EPA-SAB-EEC-85-008

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

July 31, 1985

OFFICE OF THE ADMINISTRATOR

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

Dear Mr. Thomas:

In late November, 1984, the Science Advisory Board was asked to review the technical basis for the development of a "decision rule" for determining whether or not specific hazardous wastes should be restricted from land disposal. This review was assigned to the Environmental Engineering Committee.

In the course of its review, the Committee examined two proposed approaches to developing the decision rule, one proposed by the Office of Solid Waste, and the other by the Office of Policy Analysis in OPPE. We have already sent you our report on the OSW version, and are pleased to now forward our review of the one proposed by OPA.

The Committee agrees that the OPA approach, because of its complexity and data-intensiveness, will not be applicable to all waste-banning decisions. The approach should be useful, however, on a waste- and site-specific basis for comprehensive comparisons of the risks of alternative hazardous waste disposal options.

The Committee has been particularly pleased with the cooperation extended by the OPA staff, and we are pleased to note that they have already taken steps to implement some of the Committee's recommendations.

If you have any questions, or should you wish any further action on our part, please call on us.

Sincerely,

Raymond C. Loehr

Raymond C. Loehr
Chairman, Environmental
Engineering Committee
Science Advisory Board

Norton Nelson

Norton Nelson
Chairman, Executive Committee
Science Advisory Board

cc: R. Morgenstern
S. Napolitano
A. Fisher
J. Briskin
A. Corson
S. Bromm
T. Yosie

REPORT

of the

ENVIRONMENTAL ENGINEERING COMMITTEE

SCIENCE ADVISORY BOARD

U. S. ENVIRONMENTAL PROTECTION AGENCY

on their review of

"COMPARISON OF RISKS AND COSTS OF HAZARDOUS WASTE ALTERNATIVES: METHODS DEVELOPMENT AND PILOT STUDIES"

July, 1985

I. EXECUTIVE SUMMARY

The Committee finds that the OPPE method of comparative risk analysis has scientific and technical merit and can provide useful information to decision-makers if further developed. However, we do not find the method *per se* useful for the Nationwide waste banning decision on several hundred chemicals. It is useful on a waste- and site-specific basis in that a decision can be based on a comprehensive appraisal of comparative risks of alternatives.

The method may not have generic applicability. The method is based on the scenario approach, the selection of a specific set of sub-models required, and the output form, as characterized by comparative risks and costs among the chosen scenarios. Its generality depends on how representative the scenarios can be made. An advantage of the method is that it provides for an explicit statement of uncertainties, if the uncertainties of the component parameters and models are known or estimated.

The choice of model components and the linking mechanisms to arrive at the complete model concerns the Committee in the following ways: (1) While some suggested sub-models are tested and accepted, others are not now verified and may not in practice be verifiable; (2) The data base for some of the models needs careful analysis, for both quality and quantity. Selection of parameter values based on quality peer-reviewed research is essential to avoid misleading results.

The health-effects section of the model, as with other similar models, suffers from the data-base problems already described. In addition, however, the Committee has concerns about the methods used. Among these are the use of a non-threshold model (which introduces problems when considering chemicals which may have threshold effects); the ignoring of pharmacokinetic effects and compound interactions; and inadequate toxicological evaluation and extrapolation techniques, especially simplistic temporal, route-to-route and species-to-species extrapolations. The Committee notes that the modular nature of the model does not restrict it to the use of a non-threshold approach.

The overall OPPE method needs upgrading in the area of surface drainage modeling and most importantly in the risk assessments related to the handling and transport of wastes with respect to fugitive emissions and probability of leakage and spills.

Finally, the model makes no provision for evaluating non-human environmental effects except for a "qualitative" evaluation. However, we are informed by OPPE that improvements are being made.

It is important to note that OPPE has responded at length to many of the comments and concerns expressed by the Committee in written summaries and in discussions with the Committee, and is studying ways of improving the method. The Committee commends OPPE for undertaking this major piece of research and encourages further work. The basic idea, if the concerns expressed can be taken into proper account, is sound for identifying the comparative risks of hazardous waste disposal options. With Agency policy interest in risk assessment strong, a properly developed method will be of real value.

II. INTRODUCTION AND HISTORY

At a meeting of the Environmental Engineering Committee on August 16, 1984, Mr. Alan Corson, Office of Solid Wastes, briefed the Committee on the development of a decision rule for restricting certain hazardous wastes from land disposal as governed by the proposed amendments to the Resource Conservation and Recovery Act. Two main approaches were under way: One incorporating a simplified predictive modeling approach (referred to as the OSW model), the other a more complex modeling framework based upon comparative risk assessment (referred to as the OPPE model).

