UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

WASHINGTON, D.C. 20460

SAB-EEC-88-030

OFFICE OF
THE ADMINISTRATOR

July 12, 1988

Honorable Lee M. Thomas
Administrator
U.S. Environmental Protection Agency
401 M Street, S.W.
Washington, D.C. 20460

Dear Mr. Thomas:

The Science Advisory Board has reviewed the Unsaturated Zone Code (FECTUZ) for the Office of Solid Waste's Fate and Transport Model. The Office of Solid Waste sought to develop a code which would account for the attenuation of chemical constituents in the unsaturated zone and have potential uses in the Toxicity Characteristic and Concentration-Based Listing rulemakings. FECTUZ is a model package consisting of an analytical code and a finite element numerical code; each code contains a flow module and a transport module. In requesting the review, the Director of the Characterization and Assessment Division asked the Board to address three issues: the dimensionality of FECTUZ, the appropriateness of the assumptions underlying the code, and code implementation.

The Unsaturated Zone Code Subcommittee of the Science Advisory Board's Environmental Engineering Committee reviewed the documentation for the code at open meetings December 10, 1987 in Denver and January 19, 1988 in Washington.

The Subcommittee concluded that the dimensionality of the code (one-dimensional transport in the vertical dimension) is probably adequate for situations in which the porous medium can be considered relatively homogeneous, without substantial stratification and that the one-dimensional limitation may not be a serious one from the standpoint of asymptotic, steady state analysis of groundwater protection, since the primary effect of lateral spreading would be to retard downward mobility and hence to increase the time available for transformation of the contaminant, thus reducing the amount that reaches the water table.

The Subcommittee believes that there are no serious problems associated with treating the fluid as incompressible, isothermal, and homogeneous. The acceptability of all the other assumptions hinges on the application of the model. Certain classes of phenomena are not well enough understood to be incorporated into a management model of the kind reviewed here. Because of the importance of these phenomena to site-specific applications, there is an urgent need for scientific research to clarify the scientific principles underlying these phenomena. Such research would have benefits beyond this model. The FECTUZ model package is also subject to limitations imposed by its simplifying assumptions and the scarcity of data necessary for parameter estimation. Both versions of the model are incomplete in the sense that several potentially important governing processes are neglected altogether. The Subcommittee believes these limitations are not so debilitating as to preclude its employment for generalized regulatory development applications, but believes that the inability to take into account several potentially relevant processes casts serious doubt on the advisability of site-specific applications. It is recommended that the Agency mount directed and continuing efforts (a) to improve the knowledge base concerning relevant processes which have been neglected on grounds of inadequate understanding, and (b) to seek expert consensus in these areas, especially biotransformation, immiscible transport, and fracture transport.

The Subcommittee finds that for the intended tasks in regulatory development, the composite model consisting of FECTUZ-A and EPA-SMOD is acceptable from the standpoint of simplicity and computational ease. Where Monte Carlo replication of the model is planned, the overall uncertainty of the transport model should be addressed because the Monte Carlo methodology is not able to account for uncertainties arising from incompleteness or deficiencies in the underlying model. However, for site-specific decisions where the accuracy and completeness of representation of transport and transformation processes is of paramount importance, the FECTUZ model seems bound to be inadequate, especially the analytical version owing to its implicit simplifications and its inability to take into account temporal variations, site-specific conditions and heterogeneity. The Office of Solid Waste should take special care to warn potential users against site-specific applications of the composite model, because there is a substantial danger that such usage could be misleading and detrimental to the protection of groundwater quality.

Additionally, the Subcommittee has expressed concerns and made suggestions relating to how the Agency establishes the need for the development of a new model, how existing models are evaluated, and on the existence and use of adequate in-house capability for evaluating issues related to transport model development and application.

The attached report contains more detailed responses to these issues.

We are pleased to have had the opportunity to be of service to the Agency and look forward to a written response to our report.

