Vadose Zone Modeling Workshop Proceedings, March 29-30, 1993

R. Khaleel

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**Westinghouse
Hanford Company**

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VADOSE ZONE MODELING WORKSHOP

BACKGROUND

At the Hanford Site, the record of decision for remediation of CERCLA sites is largely based on results of the baseline risk and performance assessment of the remedial action alternatives. These assessments require the ability to predict the fate and transport of contaminants along appropriate exposure pathways which, in case of the Hanford Site, includes the migration of contaminants through the vadose zone to the water table. Listed below are some of the requirements, as prescribed by the regulators, relative to CERCLA risk and performance assessment at Hanford.

- o *"Assumptions and approximations used in the models or input data must be clearly documented by a thorough audit trail and the predictive uncertainties associated with these approximations should be quantified. This will aid in the understanding of model results and will provide a framework in which the predictive models can be improved as more and better data are collected and a better understanding of the site evolves."*
- o *"Data input to predictive models shall be of a quality acceptable to the regulators and of sufficient quantity to statistically describe spatial and temporal variability. This requirement will assure that uncertainty due to variable input can be quantified and, as more and better data are collected, gradually reduced."*

The information required in support of site characterization and risk assessment tasks for the RI/FS work at various operable units includes, among others, a characterization of soil hydraulic properties and development of vadose zone flow and transport models. Due to the broad scope and complexity of these tasks and their application to most, if not all, operable units, they fall outside the scope of any individual operable unit RI/FS work plan and are better addressed in a well-organized, comprehensive, and coordinated site-wide effort. The tasks identified in the TPA milestone M-29-02 document, "Groundwater Model Development Plan in Support of Risk Assessment," DOE/RL-91-62, December, 1991 are in support of the requirements prescribed by the regulators.

A workshop was organized by the Environmental Risk and Performance Assessment Group, Westinghouse Hanford Company on March 29-30, 1993 at the Richland Best Western Tower Inn. During the workshop, an assessment was made of the need for and scope of various tasks being conducted or planned as part of the Hanford Site waste isolation performance assessment/risk assessment activities. Three external, nationally-recognized experts served as part of a review panel for the workshop: a. Professor Lynn Gelhar of MIT, b. Professor Peter Wierenga of University of Arizona, and c. Dr. Rien van Genuchten of U.S. Salinity Laboratory, Riverside, California. The technical experts provided their perspectives on the current state-of-the-art in vadose zone flow and transport modeling. In addition, the technical experts provided an outside independent assessment of the work being performed or planned in support of various activities identified in TPA Milestone M-29-02.

This document includes the following:

- o Recommendations from the three peer reviewers.
- o Areas of expertise of the three peer reviewers.
- o Workshop agenda.
- o Copies of viewgraphs (where available) from presenters at the workshop.
- o Workshop minutes.
- o List of workshop attendees.

RECOMMENDATIONS FROM THE THREE PEER REVIEWERS

WHC-MR-0420

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Agriculture

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April 13, 1993

Dr. Raz Khaleel
Westinghouse Hanford Co.
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Richland, WA 99352

Dear Raz:

Enclosed is my report about the Vadose Zone Modeling Workshop. I trust that my comments are interpreted in a constructive manner and eventually will help to improve interactions and productivity at the site.

Please let me know how else, at any point in the future, I can help your program at WHC. Again, I enjoyed the discussions in Richland and hope that something constructive will come out of the meeting.

Sincerely yours,

Rien van Genuchten
Research Leader

Enclosures

Comments by M. Th. van Genuchten regarding the

VADOSE ZONE MODELING WORKSHOP

ENVIRONMENTAL RISK AND ASSESSMENT GROUP
WESTINGHOUSE HANFORD COMPANY
RICHLAND, WA

March 29-30, 1993

My comments below are based on information provided in TPA Milestone M-29-02 document "Groundwater Model Development Plan in Support of Risk Assessment, "DOE/RL-91-62 (December 1991), and on information given by investigators during the above two-day workshop (March 29-30, 1993). This material was insufficient for me to get a clear view of the scope and depth of all activities. Hence, several of my comments are of a very preliminary and somewhat superficial nature. Nevertheless, I hope that they will benefit ongoing and planned activities at the Hanford Site. Several comments directly or indirectly address organizational and program integration issues, while others focus on more specific technical issues.