In response to an Agency request for review of these approaches, a Subcommittee chaired by Dr. J. William Haun was appointed to conduct the review on an accelerated time schedule. The Subcommittee was assisted by several consultants (for a full list of the Subcommittee, see Appendix A). The full Environmental Engineering Committee completed a report to the Agency on its review of the OSW approach in April, 1985.

By letter dated January 7, 1985, and at a meeting of the Waste Banning Subcommittee (denoted above), on January 31, 1985, Dr. Richard D. Morgenstern, Director, Office of Policy Analysis, OPPE, presented the draft Final Report on "Comparison of Risks and Costs of Hazardous Waste Alternatives: Methods Development and Pilot Studies" (EPA Prime Contract No. 68-01-6558, Subcontract No. 130.155, Work Assignment No. 24), which forms the basis for the OPPE model. Dr. Nicholas Nichols, Dr. Ann Fisher, Ms. Jeanne Briskin and several contractor representatives also provided the Subcommittee with details of the method and background. The Subcommittee again met on February 25 and February 27 with Dr. Fisher and other members of the OPPE project team.

As a result of this activity, responding to the urgent need of Agency staff for a preliminary response, a Letter Report on the review to date was issued by Dr. Terry Yosie, Staff Director, SAB, on behalf of the Environmental Engineering Committee on March 8, 1985. This report constitutes the detailed basis for that Letter Report.

The scope of the review as originally suggested by OPPE, which focused primarily on the reasonableness of the sub-models and their integration, is shown in Appendix B. In addition, based on the early discussions, Dr. Loehr developed a more general list of issues for the Subcommittee. This list is shown in Appendix C. Both Lists were used by the Subcommittee in its conduct of the review.

III. DESCRIPTION AND EVALUATION OF THE MODEL

As a result of the recent (11/84) amendments to the Resource Conservation and Recovery Act (RCRA), EPA is required to establish which wastes, of those specified in the Act, are not to be banned from disposal in certain land disposal facilities. It is believed that the required rule must be "generic," i.e., of National scope and not of a site specific nature.

The research described in the draft study report was designed to: (a) "test the viability of comparative risk assessment for hazardous waste management alternatives," and (b) "serve as a basis for making land disposal prohibition decisions for hazardous waste streams" (p. 1-2). The study contributed to the development and demonstration of comparative risk assessment methods by using a pilot study approach.

The model proposed is utilized for a specific waste by selecting a number of possible disposal technologies (scenarios) considered appropriate for the particular waste. For each waste and waste treatment scenario, existing models are used in combination to estimate waste releases, environmental transport of the released components of concern, and to identify the potential population exposed, and estimated doses to exposed individuals in that population. Further, the model then develops dose-response relationships for each waste component based on the best literature data available and, from this estimates human health risks by combining the exposure and dose-response information. Finally, the model is used to qualitatively evaluate ecological impacts of the selected scenarios. Using estimates of uncertainties in the human health risk estimates, an explicit estimate of the uncertainty of each overall estimate is made to permit decision-makers to take these ranges into account.

The Pilot Study considers for illustration three wastes, with four or five scenarios for management of each. While its potential utility and potential versatility were reasonably well represented in the pilot study, the method as presented represents a still-preliminary approach.

IV. EVALUATION OF THE METHOD AND ASSUMPTIONS

A. General Comments

Over the next five years, the Agency must determine which, of as many as 450, wastes or waste streams are to be evaluated to determine if they should not be "banned" from landfills. The OPPE states that the approach identified in the draft study report may be able to consider from 20 to 40 wastes or perhaps 5 to 10 percent of the wastes that may have to be evaluated. The implementation of this approach even to a small number of wastes will require significant effort involving extensive data-gathering and evaluation as well as significant judgmental evaluation of input and results. The effort to apply the OPPE method to selected wastes could be an excellent investment if it prevented suboptimal decisions that increase risks to human health or to the environment.

The approach makes an important contribution by attempting to estimate the relative risks in all media, since, if the land disposal option is banned, the wastes still have to be handled and disposed of in some manner. The approach can provide information concerning: (a) pretreatment alternatives that can be considered before land disposal, (b) the relative impact of other disposal alternatives on protection of human health and the environment, (c) relative costs involved, and (d) data and research needs that can reduce the uncertainties involved in estimating the relative risks.

It will readily be appreciated that this approach is necessarily data- and resource-intensive. Analysis of each scenario for each waste requires detailed knowledge of the available technologies of disposal and detailed knowledge of the existence and use of many submodels: fugitive emissions from landfills; solute transport in groundwater; dispersion models for air transport; dose-response and health affects, and many others.

OPPE is to be commended for undertaking such an important evaluation, for its early judgment to support such a detailed study, and for its wisdom of continued support for the study. The study clearly has had good intellectual input, the individual components appear sound, and reasonable estimates of potential health risks appear to have been obtained. The study also has considerable fallout value. Even if not applied solely to the banning decision, the technique developed will be useful in many other situations. The task of risk assessment is to make the most credible possible statements about definable relationships, reducing uncertainty, and making explicit whatever uncertainty remains. This study accomplished these goals.