Sincerely,

Norton Nelson, Chairman
Executive Committee
Science Advisory Board

Raymond Loehr, Chairman
Environmental Engineering Committee
Science Advisory Board

Paul Roberts, Chairman
Unsaturated Zone Code Subcommittee
Environmental Engineering Committee

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SAB-EEC-88-030

REPORT OF THE
UNSATURATED ZONE CODE SUBCOMMITTEE
ENVIRONMENTAL ENGINEERING COMMITTEE
SCIENCE ADVISORY BOARD

U.S. ENVIRONMENTAL PROTECTION AGENCY
ON THEIR REVIEW OF THE
OFFICE OF SOLID WASTE'S
UNSATURATED ZONE CODE FOR THE OSW FATE
AND
TRANSPORT MODEL

June, 1988

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Date: June 1988

NOTICE

BACKGROUND

Procedural

On October 22, 1987 the Office of Solid Waste (OSW) made a presentation to the Environmental Engineering Committee on its unsaturated zone code (FECTUZ) for the Office of Solid Waste's Fate and Transport Model. In developing FECTUZ, the Office of Solid Waste sought to create a code which would account for the attenuation of chemical constituents in the unsaturated zone and have potential uses in the Toxicity Characteristic and Concentration-Based Listing rulemakings. The Committee formed the Unsaturated Zone Subcommittee to conduct the review of FECTUZ. The review was formally requested in an October 16, 1987 memorandum from the Director of OSW's Characterization and Assessment Division (Appendix). The memorandum asked the Board to address three issues: the dimensionality of FECTUZ, the appropriateness of the assumptions underlying the code, and code implementation.

The Subcommittee held open meetings December 10, 1987 in Denver, Colorado and January 19, 1988 in Washington, D.C. The Environmental Engineering Committee heard the preliminary report of the Subcommittee January 20, 1988 and approved this report on April 15, 1988.

Model Structure

To summarize briefly, FECTUZ is a model package that has been developed in two versions: an analytical code and a finite element numerical code. For clarity we will refer to the two versions as FECTUZ-A (analytical) and FECTUZ-N (numerical), respectively. FECTUZ-A and FECTUZ-N each consists of two modules: flow and transport. An acronym, FECTUZ stands for Finite Element Code for Transport in the Unsaturated Zone. In fact, this acronym is a misnomer if applied to the analytical version, as it is not a finite element code. This inconsistency was confusing to the Subcommittee, is likely to mislead users, and therefore should be corrected by renaming the analytical code.

In developing the model, OSW and their consultant placed a high priority on two objectives: 1) computational efficiency, and 2) ability to deal with a wide range of soil characteristics, including highly nonlinear relationships between soil moisture and permeability. The justification for these priorities is to permit use of the model in Monte Carlo evaluations of expected concentration levels at water supply wells under a wide variety of soil conditions.

The flow module is based on the assumption of one-dimensional, isothermal flow of an incompressible, homogeneous fluid according to Darcy's Law. Vapor flow, transport through secondary porosity (fractures and fissures), and migration of immiscible liquids are neglected. A flux-type boundary condition is imposed at the top of the unsaturated zone.

Likewise, solute transport is assumed to be one-dimensional, incorporating advection and Fickian dispersion, i.e. a diffusion-like model of solute front spreading. Sorption is assumed to follow a linear equilibrium relation. First-order transformation is incorporated, but at present only hydrolysis is considered in the selection of the rate coefficient, owing to a perceived lack of knowledge concerning biotransformation processes. The documents provided are ambiguous about the nature of the transformation submodel, as they refer to "first-order decay", implying that biotransformation and chemical reactions other than hydrolysis are included. These other reactions can be incorporated within the current structure of the model, but they are not included in the current implementation.

The model is capable of performing either transient (FECTUZ-N) or steady-state (FECTUZ-A) simulations of flow and transport. However, in the proclaimed uses for regulatory development, namely Toxicity Characteristics and Concentration-Based Listings, it apparently will be used only in the steady-state mode, i.e. a constant water flux is assumed. The procedure consists of calculating the steady-state concentration at a monitoring well ouside the landfill site, with the distance to the monitoring well treated as a distributed parameter estimated from OSW's data base.