1. From the presentations at the workshop it is clear that some excellent basic and applied research is being carried out, especially in the site characterization and modeling areas. Creative work is clearly needed to conceptually understand, measure and model water flow and chemical transport at Hanford in view of the deep and highly heterogeneous unsaturated zone. Expertise to carry out the necessary work is certainly available among scientists and engineers at Westinghouse Hanford Company and its collaborators including Pacific Northwest Laboratories.

While the expertise is available, there appears to be a lack of coordination and integration of site-wide activities. Improved coordination appears needed both "horizontally" across institutional and disciplinary barriers among the researchers site-wide (Comment No. 2), and "vertically" in a program integration sense involving researchers, managers and especially regulators (No. 3).

2. Informal technical meetings or internal seminars, including workshops such as the present *Vadose Modeling Workshop*, are important mechanisms for interaction and feedback to, and dialogue among, scientists and engineers at what I would like to call the "grass-roots" level. Such opportunities for information exchange at the grass-roots level should be provided on a regular (e.g., monthly) basis, and possibly with input and scrutiny from outside researchers. The purpose of such meetings is not to satisfy regulatory milestones, but to provide feedback to, and interaction among, scientists and engineers. They provide a mechanisms to identify and address shortcomings in current research plans and procedures related to specific topics, e.g., recent developments in modeling, coordination of computer codes, review of instrumental methods, clarify data needs for modeling purposes, and provide informal reviews of progress. It is imperative that the discussions be relatively open to, and at times with active participation from

outside researchers. I believe that such informal grass-roots interaction will increase research productivity and effectiveness, and will also increase morale among the scientific staff.

3. Comment 2 pertains to interaction among scientists. In addition, I believe that there is a major need for improved site-wide program integration. Since multiple groups, institutions, and interests are involved (WHC, PNL, USGS, on-site and off-site contractors, scientists, managers, regulators), effective interaction and communication between these different parties is critical. In part because of institutional barriers, there appears to be a lack of coordination among scientists involved in field data collection activities, laboratory analyses of field samples, and modeling efforts. Lack of coordination seems to be exacerbated by a lack of communication between researchers and regulators. Researchers should be given a high degree freedom to interact with peers across institutional and disciplinary barriers. Examples which could benefit from improved coordination are area-wide characterization of the unsaturated hydraulic properties (see also comment No. 4), the modeling efforts (No. 5), and improved communication between modelers and experimentalists. It seems that at present no specific individual or group is responsible for this type of integration and communication. Hence, I strongly recommend that some type of area-wide coordination or oversight committee be put into place. It is imperative that researchers, managers and especially regulators representing different groups participate in such an oversight committee.

It is crucial for the site-wide oversight/coordination committee to realize that the ultimate goal of activities at the Hanford site is the long-term safe management and/or cleanup of radioactive and other wastes, and that these goals may go beyond satisfying certain CERCLA RI/FS procedures and TPA Milestones. The committee should ensure that data collection and modeling activities are commensurate with each other. The ultimate goal of a data collection program is not to satisfy a long list of data appearing in a pre-determined list for the RI/FS process, but for use by modelers to make risk assessments, predict future events, or investigate the appropriateness of alternative remediation strategies. In other words, data collection, sample analysis and use by modelers is an ongoing dynamic process which requires continued and intense interaction.

The committee can help immensely by facilitating communication among scientists site-wide as advocated under comment No. 2, and especially between scientists and regulators. While "data input to predictive models shall be of a quality acceptable to the regulators...", it is imperative that they also be acceptable to the scientific community at large. I am afraid that if the broader approach is not taken now, it is not unlikely that eventually the entire CERCLA RI/FS process and the usefulness of TPA milestones will be questioned. Acceptance by the scientific community at large requires scrutiny and feedback from the scientific community. This also means the participation of Hanford scientists in professional meetings and publication of research results in the

open literature. Payoff of such an open perspective are easily documented.