However, in terms of EPA needs relative to the waste banning decisions, it does not appear that the study approach can serve as the sole basis for the final decisions. The study approach can be used with one or more other approaches or methods to provide a broader perspective on those major wastes that may be banned from land disposal in order to protect human health and the environment. Such major wastes could be those that are of large volume, are of unique characteristics, may have an apparent adverse economic impact on an industry if banned from land disposal, and/or appear likely to cause a potential adverse human health and environmental impact if disposed of in another way. Other approaches may be able to more quickly evaluate a larger number of wastes and identify those for which more detailed evaluation is needed.

The study approach would provide the Administrator with a richer array of information on relative risks, intermedia transfer or costs when making decisions about which wastes should not be banned from land disposal.

B. Components of the Model and Model Linking

1. Random Walk Solute Transport Model

The Random Walk model was selected to predict two-dimensional contaminant transport in groundwater aquifers. The horizontal flow field in the aquifer is computed using a finite difference technique. Solute transport is calculated using a population balance technique in which many particles are released and their fate simulated. The advective transport for each particle follows the flow field and dispersion is incorporated by random displacements. As the number of particles released becomes large, the spatial distribution of particles corresponds to the concentration profile of the constituent. The technique produces a solute concentration profile which should in theory (as the number of particles becomes large) be identical to that obtained with more traditional, two-dimensional advective-dispersive models using finite difference or finite element solution methods. Linear equilibrium adsorption is incorporated through the use of a retardation coefficient, and reaction is represented with a generalized half-life (i.e., multiply results by e^{-kt}).

The Random Walk model has been used in many applications and is a well recognized tool, for example, through its use as part of the program of the Holcomb Groundwater Research Institute. This provides confidence and credibility for its use. There are, however, limitations to the model that should be recognized, particularly as regards its treatment of chemical transformations of contaminants in the soil. A detailed review of Random Walk and other groundwater transport models was performed as part of a study sponsored by the Electric Power Research Institute (Kincaid and Morrey, 1984). A summary of this Random Walk review is included as Appendix D. Based on the EPRI analysis and a review of the Random Walk Model by the Committee's consultants, there is a major area of concern about the model's applicability. The model allows for a detailed characterization of two-dimensional flow profiles; spatial heterogeneity in hydraulic conductivity, storativity, etc. As mentioned in the OPPE presentation, the model allows incorporation of pumping-remedial action, which is useful for its intended applications. Similarly, a careful representation of dispersion is incorporated. As such, transport mechanisms are well represented, and the model is very appropriate for predicting the fate of "solutes"...constituents which undergo no chemical transformation. The reaction and adsorption components of the model, however, are much more limited. In particular:

a. In the Random Walk model, both the reaction rate and the adsorption (retardation) coefficient are constant over the aquifer study area. Heterogeneity in soil conditions which might affect these factors is not considered.

b. Unlike other numerical models where the chemical interactions are formulated as part of the finite difference or finite element equations, the population balance technique used in Random Walk is expressly designed for the case of linear, equilibrium adsorption and first order decay. The Random Walk model would require significant modifications to make it applicable to more complex chemical conditions. While nonlinear, non-equilibrium adsorption and higher order kinetics are not commonly incorporated in applied groundwater models today, they may be used in the future as our scientific understanding advances. It will be very difficult to incorporate these advances in the Random Walk model.

The limited representation of chemical processes relative to the detail given to transport processes should be recognized. It may reduce the applicability of the Random Walk model for certain kinds of problems in certain locations, particularly when chemical processes are non-ideal. The level of chemical representation is no better than that provided by the OSW model (and possibly worse, depending on the resolution of item b above). This limitation should be recognized.

To summarize, the use of the Random Walk model is acceptable, with the limitations noted. In addition, it should be noted that there are a number of other numerical codes which can simulate two-dimensional advective-dispersive transport. Those models utilize more traditional solutions of the material balance equation at a grid point or cell, and like the Random Walk model, can allow for non-homogeneous flow conditions, pumping wells, etc. Some users may be more familiar with the conceptual basis for these models, and they may be easier to adapt to situations where the use of more complex chemistry is appropriate. As such, alternative numerical models should be considered in future applications.

A final consideration applicable to the use of any numerical groundwater model, regards the limited level of validation, particularly for complex field conditions where constituents undergo chemical transformation. Successful attempts to verify models in the field have been made in recent years, though validation remains difficult and expensive. Some degree of field calibration and verification is recommended.