Intended Uses of the Model

The questions posed to the Science Advisory Board cannot be addressed properly without a clear idea of the prospective uses of the model. In delineating the intended applications, OSW informs us that they envision using FECTUZ in the immediate future mainly as a tool in developing regulations for disposal to municipal landfills: i) for use by the regulated community to assess whether a waste is hazardous (Toxicity Characteristic); and ii) for use by OSW to reassess previous listings, to set concentration criteria, and to delist substances if appropriate (Concentration-Based Listing). It is implicit that, in these applications, FECTUZ will be used in combination with the saturated zone groundwater flow and transport model, EPA-SMOD, which is a two-dimensional, steady-state model. A previous version of the model was reviewed by the Environmental Engineering Committee of the SAB. As such, the steady-state version of FECTUZ (what we refer to above as FECTUZ-A) will be used.

Concerning other uses of the FECTUZ model, OSW states that it "does not have any other specific uses planned for the FECTUZ Code at this time. However, two site-specific uses are possible. These are use in decisions on ACLs (alternate concentration limits) and in Clean Closure decisions." It is implicit that, in these site-specification applications, the intended use of FECTUZ will require the more sophisticated dynamic mode (what we refer to above as FECTUZ-N) in conjunction with a dynamic numerical simulation model for the saturated zone. The use of the more detailed models is intended to allow incorporation of site-specific soil and geological properties in these applications.

If EPA changes its assumption to include a liner in its assumed landfill, the liner effect should be incorporated in FECTUZ, as it will control flow.

RESPONSES TO QUESTIONS POSED BY OFFICE OF SOLID WASTE

Dimensionality of FECTUZ Code

The dimensionality of the code (one-dimensional transport in the vertical dimension) is probably adequate for situations in which the porous medium can be considered relatively homogeneous, without substantial stratification. However, in soil layers or zones with low permeability relative to the surrounding media, considerable lateral spreading may occur, particularly if free-phase hydrocarbons are present (Mull, 1971; Schwille, 1984). The one-dimensional limitation may not be very serious from the standpoint of an asymptotic, steady state analysis of groundwater protection, since the primary effect of lateral spreading would be to retard downward mobility and hence to increase the time available for transformation of the contaminant, thus reducing the amount that reaches the water table. On the other hand, this same phenomenon could lead to circumstances in which the unsaturated zone accumulates contamination to a greater degree prior to detection in groundwater monitoring wells, compared to the case without stratification.

Appropriateness of FECTUZ Assumptions

The Subcommittee believes that there are no serious problems associated with treating the fluid as incompressible, isothermal, and homogeneous. The reliance on Darcy's Law is a widely used expedient that is justifiable at the level of regulatory development applications, but may be unsatisfactory in site-specific applications if transport through secondary porosity or migration of immiscible liquids plays a role. These factors are discussed below under the category of processes neglected in the model.

Neglecting hysteresis effects (physical effects which lag their cause) in the relative permeability relationships is permissible under asymptotic (long-term, steady state) conditions. However, the omission of the differences in relative permeability relations between imbibition (saturation with liquid) and drainage will result in a gross misrepresentation of transport under nonsteady conditions, especially for soils having strongly nonlinear characteristics. Hence, this simplification will hinder accurate simulation of nonsteady-flow situations with FECTUZ-N, even though the numerical model is otherwise capable of handling nonsteady inputs.

The formulation of the dispersion term according to Fick's Law is a representation that is commonly practiced in transport modeling, and is acceptable in most situations. This representation is certainly adequate for simulations at the level of regulatory development. Substantial deviations from Fickian behavior must be anticipated in strongly heterogeneous or stratified media, however, and should be taken into account in site-specific applications under such circumstances. Even more serious inadequacies will arise if transport in secondary porosity is significant, as discussed below.

