread low-levels of contamination over a larger area and volatilization may lead to mass losses to the atmosphere. The conceptual model under consideration is that of contaminant migration from a landfill. For this scenario it is usually appropriate to picture the source as being vertically and laterally confined with respect to vapour transport. That is, a low-permeability cap should prevent significant losses to the atmosphere and limit lateral migration. Neglect of atmospheric losses will be conservative, but not overly so if source concentrations are based on measured values within the landfill. Neglect of diffusive vapour transport may lead to a slight underestimation of concentrations in the lateral direction; however, over long periods of time, such concentrations are likely to be orders of magnitude less than those due to groundwater transport.

4). *Is the representation of flow and transport through fractured media by using the equivalent hydraulic conductivity approach justifiable for a model which is implemented on a nationwide basis using the Monte Carlo approach?*

Over long timeframes fractured media should behave in a manner that is similar to "heterogeneous" media, but the effect may be accentuated. Thus, the following discussion on the incorporation of heterogeneities is relevant to this question.

5). *Is the technical approach planned to be used for factoring in the effects of heterogeneities in aquifers on the subsurface flow and transport of chemical constituents adequate using the Monte Carlo procedure?*

Based on the results of simulations presented in the background documents, the increased dispersion that is attributed to heterogeneities does not appear to have a large impact on the gross results of Monte Carlo simulations. Such increased dispersivities must, of course, increase the uncertainty in the Monte Carlo results. This makes mathematical and physical sense because increased dispersivities, used in this way, simply imply greater uncertainty as to where the plume is located.

The net result of enhancing dispersivities to account for gross heterogeneities is that plumes become more dispersed. This approach is appropriate if the objective is to determine whether or not a particular plume might intersect a well. However, if the objective is to determine the maximum concentration that a well might be subjected to, this approach is not suitable. If this latter scenario is applicable from a toxicological viewpoint, it would be more appropriate to use smaller (i.e., unmodified) dispersivity values and bias the well locations such that they are more likely to intersect the plume. That is, an alternative approach, that would better represent the maximum concentrations that might be found in a well, would be to preferentially locate wells directly downgradient of the source.

Editing Oversights

HWIR99 is not defined.

Figure 3.1 does not include definitions of x_u and x_d.

In several places the text claims that the saturated zone model can consider both linear and nonlinear sorption processes (e.g., implied last paragraph page 4; stated twice on page 17). From the reviewer's understanding of the numerical method, along with contrary claims elsewhere in the text (e.g., pages 4 and 25), this is not true. The model only considers a linear sorption model in the saturated zone.

It would appear that the source for the saturated zone can only be square. This should be documented.

The termination criterion discussed under Section 3.2.3 implies that the source concentration can only decrease. Is this true?

NTSCRW and NTSFST are not defined in Table 3.3.

The domain discretization is not described in the model validation sections (pages 41 and onward). It is relevant to both the model and independent testing.

The third equation on page D-7 should indicate a range of validity of $x > x_d$, rather than $u > u_d$.

Overall, references to the scientific literature are somewhat sparse.

A reference for equation 2.22 and the evidence that supports its use should be supplied.

A reference or further explanation should be provided for equation D.23 on page D-8.

There a small formatting problems with references in a number of places.

References

Domenico, 1987. An analytical model for multidimensional transport of a decaying contaminant species. Journal of Hydrology, 91(1987), 49-58.

Appendix

The following documents were supplied for background information.

US EPA, 1996. EPACMTP Background Document, Washington, DC 20460.
US EPA, 1997. EPACMTP User's Guide, Washington, DC 20460.
US EPA, 1996. EPACMTP Background Document for Finite Source Methodology for Chemicals with Transformation Products, Washington, DC 20460.
US EPA, 1996. EPACMTP Background Document for Metals, Washington, DC 20460.
US EPA, 1997. Test and Verification of EPACMTP, Washington, DC 20460.
SAB Report: Review of EPA's Composite Model for Leachate Migration with Transformation Products - EPACMTP. Prepared by the OSWER Exposure Model Subcommittee of the Environmental Engineering Committee, Science Advisory Board, Washington, D.C. EPA-SAB-EEC-95-010, August, 1995.
Response to the SAB Report: "Review of EPA's Composite Model for Leachate Migration with Transformation Products - EPACMTP. Prepared by the OSWER Exposure Model Subcommittee of the Environmental Engineering Committee, Science Advisory Board, Washington, D.C. EPA-SAB-EEC-95-010, August, 1995."
US EPA, 1998. A Study to Assess the Impact of Fractured Media in Monte-Carlo Simulations, Washington, D.C. 20460.
US EPA, 1999. Incorporation of Heterogeneity into Monte Carlo fate and transport simulations. Washington, D.C. 20460.
US EPA, 1997. Implementation of the Vapor-Phase Migration Simulation Module for the EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP). Washington, D.C. 20460.