2. Modeling of Unsaturated Zone Transport

In the analysis presented in the OPPE report, the McWhorter-Nelson model is used as a basis for modeling transport in the unsaturated zone. The McWhorter-Nelson model, however, computes only a water recharge rate - no contaminant transport mechanisms are included. Contaminant transport is calculated in the OPPE examples by considering only the hydraulic residence time in the unsaturated zone associated with the computed recharge rate. This results in a step break-through profile, with no consideration for the effects of dispersion, adsorption (retardation), or reaction. Significant adsorption or reaction may considerably alter the pollutant washout profile from the unsaturated zone. An analysis which ignores these processes is not consistent with either the current state-of-the-art of unsaturated zone modeling, or the level of sophistication used in other components of the risk assessment. As noted in the OPPE report and the supporting MRI documents, there are models available for the unsaturated zone, such as the analytical PESTAN model, which incorporate dispersion, retardation, and decay. These should be utilized to generate more realistic estimates of the temporal breakthrough profile from the unsaturated zone.

3. Atmospheric Transport/Dispersion Models

Air pollution impacts are simulated using Gaussian plume models incorporating wind speed and direction, transverse and vertical diffusion (as a function of atmospheric stability class), terrain adjustment in certain cases, and plume-depletion and particle deposition processes. The selection of the Industrial Source Complex (ISC) Long-Term Model for area sources and the ATM model for point sources appears to be based on a careful and credible review of the current state-of-the-art of air modeling, and a full consideration of the capabilities of existing models. The ability to link the ATM model to population exposure estimates through the Graphic Exposure Modeling System (GEMS) is particularly beneficial. It is worthwhile to note that long-term average concentration profiles are sought (rather than short-term "event" concentrations), therefore, long-term versions of the models are utilized. The long-term versions use integrated forms of the Gaussian plume model based on the joint frequency distribution of wind speed, stability class, and wind direction.

Although the models selected represent the state-of-the-art in Gaussian plume modeling, there has been concern expressed among SAB members that the level of validation for this class of models has been limited.

4. Uncertainty Analysis

The propagation-of-error technique for evaluating uncertainty is formulated on the basis that links between model components occur in a multiplicative fashion. The assessment may effectively be represented by an equivalent, simplified model of the form:

$$\text{Risk} = \text{Pollutant Release} \times \text{Transport Factor} \times \text{Exposure} \times \frac{\text{Response}}{\text{Dose}} \times \text{Health Effects Factor}$$

Uncertainties in each component are assumed to be independent and are routed logarithmically. The method is correctly developed and implemented, assuming the multiplicative assumption is adequate. The technique has a number of desirable features, including its simplicity and direct use with "order-of-magnitude" judgments of uncertainty bounds. There may, however, be a need for a more careful consideration of the implications and limitations of the multiplicative assumption. This discussion is relevant as well to the integration issue (Appendix B, 2; Have the models been integrated (combined) without violating scientific principles? Is the integration consistent with the state-of-the-art?).

Two issues may be raised to illustrate possible difficulties with the multiplicative assumption for model linking. The first arises if and when thresholds are incorporated in the dose-response functions for health effects. A more sophisticated uncertainty routing procedure would then be required to account for the probability of zero impact (e.g., below threshold). The second issue relates to the temporal aspects of the analysis resulting from the stochastic nature of pollutant release in the Pope-Reid landfill liner failure model. (We were asked not to review the Pope-Reid model itself, but the incorporation of the model in the overall framework is important.) In the OPPE report, the results of replications of the Pope-Reid model are averaged to obtain a nominal temporal profile of pollutant release. It is then assumed that the use of a multiplicative uncertainty factor can capture the full range of uncertainty in both the amount of pollutant released and its temporal distribution. The validity of this assumption is not intuitively obvious, and needs to be demonstrated with a more detailed set of example simulations. In particular, it would be useful to evaluate transport simulations for each of the Pope-Reid replication outputs. The resulting "exact" distribution of concentration-exposure can then be compared to the lognormal distribution derived from the multiplicative assumption. This analysis is computationally intensive and should not be performed for all cases. Rather, the comparison should be demonstrated once to evaluate the adequacy of the simplified integration assumption; to build confidence in its use (or provide guidance for a better alternative).

The use of "one standard deviation" in the uncertainty analysis results in an 84 percentile concentration. This is fine so long as the scenarios are considered only in a comparative sense. If, however, the absolute level of impact is also evaluated (as is apparently the case from the OPPE report), then 84% seems too low for an "upper limit." The OPPE has indicated that it concurs with this suggestion and intends to use a wider confidence interval.