The treatment of sorption as conforming to the linear equlibrium assumption is also adequate for dealing with most situations of trace organic contaminant transport in a homogeneous medium. However, in concentrated leachates, cosolvent effects and facilitated transport maybe significant. Cosolvent effects occur when chemicals are more readily dissolved in the fluid phase due to the presence of other chemicals in the contaminant stream. Facilitated transport occurs when contaminant mobility is increased due to interactions with other dissolved organic substances such as naturally occuring humic acids. These processes tend to increase the mobility of the contaminants through the unsaturated zone and along the ground water flow path. The linear equilibrium assumption is usually inadequate for contaminants such as trace metals, for which selective cation exchange is the dominant sorption mechanism. Moreover, in fractured or strongly stratified media, it is questionable whether equilibrium will be obtained for contaminants of any kind, as diffusional limitations govern the exchange between the mobile fluid and the matrix or immobile zones. Ignoring these complexities is justifiable in regulatory development applications, but certainly not in site-specific applications.

Solute transformation according to a first-order rate expression likewise can be justified as an expedient in simulations supporting regulatory development. The first-order rate formulation is an acceptable approximation for many chemical reactions, and in some instances for biotransformation processes. On the other hand, the transformation submodel and its associated data base are inadequate in some respects, and the FECTUZ documentation does not clearly recognize those inadequacies. At present, only a single transformation mechanism is incorporated: chemical hydrolysis. Although hydrolysis rates of many compounds are strongly dependent on pH, the model is not capable of predicting the pH in the leachate plume, relying instead on estimates of the pH of native groundwater. The data-base for this estimate currently relies on sampling data from saturated zone measurements. This is inappropriate for use in an unsaturated zone model. However, even if native unsaturated zone data were collected, this would not account for the effect of the leachate on the pore-water pH. This deficiency could lead to inaccuracies of several orders of magnitude in estimating hydrolysis rate constants. Further, the analysis could be seriously biased in the direction of overestimating transformation rates for compounds for which base hydrolysis is the dominant mechanism, if the majority of leachate plumes are acidic.

Similarly, biotransformation could be included as a simple first-order rate process. However, consensus is lacking for generalized prediction of transformation rate constants, as these depend strongly on conditions such as organism adaptations and concentrations, pH, and the presence or absence of electron acceptors (oxygen under aerobic conditions), toxicants, essential nutrients, etc. which are site-specific. Site-specific applications of the FECTUZ model package can lead to overestimates of solute transport since site-specific biotransformation analyses generally result in biodegradation being a primary process influencing chemical fate. Hence, estimates of chemical transport made without considerations of biotransformation are almost always so overly conservative as to affect regulatory decisions. Generalized chemical transport predictions will necessarily suffer due to lack of generally applicable biotransformation rate constants; however, site-specific analyses should include all of the fate processes for which specific data can be reasonably obtained.

Implementation of the full range of transformation possibilities, including the uncertainties in conditions that influence the rate constants, would magnify enormously the uncertainty spectrum of predicted outcomes in Monte Carlo simulation.

The transformation submodel considers neither chain reactions nor the formation of hazardous daughter products. Including transformation reactions without considering the possible formation of hazardous intermediate products can bias the results of simulations toward underestimating the risk of serious contamination of groundwater resources. In regulatory uses, including both toxicity characteristic assessment and concentration-based listings, it would be dangerous to use the transformation submodel without considering byproduct formation where relevant. It is recommended that the transformation submodel be decoupled in the analysis of any compound known to form hazardous intermediate products, unless the byproduct formation is incorporated explicity.

Important mechanisms of contaminant transport or transformation that are neglected by the FECTUZ-A model include vapor phase transport (volatilization), abiotic tranformation other than hydrolysis, biotransformation, free-phase flow of organic liquids, and fracture flow. Further, FECTUZ does not permit nonlinear equilibrium relations for sorbing solutes, nor does it allow for competition or similar interactions that may arise in multisolute systems, especially cosolvent effects.