ATTACHMENT D

Peer Review of "Vadose Zone and Saturated Zone Modules Extracted From EPACMTP for HWIR99" by:

Frank Schwartz
Ohio State University

Title: Peer Review – Ground Water Modules

By: Frank W. Schwartz

Date: November 20, 1999

This review is organized according to the charge to the panel.

1a. *Are the vadose zone and saturated modules extracted from the EPACMTP reasonable for use in the HWIR Multimedia, Multipathway, and Multireceptor model for nation-wide implementation?*

The modules extracted from EPACMTP are reasonable for use in the HWIR implementation. The modules capture many of the key processes involved with contaminant transport in saturated and unsaturated systems. The methods used in formulating and solving the equations appear robust, yet are sufficiently simple to minimize burdens in using these relatively sophisticated codes. The treatment of the processes and details of the mathematical approach are well documented in various reports. The EPACMTP family of codes has been around long enough to have a good history of verification checks and independent peer reviews. From a modeling perspective, the coupling of the vadose zone and saturated models appears to work well and certainly simplifies the modeling approach.

This review does not look in detail at the various data used in applying the model. The important question is whether the relatively sophisticated model treatment is adequately supported by data. In other words, an elegant model, which might only be supported by mediocre data, overall doesn't provide a net gain in the rigor of the overall analysis. Obviously, other reviewers were concerned about this point, especially in assessing whether the treatment of biodegradation of organic compounds is conservative and/or realistic.

The collection of reports alludes to some validation testing, where model assessments are compared with the known behavior of plumes at real sites. There appears to be some need for additional work to demonstrate that this overall modeling approach can capture the behavior of the differing settings to which it is being applied. Such check in essence validates the modeling approach and the supporting data, as a complete package. For example, it is not clear to me that the vadose zone/aquifer concept reasonably represents all settings in a generic manner.

1b. *Is the mathematical formulation and the solution of the pseudo three-dimensional saturated zone module appropriate for use in the 3MRA model?*

The HWIR99 report explains that the more rigorous treatment for flow and transport in the saturated zone was too computationally intensive for routine applications in Monte Carlo simulations, which prompted an effort to develop a simplified but more efficient approach. The report is vague on the need and justification of the simplifications in the first place. For example, since 1995 when EPACMTP became more commonly used, processor speeds and memories have expanded to the extent that most of us have junked the 1995-type equipment. Are Monte Carlo analyses still out of the question with the newest computers, and has there been a diligent effort to speed up or to optimize the original 3-D approach (e.g., different computers; different compilers; smaller grids; fewer realizations; eliminating some MC calculations by scaling approaches etc)?

From a reviewer's point of view, justification for the decision to create a simplified but less accurate module has not been provided. Similarly, it would be useful to provide users with comparative numbers on the efficiency of the various approaches.

Indications are that the formulation of the pseudo three-dimensional model is appropriate for use in the package. If an optimized numerical approach for solving the flow and transport problems is really not practical then the analytical/numerical approach would seem to provide the only viable approach. It is not exactly clear how much speedup has been achieved through the simplifications.

The simplified approach has been successful in meeting the need to speed the code up, yet retain most of the key processes. There have been good ideas implemented here, which overcome the process limitations associated with pure analytical solutions.

2a. *Is the pseudo-three dimensional module reasonably verified for practical purposes?*

The report shows that for a few test cases the module can reproduce results of a more rigorous model with fair to good accuracy. The report probably overstates the quality of the fits obtained in the cross-verification trials.

I think that the verification testing shows the potential of the simplified approach. However, more convincing results are required because in a Monte Carlo framework extreme parameter associations may be created. The main problem is that the cause of the "errors" has not been elucidated in detail. For example, assuming mass to come out of a downstream patch produces an error that affects the timing and perhaps the concentration. One could surmise that larger sources than the one analyzed would have a greater error, while smaller sources might be subject to smaller errors. These conceivably could be worse fits generated for problems that had more of a three-dimensional flow configuration (perhaps higher recharge cases).