I am stressing these points in part also because of my impression that much work is being done to physically get soil samples from the field, but that a comprehensive analysis of the samples and their use in RI/FS modeling is not commensurate with the expensive field sampling program (notable regarding the deep drilling effort).

4. This comment relates to hydraulic properties measurements. Hydraulic property estimation is an area of work where area-wide coordination is a especially important. A wealth of high-quality data is currently being collected, but by different groups, for different purposes, and for different waste sites. I propose that a site-wide hydraulic or soils database management system be established. This database should be continually updated and regularly distributed among the various parties and researchers involved (including modelers, field people, laboratory personnel). The database should contain all measured hydraulic and related data such as the measured particle-size distributions and other information affecting the hydraulic properties.

The database eventually may yield enough information to correlate the hydraulic properties with soil textural information at the Hanford site. While fractal approaches appear useful, other approximate indirect methods also exist which correlate the hydraulic properties with soil texture and related properties such as organic matter content, bulk density, and soil mineralogy (Rawls et al., 1992; Baumer, 1992, Carsel, 1992). Again, a site-wide database is a prerogative for such an effort.

Area-wide coordination of hydraulic measurements also will permit comparisons of different methods for measuring the hydraulic properties of soils, e.g., predicted results based on measured retention data (Khaleel), and measured results obtained using Tempe-cell type samples (Relyea), and the centrifuge method (Conca).

Some other comments related to the hydraulic properties:

- a. Hydraulic properties currently are measured mostly on small cores. I believe that it is important that eventually a field experiment be carried out to measure the unsaturated soil hydraulic properties in situ. The standard approach would be to implement a instantaneous profile type (or gravity drainage) experiment, although other methods are also available. Several promising scaling procedures (Shouse et al., 1992; Vogel et al., 1991) are now available for analyzing the hydraulic properties of layered or otherwise heterogeneous soil profiles. Although the in-situ experiments are generally limited to measurements in the upper few meters of soil (they could be easily extended to deeper layers at Hanford), they should give more realistic field estimates of the hydraulic properties, and provide a comparison with the core measurements in the laboratory. The field experiment could be implemented using neutron probes, tensiometers were applicable (may not work well in gravel), TDR, and other instrumentation.

- b. There should be a site-wide delineation/inventory of soil textural heterogeneities and their hydraulic characterization using a combination of direct and indirect measurements. Some of the small core hydraulic data by Conca show extensive vertical differences in hydraulic conductivity. This information could be extrapolated laterally using information of soil textural stratification and, with some additional theoretical work, provide a means for estimating the anisotropy in the macroscopic scale hydraulic conductivity. The bottom line here is to synthesize/extract as much information as possible from available field samples, especially the very expensive samples coming from the deep boreholes. Again, this effort requires some creative and publishable developmental research.
 - c. The accuracy of the predicted hydraulic conductivity functions obtained with the van Genuchten-Mualem equations should be validated at low water contents. The predicted conductivity equations should be matched with a measured value (or measured values) at relatively low water contents (data of the type collected by Conca provide appear excellent for this purpose). Matching the equations at saturation is not realistic because (1) the saturated hydraulic conductivity, K_s , may be a poor indicator of unsaturated hydraulic conductivity at low water contents because of the dominant effects of soil structure on K_s and (2) the need for extrapolating to conductivities close to the average recharge rates at the Hanford Site. Some of these issues are discussed by Luckner et al. (1989).
 - d. An accurate description of the hydraulic properties at low water contents is important. A two-phase (air-water) flow description may be needed for the prevailing water contents at Hanford. If the single-phase Richards' equation is used, problems surrounding the residual water content (θ_r) must be addressed. I know that some work in this area has been done by Gee and colleagues at PNL, or is being done, but this was not discussed at the workshop.
 - e. Anisotropy in the unsaturated hydraulic conductivity may not be an important issue for steady-state vertical flow simulations. However, anisotropy is important for single high-intensity point infiltration events when the soil profile controls the infiltration rate (e.g., spills and leaks such as those at the 241-T-106 tank site).
 - f. Similarly, very precise estimates of the hydraulic conductivity may not be needed for long-term flow simulations close to steady state. The most important issue is then having accurate estimates for the recharge rate (q_0) and precise estimates of the effective water contents throughout the vadose zone.
5. Area-wide coordination is also needed in the modeling area. It may be worthwhile to implement a centralized modeling group which continually improves and updates adopted computer codes, and which provides support to smaller units involved in the application of models to specific waste sites. It is my feeling that the use of public-domain codes should be preferred (e.g., the PORFLO set of codes), so that there is in-