Neglecting such potentially important mechanisms raises questions as to whether the model can provide accurate estimates of the central tendency, whether the overall effect of the omissions may tend to underestimate the threat to groundwater quality, and whether the range of uncertainty may be substantially underestimated.

For organic contaminants, the first three mechanisms -- vapor phase transport, abiotic transformation, and biotransformation -- serve mainly to reduce the amount of contaminant which would otherwise reach the water table. Hence, neglecting these processes in the FECTUZ model does not increase the risk of protecting groundwater resources inadequately if the model is used as a basis for regulatiory decisions. However, transport in fractures or macropores, free-phase flow of immiscible organic liquids, and cosolvent effects would allow contaminants to migrate more rapidly than would be predicted by the model, and thereby reduce the contaminant's residence time in the unsaturated zone, thus reducing the opportunity for transformation.

Transport in fractures is a phenomenon that has only recently attracted attention as an important mechanism of contaminant migration. In a recent review, Jury (1987) states that "in any natural setting, interaggregate structural features such as soil macropores, cracks, plant root holes, or animal burrows will be interspersed with the bulk structural characteristics" and that "these geometric features, although very small in volume, can have a significant effect on the transport of chemicals and particularly on those which are highly absorbed." In general, it can be expected that, in systems that possess substantial secondary porosity in the form of fractures or macropores, transport will be characterized by early breakthrough and extended tailing of contaminants (van Genuchten, 1985). Fracture transport is of special significance in media of low permeability such as clays, which furthermore are prone to fracturing owing to their tendency to swell or shrink in response to changing chemical conditions or moisture content. Hence, this mechanism is likely to be of great importance precisely in the kind of media that we tend to rely on to isolate waste disposal sites. Despite this recognition of the potential significance of fracture transport, there is a dearth of conclusive confirmatory evidence, because of the extreme difficulty of conducting the necessary investigations, which would need to be conducted at field scale. At present, various modeling approaches are being explored to deal with this problem, including deterministic models based on advection in fractures with diffusion into the matrix and stochastic models that rely on probabilstic representation of transport, but experimental evidence suitable for model verification is meager. A recent review by van Genuchten and Jury (1987) summarizes the promise and limitations of modeling approaches, concluding that rigorous, structure-oriented models are presently too complex for routine use in management. In summary, our inability to formulate an adequate model for this transport mechanism is a severe hindrance to modeling transport at sites where secondary porosity exists in substantial measure. The importance for transport notwithstanding, it is understandable that fracture flow has not been corporated into FECTUZ.

The migration of free-phase organic liquids in the subsurface has been incorporated in several models (Corapcioglu and Baehr, 1987; Hochmuth and Sunada, 1986; Abriola and Pinder, 1985; Faust, 1985). These models could be used in conjunction with or in place of FECTUZ if the presence of free-phase organics is suspected. Leakage of free-phase organics into the subsurface might occur if the low-permeability clay liners used at landfill sites are attacked by the waste. Brutsaert (1987) showed that some solvents can cause these clay liners to shrink and develop cracks that could allow breakthrough of the solvents and associated contaminents. Another aspect of contamination by free-phase organics that cannot be modeled with FECTUZ is the long-term contamination of groundwater caused by dissolution of residual hyrocarbons trapped in the capillary fringe (Pfannkuch, 1983).

In summary, the FECTUZ model package is subject to limitations imposed by its simplifying assumptions, our lack of understanding of important phenomena, and the scarcity of data necessary for parameter estimation. Both versions of the model are incomplete in the sense that several potentially important governing processes are neglected altogether. The Subcommittee believes that these limitations are not so debilitating as to preclude its employment for generalized regulatory development applications, but believes that the inability to take into account several potentially relevant processes casts serious doubt on the advisability of site-specific applications.