I think that more work has to be done in understanding what simplifications create what errors. This knowledge would provide a basis for evaluating the likely performance of the code as it is applied in Monte Carlo situations and to different geographic regions.

2b. *Will the results derived using the pseudo three-dimensional version of the module be practically reasonable with the Monte Carlo framework for a nation wide implementation of the model ...?*

As stated above, there are positive indications that results using the simplified module would be appropriate. The simplified approach is not always conservative vis-à-vis predictions, but the discrepancies appear to be relatively small. The biggest problem, in my opinion, is that without a clear understanding of the origin of the discrepancies, it is unreasonable to extrapolate from just a few verification trials.

3. *Is it reasonable to make this simplification in order to implement the model without utilizing the volatilization ...*?

Volatilization has the ability to expedite transport away from the source and effectively increase the footprint of the source. Indications from the 1997 report are that the effects of volatilization are relatively unimportant on a nationwide basis. This finding is reasonable and probably valid as a general conclusion.

I would note, however, that in the modeling approach, transport associated with volatilization is modeled primarily as a diffusion process. The few field studies on this topic suggest that at DNAPL sites there is a component of density-driven flow that significantly overwhelms diffusive-type transport. Migration laterally can be much larger and migration to the water table is more rapid than is the case with dispersion. It still would not likely make a big difference. The overall mass flux in the vapor phase into the saturated zone would likely be small irrespective of the vapor transport mechanism. The main point here is that one analysis probably can't form the basis for doing away with volatile transport. However, my feeling is that the process can be dismissed.

4. *Is the representation of flow and transport through fractured porous media by using the equivalent hydraulic approach justifiable for a model, which is implemented on a nationwide basis using the Monte Carlo approach?*

The approach to simulating fractured rocks involves considering sites of one of three types and adjusting the hydraulic conductivity within the Monte Carlo simulation. The results are more or less obvious namely that there is no change in peak concentration as compared to media without fractures. The plume would move somewhat faster with more or less the same plume shape – giving rise to similar concentrations at the receptor well. The fracturing fundamentally doesn't do much to alter the transport. This model of fracturing would show important effects when the contaminant parent/daughter degraded with a relatively short half-life.

This simple fracture model likely does not capture the important interaction between the character of the fracturing and the transport. The dispersivity would depend on the geometry of fracturing, along with the retardation factor. Fracture zones might exist that essential channelize flow to the receptor well in worst cases or cause the plume to miss the well under more favorable conditions. I think that considerably more effort will be required if it is essential to add fractures to the analysis. The present analysis is not particularly convincing of its simplicity and lack of realism.

5. *Is the technical approach planned to be used for factoring in the effects of heterogeneities in aquifers on the subsurface flow and transport of chemical constituents adequate using the Monte Carlo procedure?*

The approach used for representing the effects of heterogeneities needs rethinking and more development work. The theory for this correction-factor approach comes from a July 1999 report on "Incorporation of Heterogeneity into Monte-Carlo Fate and Transport Simulations". This report explains an analysis approach that provides theory to develop a correction-based approach for Monte-Carlo simulations. I have concerns about the analyses presented in that report, the most serious of which I outline as follows.

Dispersion at the macroscopic scale is created by heterogeneity in hydraulic conductivity. There is theory that lets one estimate dispersivity values from the heterogeneous structure of the porous medium – variance in log K and correlation length scale. If you build a heterogeneous field, then macroscale dispersivity is automatically created in the transport. Given that the heterogeneity accounts for macroscale dispersion, the dispersivity value that needs to be defined in the model is the local-scale value, which will be small e.g., 0.1 m. In the 1999 report, both large dispersivity values and heterogeneous medium coexist, which is an important conceptual error. The existence of a dispersivity of say 100 m implies that there is heterogeneity with a correlation length scale of 10s to 100s of meters (depending upon the variance in log K) that is not considered. If in fact big dispersion exists at sites, then big-scale heterogeneity will exist as well; this heterogeneity is not represented in the analysis.