house expertise and less reliance on outside contractors. This will also facilitate a more immediate and expeditious adaptation of the models to the various waste sites. Again, this approach presumes that institutional barriers can be eliminated or kept to a minimum.

6. This comment addresses model validation and calibration. First of all, the possibility of true *model validation* is increasingly being questioned in the scientific literature. I believe that TPA Milestone M-29-02 document (DOE/RL-91-62) provides a realistic assessment of what can be done in the groundwater and vadose zone modeling area, except that the term "validation" should not be interpreted in the most strictest sense of truly being able to validate a particular model. The usefulness of the term "model validation" has justifiably been questioned (e.g., Konikow and Bredehoeft, 1992), although not by all (Maleszewski and Zuber, 1992; Beven, 1989). At a minimum, there should be a clear distinction (Narasimhan, 1987) between model verification (accuracy of the numerical methods used for solving certain differential or other equations), and model validation (accuracy and applicability of conceptual processes embedded in the adopted differential equations).

With all its shortcomings, it appears that the Richards' equation is still the model of choice for simulating variably-saturated flow, although variants are possible (e.g., for two-phase flow simulations involving water and air at very low water contents, or stochastic approaches). Some of the processes which likely will not be included accurately in the near future are, among other things, macropore flow, unstable flow at soil textural interfaces, small-scale heterogeneities; chemical and temperature effects on hydraulic properties (notable for liquids leaked from the tanks, two-phase air-water flow at low water contents), and root growth and root water uptake as a function of water stress. These complexities show that one must remain modest about model predictions, and that a high level of uncertainty will remain. It also means that model validation is a fairly site-specific exercise and, unless demonstrated otherwise, should hold only for similar initial and boundary conditions (e.g., similar recharge rates) as used for the calibration exercise.

The best use of models, then, is to consider them to be pragmatic tools in research and management. Ultimately, models are the most effective tools for getting a better understanding of the unsaturated zone at the Hanford site. Any prediction should be treated with some suspicion, yet as being the best available estimates, subject to continuous adjustment. No model should ever be declared "valid". This is because no model, however sophisticated, will ever represent reality since a model, by definition, is an approximation of reality.

For the above reasons, model calibration at the Hanford site should be a continuous, never-ending effort. An excellent example of model calibration involves the work by Gee and colleagues at PNL on estimation recharge (see also Comment No. 9). This type of model calibration and model use (not validation) could provide a good example

for other activities (e.g., modeling and model calibration at the tank farm).

8. The tailing (elution) part of the nitrate distributions below the 241-T-106 tank leak site may provide unique data for model calibration.
9. Current work by Gee and colleagues at PNL on recharge measurements (and related model calibration) is critical and should continue with a high level of priority. Real payoffs of this work is (was) only possible after many years or decades of persistent work. This research is now showing significant results. Perhaps different tracers could be added (e.g., Cl or Br at intervals of several years) to provide additional information many years from now. I disagree with Gee's disappointment that suddenly recharge was observed, but not "predicted" with the previously calibrated Richards' equation. This discrepancy does not validate or invalidate Richards equation (we know that Richards' equation has its problems but, again, it may be the best model available at present). I advocate a more pragmatic approach. The issue here is not the "validity " of the Richards' equation but how best to use this equation for analyzing the data, and then to extrapolate in time (or space), i.e., its use as a long-term management tool. Model calibration should continue in this case also because the initial calibration did not include time periods during which recharge was high. [Was there some preferential flow in the lysimeters? What about along the walls? Or could it be that the lysimeters were not completely at equilibrium until this relatively wet winter?].
10. Actual water contents should be used when simulating transport in the surface sandy gravel systems near tank site 241-T-106. While water contents and hydraulic properties may be measured without the gravel and stones, they must be corrected before their use in the actual simulations. Otherwise they will underestimate the actual pore-water velocities ($v = q_0/\theta$) in the simulations of contaminant transport below the leaking tank site.
11. A do-nothing baseline attitude may be unacceptable for certain situations. This is especially true for the high infiltration situation at the 241-T-106 tank leak site. The surface silty sandy gravel backfill layer induces 5-15 cm recharge per year, while the sloping (?) tank surface may further increase point recharge. This situation irreversibly promotes infiltration and increases the rate of transport of radioactive and chemical wastes into and through the vadose zone. This issue is a high-priority one and should be addresses without delay. Common sense says that some action is needed here.
12. Modeling radionuclide transport using the K_d approach may not be accurate. For example, Cs transport may be controlled by major ion chemistry. Complexing with chelating agents/solvents such as EDTA may lead to significantly lower K_d 's, and hence increased transport rates. Also, retardation factors (R) are functions of the water content and should not be taken constant over the whole profile or versus time.