Compatability With Comprehensive Transport Model

This question is conceptually difficult to answer, because the scope of modeling objectives is subject to change. The Office of Solid Waste should recognize that the requirements for a model to be used in regulatory development are different from those for other more site-specific applications for which the unsaturated zone transport code is intended to be used as a tool. Further, the Subcommittee has been informed by OSW that the existing model for groundwater transport (EPA-SMOD) is an analytical code that is compatible only with the analytical version of FECTUZ. Hence the comprehensive transport model is subject to the same limitations as FECTUZ-A, namely it is suitable only for steady-state simulations of transport in a homogeneous medium. The Subcommittee is hindered from answering the question of compatability in detail, because OSW has not provided updated documentation on the current version of EPA-SMOD.

In order to derive any benefit from the non-steady state capabilities of the FECTUZ model, the Agency would need to couple it with an appropriate peer-reviewed dynamic saturated zone model. Full use of non-steady state capabilities will be particularly important if EPA modifies its assumption of an infinite contaminant source.

For the intended tasks in regulatory development, the composite model consisting of FECTUZ-A and EPA-SMOD is acceptable from the standpoint of its simplicity and computational ease. Indeed, for the kinds of tasks contemplated in regulatory development applications, an even simpler, steady-state model relying on analytical solutions, such as the RITZ Model described at the December 1987 meeting of the Subcommittee, would probably be a suitable compromise between adequacy of representation and computational efficiency. If the situation is to be simplified by assuming steady, one-dimensional flow and considering only the asymptotic condition at very long times, it is not necessary to consider dispersion in the unsaturated zone, and the nonlinearity of the soil's permeability relation is of minor importance.

Hence, if the transport in the unsaturated zone is restricted to a one-dimensional, steady-state situation, some of the complexities of FECTUZ could be avoided in the interest of computational efficiency. Rather, in such an asymptotic analysis, predicting the extent of transformation is the crux of the matter, because in the long-term steady state, all of the solute that is not transformed ultimately will reach the water table. Assuming a first-order reaction, the extent of transformation depends on the product, kt, of the transformation rate constant times the solute's residence time. The transformation rate constant k depends on the reactivity of the solute as well as on chemical conditions. The solute residence time is influenced mainly by advection and sorption. Dispersion influences the residence time distribution but not the average residence time, and might be safely neglected as a factor of secondary importance in a steady-state analysis of the kind contemplated by OSW for regulatory development purposes, in the sense that its influence is much smaller than the potential impact of transformation processes.

For site-specific decisions where the accuracy and completeness of representation of transport and transformation processes is of paramount importance, the FECTUZ model seems bound to be inadequate, especially the analytical version, FECTUZ-A, owing to its implicit simplifications and its inability to take into account temporal variations, site-specific conditions and heterogeneity. The Subcommittee feels strongly that OSW should take special care to warn potential users against site-specific applications of the composite model.

There is a substantial danger that such usage could be misleading and detrimental to the protection of groundwater quality.

Validation

The flow module of the FECTUZ model package has been validated for extreme conditions of soil characteristic nonlinearity, and can be considered to represent state-of-the-art modeling capability. However, the Subcommittee has seen no evidence that the combined flow and transport model, including the transformation module, has been confirmed by comparing to observations in a real system. Neither has the comprehensive model, combining transport in the unsaturated and saturated zones, been validated by comparing to observed field behavior. Given this lack of validation, OSW should be cautious in authorizing general use of these models for any purpose. The Agency should initiate a concerted effort to gather or generate the needed field data to allow validation of the proposed groundwater models.

Uncertainty Analysis with FECTUZ

The FECTUZ model is to be applied in conjunction with EPA-SMOD to determine the degree of uncertainty associated with Toxicity Characteristic and delisting decisions. The intent of the uncertainty analysis in the rulemaking procedure is to identify the fraction of potential land disposal sites across the United States where a given leachate concentration will result in exceedances of a health-based standard. So long as this fraction is low, eg., below 5 or 1 percent (the actual value used is a policy decision), then the allowable leachate concentration is considered to be protective for hazardous waste classification. Monte Carlo replication of the model is thus intended to characterize the range and distribution of soil transport conditions encountered throughout the United States.