The report does not consider correlation in the hydraulic conductivity field, as is normally represented by a correlation length scale. This treatment implies that the correlation length scale is much smaller than the size of the grid blocks, or 10 m. Thus, the heterogeneity that is being modeled is of small scale, which as expected produced very little impact on the transport. The simulation results with large dispersivity are simply saying that there is a large scale heterogeneity present, which swamps the smaller effects. It makes little sense to effectively include the small-scale heterogeneity and not explicitly consider the more important larger scale.

The analysis that is presented in this report needs to be redone with an appropriate consideration of the role of heterogeneities in dispersion. If it is decided to run simulations with large dispersion (see my note, additional comments), then it will be necessary to include the largest scale heterogeneity and account for the correlation structure in the field. For example, large dispersivity values imply the existence of direct high permeability pathways from a source to a receptor well 100 m away from the site (see e.g., HWIR99). Similarly, high permeability pathways that miss the well will route mass in another direction. Thus the variation in concentrations observed at the receptor well could be huge when these high-permeability pathways exist.

6. *Additional Comments on Dispersion*

In the regulatory problem that is being addressed by this modeling effort, there are two processes that make a great difference to dose at the receptor well – dispersion and chemical destruction of contaminants. This conclusion assumes that the well is always hit by the plume. (Not the same assumption as EPACMTP.) Dispersion can thin the mass before it reaches the well and the chemical processes break it down. Because dispersion is operative for all contaminants, it will be a key process in determining the dose from wells. In reading all the documents, it is not clear that there is a consistent and appropriate treatment of dispersion. I'll discuss points in the following section.

Detailed field tracer tests over 100-300 m show that dispersion is a relatively insignificant process. Dispersivity values are often small in sand aquifers (less than 1 m). Larger values obtained in many tests are generally discounted by Gelhar as being overestimates due to errors. Vertical transverse dispersivity is usually small with diffusion-scale numbers. Thus, overall plumes from relatively large sources should not be impacted by dispersion.

Many of the test cases in the present reports are based on appropriate dispersion values (e.g., HWIR99). There are other documents where the dispersivity approach is of concern. The EPACMTP document (1997) (Table 7.5) probably overestimates dispersivity values for travel distances of 150 m. For greater distances, dispersivity values are scaled as a function of travel distance. According to Equation 7.9 (which contains a serious typo) at a distance of 2000 m the longitudinal dispersivity would be about 70 m and the vertical transverse dispersivity would be 0.4 m. These are large values, along with the values used in the Heterogeneity report (July, 1999).

The problem as I see it comes to the distance scaling of dispersivity values. I think if one believes the geostatistical origins of dispersivity, one also ought to believe in a single constant asymptotic dispersivity value that applies to the aquifer. It may take some travel distance (e.g., 10-100 correlation lengths) to reach this dispersivity but eventually it will be attained. For dispersivities to increase constantly along a unit, the correlation structure of the unit would need to keep changing. This might occur but has never been documented. Similarly, there should be no reason to scale vertical transverse dispersivity values. A plume cannot magically assume some capability to spread vertically once it has moved away from the source. In summary, I think that the EPA's thinking on dispersion as applied in this work and elsewhere is wrong.

The Yucca Mountain project looked at far-field modeling for 20 to 30 km away from the repository. Simulations involving modestly large longitudinal values, 100s of meters over the travel distance were scrapped in favor of a stream-tube model that severely minimized the effects of dispersion. My recollection is a factor of 2x or 3x reduction in the source concentration over 20-30 km due to dispersion.

7. *Recommended Improvements for Next Six Months:*

(a) I think it would be important to revisit the basic concepts of dispersion (see 6.) with a view to producing a more defensible agency stance on this important issue.

(b) The pseudo three-dimensional approaches are promising to make the Monte Carlo analyses more tractable. I would recommend work to optimize the original 3-D code to see whether limitations of 1995 have perhaps gone away with more powerful compilers and computers. It is not clear that the compiler being used is by any means the fastest one around.

If the pseudo three-dimensional approach is followed, it will be necessary to know more precisely where the deviations are being produced. Knowing more about the error will enable one to evaluate the extent of errors produced in a Monte Carlo analysis. The work on this topic so far has been necessary but not sufficient.

(c) The analyses of heterogeneities and fractures are wrong and simplistic, respectively. If it is felt that these features need to be considered in the complete evaluation, then more work will be necessary. I think the progress in dispersion [recommendation (a)] will contribute to the understanding of the impact of heterogeneities. If one needs to choose between the two, I would suggest work on heterogeneities.