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MEMO

4 April 1993

TO: Raz Khaleel, WHC, H4-14
FROM: Lynn Gelhar
RE: Vadose Zone Modeling Workshop, 29-30 March

Enclosed are copies of the transparencies I used during my talks at the workshop. In the following I have outlined a few quick points reflecting my initial impressions about the material presented at workshop. Please recognize that these comments are based on the limited written information. I may alter some of these points after having reviewed more explicit data and results.

- 1) Judging from the 200-BP-1 modeling effort, the parameters for the vadose zone modeling are not being derived in any systematic way from the field data on unsaturated hydraulic properties which are being collected at that site. The selection of parameters for the presumed homogeneous zones seems to be largely arbitrary and subjective, and consequently the model does not seem very defensible to me.
- 2) The elaborate model being used in the 200-BP-1 simulations seems to be far too complex and basically is incompatible with the crude input parameters which are being used. It would be more reasonable to begin with a series of simplified screening models of increasing complexity which are used systematically to identify the dominate transport process for this site.
- 3) It doesn't seem that the site characterization /data collection effort at the 200-BP-1 site is being designed at all to meet the needs of the modeling work. It seems to me that there should be much closer coordination between the field sampling activities and the modeling efforts.
- 4) A stochastic framework to design field sampling programs, evaluate

R. Khaleel
4 April 1993
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model parameters from small-scale field data, evaluate predictive capabilities of models, and assess model uncertainty would seem to be a much more defensible framework than the largely ad hoc and unrelated approaches which are currently being used to address these issues. The stochastic approach continues to be controversial, but I don't see any serious alternatives being put forth to address these issues in a unified fashion.

- 5) The program to measure unsaturated hydraulic conductivity is producing important new data that are essential if you are to be able to predict multidimensional transient flow and transport. The data clearly show that the standard van Genuchten/Mualem method (based on saturated conductivity and moisture retention data) fails dismally as a predictor of unsaturated hydraulic conductivity. This is in line with our experience and strongly suggests that unsaturated hydraulic conductivity must be measured directly.
- 6) The 200-BP-1 site seems to be marginal as a case study for model evaluation (validation); the currently available site characterization data are not likely to be adequate for this purpose.
- 7) The Injection Test Site experiment has a much better prospect of being useful for model evaluation; this effort should be continued and expanded. Some additional drilling to assess current moisture (neutron logging) and solute (cores) distributions would allow evaluation of independently developed model predictions.
- 8) Reliable predictions of recharge are central to most of the vadose zone modeling efforts. Continued field experimentation at the Hanford site on this problem is very important.
- 9) Formal and informal communication, coordination and cooperation among those working on the vadose zone at Hanford should be enhanced. The vadose zone seminar suggested by Pete Wierenga would certainly be worthwhile.

THE UNIVERSITY OF
ARIZONA

TUCSON ARIZONA

April 12, 1993

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Dr. John A. Rawlins, Manager
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P.O. Box 1970
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Dear Dr. Rawlins:

Please find enclosed my outside, independent assessment of the activities of the Environmental Risk and Performance Assessment Group of Westinghouse Hanford Company as presented at the Workshop on March 29 and 30, 1993.