A particular problem with the Monte Carlo methodology described above is that it is limited to evaluations of parameter uncertainty: it is not able to account for uncertainties which arise due to incompleteness or deficiencies in the underlying transport models such as those described previously for the FECTUZ model. Unfortunately, this is the case for virtually all model uncertainty analyses performed today, as effective methods for representing and evaluating the uncertainty in model structure are not currently available. Implicit in the use of parameter uncertainty techniques is the assumption that the variations in parameter values used in the Monte Carlo analysis somehow capture the overall uncertainty in the model itself. This may not always be the case, depending on the potential impact and importance of omitted or misrepresented processes in the model.

The overall uncertainty of the transport model should be considered. First, there needs to be a more detailed discussion of omitted processes and their potential impact in the EPA reports. Second, it should be recognized that in the current application, the Monte Carlo distributions are formulated to represent only the spatial variability of parameters across the United States. The distributions do not reflect uncertainties, either in the parameters themselves or in the overall output of the model. To obtain a reasonable, conservative level of regulation, it may thus be necessary to superimpose overall judgments of model uncertainty on the model results. For example, the distribution of unsaturated zone travel times may be modified to account for the occurrence of direct macropore or fracture transport. The consideration of model uncertainty is certainly a new and difficult area, however, some initial steps incorporating basic engineering judgments are appropriate if uncertainty analysis techniques are to be used and trusted for regulatory development.

ADDITIONAL ISSUES

The Subcommittee is concerned about several other issues related to the development and use of FECTUZ that arose in the course of its deliberations:

1. How does OSW proceed in establishing the need for the development of a new model? How are existing models evaluated, including those recently developed within EPA and at other Federal agencies such as USGS and ARS?

2. Does OSW have adequate in-house capability for evaluating issues related to transport model development and application, and does OSW capitalize on the expertise available elsewhere within EPA?

These and other issues related to the use of models by the EPA have been of concern to the Environmental Engineering Committee during reviews of other programs within the Agency. The problems appear to be common to many of the modeling studies we have reviewed. The EEC is in the process of developing a generic resolution on the proper selection and use of models by the Agency, where these issues are addressed.

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Yaron, B., G. Dagan, and J. Goldschmid, editors, Pollutants in Porous Media: The Unsaturated Zone Between Soil Surface and Groundwater, Springer Verlag, 1984.

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

WASHINGTON, D.C. 20460

OCT 16, 1987

OFFICE OF
SOLID WASTE AND EMERGENCY RESPONSE

MEMORANDUM

SUBJECT: Science Advisory Board Review of the Unsaturated Zone Code for the OSW Fate and Transport Model

FROM: Sylvia K. Lowrance, Director
Characterization and Assessment Division (WH-562B)

TO: Dr. Terry F. Yosie, Director
Science Advisory Board (A-101)

The purpose of this memo is to transmit for your review a code for the simulation of flow and transport of chemical constituents through an unsaturated zone. The code accounts for the attenuation of chemical constituents in the unsaturated zone and has potential uses in the Toxicity Characteristic (TC) and the Concentration-Based Listing rulemakings. The code was developed to fully explore the comments received on OSW's TC proposal (51 FP 21648, June 13, 1986). As we have indicated to you earlier, the TC proposal would modify the existing toxicity characteristic by: (1) introducing a new leach procedure -- Toxicity Characteristic Leaching Procedure (TCLP); (2) adding 38 organic compounds to the list of TC constituents; and (3) using a ground-water fate and transport model to establish dilution/attenuation factors for the specific organic compounds. The ground-water fate and transport model used in the TC proposal was reviewed by SAB as part of the land disposal restrictions ground-water screening procedure in 1985.

In the TC proposal, the ground-water model did not incorporate an unsaturated zone. The model assumed that the bottom of the landfill was directly in contact with the water table. Consequently, any attenuation of chemicals in the unsaturated zone was ignored in the model. OSW made this assumption at that time because of a lack of adequate data to characterize the unsaturated zone for the implementation of the model on a generic basis. Because of this, OSW opted to be conservatively protective of human health and the environment.