C. Toxicological Risk Assessment

Conceptually, the methods of health risk assessment as outlined in the OPPE report are appropriate tools. Quantitative risk assessment and quantitative uncertainty analyses are both desirable approaches. The dose/response assessment proposed by OPPE is innovative in that it estimates dose response functions for a spectra of adverse effects. Most other approaches used by the Agency either estimate dose/response functions for only a single effect, usually cancer, or are restricted to the estimation of an acceptable exposure limit (e.g., ADI, ambient water quality criteria, drinking water criteria). For the purposes of comparing risks with costs of hazardous waste alternatives, the estimation of dose/response functions for all significant effects should be encouraged if it leads to more fully and clearly using the available toxicity data. With several significant modifications, the OPPE approach could serve as a useful decision-making tool. As currently written, however, it has some serious flaws and could mislead rather than assist the decision-maker.

Concerns related to the OPPE methodology include: The use of a non-threshold model for all effects, the use of maximum likelihood estimates, and simplistic temporal, route-to-route, and species-to-species extrapolations. In addition, several areas in the methodology and application of the methodology require clarification. These include: the rationale for combining effects (i.e., independent vs. graded series); how quantitative estimates of uncertainty are made (mathematic or judgmental) as well as the validity of such estimates; details of how effects on which incidence data are not available will be handled in the risk assessment (in the case studies, such effects are ignored), and how data on pharmacokinetics and compound interactions will be used (in the case studies, such data are not considered).

These concerns have been discussed with OPPE personnel and their contractors. OPPE has indicated a willingness to alter their approach to constructively address these issues.

D. Fugitive Emissions, Leaks and Spills

The OPPE study attempts to address the risks from production of fugitive emissions, transportation over interstate highways and atmospheric emissions from capped landfills. Each of the primary references is based on a minimum of information. Indeed, OPPE shares in these SAB concerns (stated in a follow-up letter to the EEC). In addition, as off-site landfill and deep-well injection alternatives force more chemical wastes to be stored, transported and re-stored before ultimate disposal, the probability of risks will be magnified over previous experience. The inclusion of small-generator wastes, all of which will have to be transported, will further exacerbate the problem. The OPPE methodology needs a major effort to gather the information to adequately address these issues and their ramifications.

E. Application of the Model

The Committee is concerned that many of the specialized models (or submodels) required to apply the method may not be adequately verified or even verifiable. An example is the estimation of exposures resulting from handling of wastes in transportation, which both the Pilot Study and one's intuition would indicate as a major route of population exposures. One advantage of the OPPE framework is that its modular nature permits the substitution of improved models and data as they become available.

APPENDIX A

U.S. ENVIRONMENTAL PROTECTION AGENCY
SCIENCE ADVISORY BOARD
ENVIRONMENTAL ENGINEERING SUBCOMMITTEE

WASTE BANNING SUBCOMMITTEE

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Questions for SAB Review

1. Because of the many steps in the health risk assessment process, several models were used. Is the use of each of the following reasonable?

   a. The Farmer et al. equation for fugitive emissions from landfills;

   b. The Random Walk Solute Transport model for groundwater movement;

   c. The Industrial Source Complex Long-Term model for dispersion of air emissions from area sources;

   d. The ATM component of GEMS for dispersion of air emissions from point sources;

   e. The multistage model, with the one-hit model as a backup when data are limited, for dose-response functions;

   f. The Carcinogen Assessment Group potency factors, Wiebull model, and modified acceptable-daily-intake approach as sensitivity checks for the dose-response function selected; and

   g. The propagation-of-errors approach for evaluating uncertainty in the health-risk estimates.

2. Have the models been integrated without violating scientific principles? Is the integration consistent with the state of the art?

3. How can this approach be improved to better estimate risks for each management strategy for a given hazardous waste stream?

APPENDIX C

QUESTIONS RAISED BY DR. RAYMOND C. LOEHR
on
Proposed OPPE Method

Following are basic questions to which the Subcommittee can respond or comment:

1. Specific questions related to the specific model/approach with respect to its scientific, fundamental credibility (basically, is the approach scientifically sound).

2. Is this model/approach likely to address the important questions facing EPA, i.e. will the correct need be addressed?

Generally, the SAB is asked to respond to type (1) questions. This generally skirts the real basic issue and we should attempt to address the type (2) questions.

Therefore, in addition to the questions that have been placed before the Subcommittee, the Subcommittee should also consider addressing the following questions:

1. To what extent does the Subcommittee feel that this approach can be used for the banning decision - i.e., from the scientific or engineering basis and not from the policy aspects?

2. Are the'nodels that are proposed to be used the appropriate ones for the intended use? Have they been adequately peer-reviewed and verified by independent data?

3. Is the data base to be used adecuate from the standpoint of accuracy, OA/OC, etc.? Is there sufficient data that can be used with this approach?

4. Are there adeouate other models that can be used for other land disposal approaches, such as land treatment, waste piles, surface impoundments and all land disposal approaches listed in the RCRA amendments, i.e., really address whether the model/aproach can be used for other land disposal methods besides landfill?