I don't believe that I ever got the Tri-party agreement milestone M-29-02 document and so I cannot comment on this document.

I did get the "Groundwater Model and Development Plan in Support of Risk Assessment" published December, 1991. This document is well written and complete and shows a good insight in models, model development, and validation issues.

If you have further questions on my report of the Workshop, please contact me at my office in Tucson, (602) 621-7228).

Sincerely yours,

Peter J. Wierenga
Professor and Head of Department

PJW:jer
Enclosure

Comments by Peter J. Wierenga, University of Arizona
Third Party Review
Environmental Risk and Performance Assessment Group
Westinghouse Hanford Company

March 29 and 30, 1993

The purpose of the Workshop was to review the activities of the Environmental Risk and Performance Assessment Group of Westinghouse Hanford Company. Many of the activities conducted by this group were represented in a clear and adequate way. However, this reviewer would have greatly benefited from an overview at the beginning of the workshop of the waste disposal problems at the Hanford site, before the presentations of individual programs. A map showing the major problem areas would have been most helpful. Without such an overview, it becomes difficult for outside reviewers to place a particular site within the context of the waste disposal problems at the Hanford site.

It would have also been most useful to have a high official of DOE give a presentation on what DOE plans to do, over the next several years, about improving the waste situation at the Hanford site. Without such an overview, it appeared that the present studies are done somewhat in isolation and that the group is working in a vacuum. This comment is similar to the comment made by Dr. Weeks during the third-party technical review conducted in 1989. In the 1989 report, Dr. Weeks commented that a well-thought out staged data collection program in support of site-wide system understanding seems to be lacking. From the two-day workshop in March, 1993, it is not clear that such a well-thought out data collection program is now in place, although considerable data on vadose zone hydraulic properties are now being generated.

A second comment, which was also made by Dr. Weeks in 1989, is that people responsible for data collection in the field or in the laboratory are not closely working with people responsible for model development and testing. In programs such as these, it is absolutely imperative that modelers and experimentalists work closely together. The experimentalists need to know which data are required for the various models and the modelers need to know which data realistically can be expected from the experimentalists.

The lack of interaction between modelers and experimentalists seems to go beyond just these two groups. This reviewer perceived a lack of interaction between scientists operating at the Hanford site. Collaboration between various scientists at Westinghouse and at PNL also needs to be encouraged. This can be accomplished by seminars, workshops, and funding of cooperative projects. For example, a seminar series on vadose zone hydrology could be considered.

More specifically, the following:

1. Modeling should be site specific. It might also be useful to employ simplified models including analytical solutions, as first approximations to understanding the phenomena observed at a particular site. Many analytical and numerical models already exist, which

observed at a particular site. Many analytical and numerical models already exist, which could be used with good success without much modification. Lynn Collard and John Smoot showed good use of existing models.

2. In applying models to existing data sets, one should not only look at the retarded species such as cesium or strontium, but also at nitrates. Apparently large amounts of nitrates were disposed of in the cribs. The tail ends of the nitrate breakthrough curves may reveal a lot about the displacement of nitrate containing solutions by nitrate-free solution after the cribs were no longer used. This would give insight into total amount of water percolating through the cribs. The same should be done for tritium.
3. Rather than drilling expensive holes at a limited number of sites, I would prefer to have small diameter holes drilled for neutron access tubes, to measure the distribution of water below cribs or leaking tanks. The depth distribution of water under a tank or crib, is of importance for modelling solute transport to the groundwater. During installation of neutron access tubes samples could be collected and analyzed for tritium, nitrate, cesium, strontium and other elements.
4. The group seems to have made good progress in characterizing the unsaturated hydrologic properties of the soils at a number of sites. The data from these characterizations will be useful in vadose zone predictions of flow and transport. It is recommended, however, to consider using faster methods for determining the unsaturated hydraulic conductivity as a function of water content or tension. In particular, the upward infiltration method and the centrifuge method should be looked at in a systematic manner. Although neither of these methods have been around very long, they look promising and will greatly improve the speed with which the data can be obtained.
5. Dr. Glendon Gee has done an outstanding job in collecting data on recharge at the Hanford site. This work should be supported and continued for many years. Recharge is the driving force for contaminant movement to the groundwater table and a clear understanding of recharge under the various soil and vegetation conditions at the Hanford site is of great importance.
6. Scenarios should be developed to cover the cribs and tank sites to reduce recharge at these sites. This work should be started as soon as possible to reduce further pollution of groundwater at the Hanford site. Models such as UNSATH which take into account evaporation and evapotranspiration could be used for refining the various scenarios.
7. It would be useful to test all models used at the Hanford site with data from the Las Cruces Trench Site. Several scientists are presently testing their model with data from the Las Cruces Trench Site. Testing of models used at the Hanford site on this data set would give these models further credibility.