The Agency received numerous comments on the absence of unsaturated zone in the model. The commenters stated that the assumption was unrealistic and landfills are not directly connected to the saturated zone. In addition, since the proposal date, the Agency has obtained data, as part of OSW's Solid Waste Landfill Survey, on the distribution of unsaturated zones at the municipal landfill sites in the U.S. These data indicate that at least 95 percent of these sites have unsaturated zones. Therefore, in order to fully explore the comments on the TC proposal, OSW has developed an unsaturated zone code (FECTUZ).

FECTUZ is a finite-element code for the simulation of water flow and solute transport in the unsaturated zone (variably saturated porous media). The code allows for a wide range of nonlinear flow conditions and handles various transport processes, which are considered in the saturated zone code, including hydro-dynamic dispersion, advection, sorption, and first order decay. The code allows for consideration of heterogeneities in the vertical dimension (layering) in the unsaturated zone.

SPECIFIC AREAS FOR SAB REVIEW

We are interested in SAB's evaluation of the FECTUZ code and have identified the following specific areas for Board's review:

1) DIMENSIONALITY OF FECTUZ CODE

FECTUZ code is one-dimensional in the vertical dimension for the following reasons:

(a) The flow in the unsaturated zone for all practical purposes can be assumed to be in the vertical direction; and

(b) OSW needs a code which can handle nonlinearites in the unsaturated zone and at the same time is computationally efficient because of the need to perform Monte Carlo analyses. Therefore, FECTUZ was developed as a one-dimensional numerical code (unlike the saturated zone code, which is an analytical code). Two- or three-dimensional codes will not satisfy this criteria.

(c) In addition, data to characterize the unsaturated zone for modeling in two or three dimensions are not available at this time.

Is the one-dimensional code (FECTUZ) an appropriate tool for the intended use under the circumstances characterized by the limitations of available data?

2) ASSUMPTIONS UNDERLYING THE CODE

FECTUZ code was developed based on several simplifying assumptions to represent the physical system to be modeled. The assumptions include:

(a) Flow of the fluid phase is considered isothermal and governed by Darcy's law.

(b) The fluid considered is slightly compressible and homogeneous.

(c) Hysteresis effects in the constitutive relationships of relative permeability versus water saturation, and water saturation versus capillary pressure head, are assumed to be negligible.

(d) Diffusive/dispersive transport in the porous media is governed by Fick’s law. The hydrodynamic dispersion coefficient' is defined as the sum of the coefficients of mechanical dispersion and molecular diffusion.

(e) Adsorption and decay of the solute may be described by a linear equilibrium isotherm and a first order decay constant.

(f) The code handles only single phase Flow (water) and ignores the flow of second phase (air).

(g) The code does not consider chain reactions. The porous media is considered as single-porosity soil media (non-fractured media). The kinematic sorption effects are not considered.

Are the assumptions made in the development of the code appropriate, considering its intended use and the limitations of the available data?

3) CODE IMPLEMENTATION

If we decided to incorporate an unsaturated zone into the ground water model, FECTUZ is to be implemented as an integral component of the ground water flow and transport code. The implementation of the code is described in the attachment.

We would appreciate your review of the procedure for incorporation of FECTUZ in the ground-water flow and transport model, and any specific suggestions the Board may have for improvements considering the limited data available.

Thank you for your help on this project. The code along with the necessary support materials are attached for your consideration. Please contact me (382-4637), or Dr. Zubair Saleem (382-4767), if we can be any assistance during the review process.

Attachment

cc: Matt Straus
Stephen R. Weil
R. Scarberry
Zubair Saleem

ATTACHMENTS

1. Finite Element Code for Simulating One-Dimensional Flow and Solute Transport in the Unsaturated Zone.
2. Methodology for Simulating Flow and Transport in the Unsaturated Zone.
3. Developing Joint Probability Distributions of Soil-Water Retention Characteristics -- Robert F. Carsel and Rudolf S. Parrish. Paper under publication in <u>Water Resources Research</u>.