It seems that these types of quest:ons also should be addressed by the Subcommittee.

If the Subcommittee decides to address some of the above issues, then at a future meeting it would be helpful if OPPE could address the following questions (or provide detailed discussion on these items) - it would be helpful to hear their explicit thoughts on these subjects for our consideration:

1. How would this approach be useful for the "banning" decision?

2. To what extent is it possible for the OPPE approach to be used for a generic situation, rather than on a waste-specific/site-specific situation?

3. To what extent have the models been verified, checked or peer-reviewed? Details should be provided on models such as the Pope-Reid model, or the Random-walk model, as used in their approach.

4. If the Subcommittee is to review/comment on applicability of certain models (see questions asked), then detailed information sbout the models needs to be provided to the Subcommittee.

TRANS - A Random Walk Solute Transport Model
for
Selected Groundwater Quality Evaluations

described in

GEOHYDROCHEMICAL MODELS FOR SOLUTE MIGRATION

Volume 2: Preliminary Evaluation of Selected Computer Codes

EA-3417, Volume 2
Research Projects 2485-2, 1619-1

Final Report, November 1984

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CODE: TRANS - A Random Walk Solute Transport Model for Selected Groundwater Quality Evaluations

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PROCESS AND INTERACTIONS: The processes and interactions addressed by this code are:

- Saturated groundwater flow in a singled confined or unconfined aquifer where water flow is typically horizontal. [The code addresses temporal variations in two-dimensional (x-y) flow for a variety of boundary conditions and arbitrary x-y geometry.]

- Advection of a chemical contaminant in a saturated groundwater system released from a variety of typical sources.

- Hydrodynamic Dispersion (both lateral and transverse) and diffusion of a chemical contaminant in a saturated groundwater system.

- Retardation of a chemical contaminant when it can be characterized by a constant K_d and the assumptions of instantaneous and reversible adsorption are adequate.

- Radioactive decay of a chemical contaminant.

OPERATIONAL ASPECTS: There are two main parts to the TRANS code: flow calculations and transport calculations.

Provisions for aquifer flow (potential or head) calculations are performed in four ways. Two methods (subroutines HSOLV2 and HSOLV4) compute head distributions for simple analytical problems. The third method is through the HSOLVE subroutine, which is a subroutine form of the Prickett and Lonnquist* flow model. This model is a well-documented, finite difference, groundwater flow model for simulating transient or steady-state groundwater flows in a water table or leaky confined aquifer. The fourth method supplies the aquifer's head distribution through a user-supplied program. Any other acceptable method or model can be used as long as head values are supplied for the same finite difference grid used in TRANS and for the same

* Prickett, T. A. and C. G. Lonnquist. "Selected Digital Computer Techniques for Groundwater Resource Evaluation." Illinois State Water Survey Bulletin 55, 1971.

hydraulic conductivity and effective porosity distributions supplied to TRANS. Velocity at every finite difference grid is calculated by:

$$V = KI/(7.48\ n) \tag{A-4}$$

where
- V = interstitial velocity
- K = hydraulic conductivity
- I = hydraulic gradient
- n = effective porosity.

Velocity at any other position in the system is interpolate using Chapeau-basis functions and the values at the finite difference grid points. Stability requirements for the flow portion of the model depend on the method chosen to develop the head (and subsequently the velocity) distribution. HSOLV2 and HSOLV4 are analytical solutions, but one must still ensure that adequate spatial sampling of these analytical solutions has been selected. HSOLVE uses a finite difference numerical scheme and a modified interative alternating direction method, MIADI, to solve for head distribution to a specified level of convergence at each timestep. Adequacy of a spatial and temporal time spacing can be checked in the same manner as for any finite difference or finite element scheme, by reducing grid spacing or timesteps and comparing results.

The transport model portion of TRANS uses a direct simulation technique. The concentration of a chemical constituent in a groundwater system is assumed to be represented by a finite number of discrete particles. Each of these particles is moved according to the advective velocity and dispersed according to random walk theory. The mass assigned to each particle represents a fraction of the total mass of chemical constituents involved. In the limit, as the number of particle approaches the molecular level, an exact solution to the actual situation is obtained. This kind of transport model is inherently mass conservative. Convergence can be checked by increasing the number of particles. There are restrictions, as with any numerical method, which limit the size of timestep that can be taken for both a time-dependent and spatially dependent problem. Timesteps for particles are limited such that advective plus dispersive movement is no greater than the spacing between velocity (head) nodes.

APPLICABILITY ASPECTS: The TRANS model allows the user to investigate groundwater pollution problems from a vertically averaged viewpoint for contamiants injected into wells, leaching fom landfills or arising from surface-water sources such as ponds, lakes, and rivers. The documentation for the TRANS program illustrates comparisons with theory for six problems:

1. Divergent flow from an injection well in an infinite aquifer without dispersion or dilution

2. Pumping from a well near a line source of contaminated water, with dilution but without dispersion

3. Longitudinal dispersion in a uniform one-dimensional flow with continuous injection at X = 0

4. Longitudinal dispersion in uniform one-dimensional flow with a slug tracer injected at X = 0

5. Longitudinal dispersion in a radial flow system produced by an injection well

6. Longitudinal and transverse dispersion in a uniform one-dimensional flow with a slug of tracer injected at X = 0

In addition, the documentation illustrates the use of the model for a real field-scale contaminant problem at Merodosia, Illinois.

SECONDARY CONSIDERATIONS:

Purpose and Scope

The purpose of this code (TRANS), as stated by the authors, is to provide a generalized computer code that can simulate a large class of problems involving convection and dispersion of chemical contaminants associated with fertilizer applications, hazardous waste leachate from landfilled and other sources, and injection of chemical waste into the subsurface using disposal wells. TRANS does not address density-induced convection. Concentration distribution in the aquifer represents a vertically averaged value over the saturated thickness of the aquifer.

TRANS addresses only a single aquifer. Spatial and temporal distribution of head in the aquifer can be calculated by four methods:

1. Analytic (HSOLV2) solution for a uniform 1-ft/d flow in the x direction

2. Analytic (HSOLV4) solution to the Theis formula centered at node (15, 15)

3. Numerical finite difference solution(HSOLVE) to the two-dimensional (x-y) vertically averaged groundwater flow equation* (this solution is for transient or steady-state flow)

4. User-supplied subroutine for reading or calculating head on the finite-difference grid used in the TRANS transport model.

The TRANS code was designed to solve real pollution problems and to address only single contaminants. TRANS can also handle (with slight changes in subroutine calls) radioactive decay and chemical retardation. The modifications required for decay are clear but those required for retardation are unclear. The code can handle contaminant source or sinks at every node as well as a variety of special sources, which include points, rectangles, circles, and lines. The flow model can handle impermeable boundaries (no flow), leaky

* Prickett, T. A., T. G. Namik, and C. G. Lonhnquist. "A Random-Walk Solute Transport Model for Selected Groundwater Quality Evaluations." Illinois State Water Survey Bulletin 65, 1981.

artesian source, induced infiltration (i.e., streams, lakes, and rivers), held-head boundary conditions, flow from springs, and evapotranspiration from the water table.

Operational Characteristics

The TRANS code is written in FORTRAN and run by the authors on a CDC CYBER-175. The code, for purposes of this study, was run on a Digital Equipment Corporation VAX 11/780. Other than changes to the program header, logical unit checker, and formatted character strings (which were all CDC-specific practices); conversion to the VAX required access to a system specific random number generator. A similar but not equivalent random number scheme was implemented. The authors indicate that the test problems included in the documentation examples took no more than a few seconds of CPU time, including compiling and loading on their CDC CYBER-175. TRANS used 140,800 bytes of virtual memory on the VAX; 10,363 central processing seconds were needed to perform the test problem simulation. The code, as documented, is dimensioned for a 29 x 30 finite difference grid and 5000 particles. These dimensions can be changed, however, to accommodate larger problems. Some difficulties may be encountered because instructions for increasing dimensions are not specifically discussed in the documentation.

Input Requirements

Input requrements for the code are explained with both appropriate text and in pictorial form (Figures 9, 10, 11, and 12 of Prickett et al.*). Input requirements for the code are those typically available from standard field or laboratory measurements. For the flow portion of the model they include:

- A variable finite difference grid description
- Timestep and number of timesteps to be run
- Areal distributions of
  --Permeability
  --Source aquifer potential for leaky artesian simulations
  --Aquifer bottom elevations
  --Aquifer top elevations
  --Head (initial conditions)
  --Aquitard thickness and permeability for leaky artesian aquifers
  --Simulations
  --Artesian and water table storage coefficients
- Pumping and recharge well locations and temporal rates
- Stream (river or lake) node locations, surface-water elevations, stream or lake bed thickness and permeability, fraction of node area available for transfer
- Constant head node locations and elevation for held head

* Prickett, T. A., T. G. Namik, and C. G. Lonnquist. "A Random-Walk Solute Transport Model for Selected Groundwater Quality Evaluations." Illinois State Water Survey Bulletin 65, 1981.

- Locations of springs, elevation at which spring flow begins, and slope of the spring flow versus ground-water head for the spring production line
- Locations of nodes where evapotranspiration from the water table is to be considered and the slope of the rate versus head line and the water-table elevation at which evapotranspiration effects are to be ignored.

For the transport model, additional input requirements include:

- Longitudinal dispersivity
- Lateral dispersivity
- Effective porosity
- Actual porosity
- Retardation factor or K_d
- Bulk mass density of porous medium
- Location and concentration of sources, description of source geometry, and selection of method for release of particles
- Sink locations and grouping of sink locations for summarizing outflow versus time results.

The model contains no checking of input for consistency and automatic termination for faulty or inconsistent inputs.

Output Results

Results are printed in a 132-character format with a concise and readable output layout. The code echos input parameters and produces line printer plots of head, numbers of particles, and concentrations. The code also reports the concentration of water entering sink nodes and groups of sink nodes versus time. The code produces no contour maps or output fields that can be passed on to other computer system programs for plotting and produces no mass balance summaries for water flow or transport.

Numerical Approximations

The general flow problem solution available with this code (HSOLVE) solves for head distribution in a leaky artesian or water-table aquifer for a heterogeneous, anisotropic porous medium with irregular boundaries. The actual system is approximated by finite difference methods based on a block-centered, variable finite difference grid. Medium properties in each grid block are assumed to be uniform. Approximation of the partial differential equation at each grid block by finite difference methods results in N equations in N unknown, where N is the number of grid blocks representing the aquifer. Time derivatives are estimated by an implicit finite difference method, and the water-table problem that results in nonlinear equations is solved by the modified iterative alternating direction implicit (MIADI) equation-solving method.

Once head distribution at the N grid blocks is obtained, the X and Y direction velocity midway between each grid block is calculated by

$$V = \frac{KI}{7.48\ n} \qquad \text{(A-5)}$$

where

V = interstitial velocity
K = hydraulic conductivity
I = hydraulic gradient
n = effective porosity.

The midgrid block X and Y direction velocities are then used in a bilinear interpolation scheme to estimate the velocity at any arbitrary location (x, y).

Transport is simulated by a direct simulation technique which involves movement of contaminant mass particles according to the convective velocity as interpolated from the convective velocity field described above. Dispersion is simulated by random walk methods. In the limit, as the number of particles gets extremely large (i.e., when the number of particles approaches the level at which each particle represents a molecule), an exact solution to the actual situation is obtained.

Assumptions and Simplification

We address the flow and transport separately. The principal assumptions regarding flow are:

- Darcian flow is assumed.
- Flow in the aquifer is horizontal and controlled only by hydraulic head gradients.
- Leakage between the simulated aquifer, rivers, lakes, other aquifers, and springs is a linear function of head difference with the slope of this relationship determined from the leakance parameter, K/m, where K is the permeability of the aquitard (or stream bed) and m is the thickness.
- Storage in the stream, lake, or river beds and aquitards is ignored.

The principal assumptions regarding contaminant transport are:

- The advection-diffusion equation for solute transport is assumed valid.
- Dispersion in porous media is a random process.
- Retention of a contaminant (or retardation of a concentration front) may be represented by an instantaneous and reversible sorption process.

Probabilistic or Statistical Aspects

The code solves a deterministic problem.

Available Documentation

McDonald, M. G., and W. B. Fleck. "Model Analysis of the Impact on Groundwater conditions of the Muskegon County Waste-Water Disposal System, Michigan." U.S. Geological Survey Open-File Report 78-79, 1978.

Prickett, T. A., and C. G. Lonnquist. "Selected Digital Computer Techniques for Groundwater Resource Evaluation." Illinois State Water Survey Bulletin 55, 1971.

Prickett, T. A., T. G. Namik, and C. G. Lonnquist. "A Random-Walk Solute Transport Model for Selected Groundwater Quality Evaluations." Illinois State Water Survey Bulletin 65, 1981.

Software Quality

The modular code consists of a main program, 20 subroutines, and three functions. The code listing is well annotated and the documentation report contains a complete description of each module, along with flow diagrams. Transfer of this program from one machine to another should be fairly easy. The code lacks any graphical output capability other than line printer plots. In addition, no routines are supplied to dump model output to disk files for use with generally available computer system plotting routines.

GENERAL CRITIQUE:

The documented verification test cases were easy to set up and repeat; however, direct checking of the results is not possible because a different random number generator is used on our computer system. The code does not produce any mass balance summaries.

In order to use the generated flow option of the TRANS code, one must obtain Bulletin 55 from the Illinois State Water Survey, which explains the vertically averaged solution for transient or steady flow. From an application point of view, the TRANS documents are difficult to follow. Examples are weak and the narrative descriptions are not straightforward. However, excellent code annotation compensates for limitations of the user's manuals.

Most of the data required by TRANS is typical groundwater survey information. The exception is the source term for the transport simulation, which needs a parcel release rate. This rate may be difficult to quantify for someone unfamiliar with 'random walk' models.

TRANS is very flexible with respect to problem configuration; thus, no modifications to the specified geometry were necessary. There were no problems encountered while running the code.