8. For model testing I prefer experiments on non-contaminated sites. Such an experiment should be done on a site where full control over the boundary and initial conditions is available and where the amount of water and solute added to the site can be precisely controlled. Such a site would also require adequate characterization of the physical and chemical properties before such a model testing experiment could be initiated. Testing a model at an existing site such as at a leaking crib site or a leaking tank site, is basically curve fitting, unless predictions are made and data are collected over time (e.g. 5-10 year intervals).

**AREAS OF EXPERTISE OF THE
THREE PEER REVIEWERS**

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VADOSE ZONE MODELING WORKSHOP

Panel members were carefully selected to provide a broad group of nationally and internationally recognized experts with individual and collective experience in stochastic hydrology, vadose zone hydrology, and soil physics. Further, members were selected to assure independence and, therefore, none were selected from Westinghouse, prime contractors at other U.S. Department of Energy Sites, or the U.S. Department of Energy.

Suggestions for panel members were provided by Westinghouse Hanford Company professionals and other nationally-known experts in the disciplines of interest. The technical areas of interest, the selected individuals, and their exclusive unique capabilities are as follows.

1. Lynn W. Gelhar

Ralph M. Parsons Laboratory
Department of Civil & Environmental
Engineering
Massachusetts Institute of Technology
Cambridge, MA 02139

Dr. Gelhar is a nationally and internationally recognized expert in stochastic groundwater hydrology. He is currently a professor at the department of Civil and Environmental Engineering, Massachusetts Institute of Technology. Dr. Gelhar has been awarded numerous research grants in the area of stochastic applications in groundwater hydrology by U.S. Environmental Protection Agency, National Science Foundation, Nuclear Regulatory Commission, United States Geological Survey, American Petroleum Institute, National Institute for Environmental Health, and Tennessee Valley Authority. He has received several highly-prestigious awards and honors from technical and professional societies. Dr. Gelhar has published extensively in peer-reviewed journals such as Water Resources Research, American Society of Civil Engineers, and Ground Water. His unique expertise in stochastic applications was of special interest to the vadose zone modeling workshop in addressing issues such as uncertainties in estimates of groundwater travel times and radionuclide release rates.

2. Peter J. Wierenga

Department of Soil and Water Science
University of Arizona
Tucson, AZ 85721

Dr. Wierenga is a nationally and internationally recognized expert in vadose zone hydrology. He is currently a professor and Head of the Department of Soil and Water Science, University of Arizona. Dr. Wierenga has been awarded numerous research grants by federal agencies such as U.S. Environmental Protection Agency, U.S. Department of Interior, National Science Foundation, and Nuclear Regulatory Commission. He has received several highly-prestigious awards and honors from technical and professional societies. He has conducted experiments at a variety of scales including laboratory columns and field scales. Dr. Wierenga was the Principal Investigator of the Las Cruces Trench

Site experiments. These experiments were designed to test a variety of models for predicting flow and transport in the vadose zone. Under his guidance, a large set of field data was collected and this data is now being used to test a variety of models. Several groups in the country are participating in this model validation effort including several national laboratories. Dr. Wierenga has published extensively in peer-reviewed journals such as Water Resources Research, Soil Science Society of America, and Soil Science. His unique expertise in vadose zone hydrology was of special interest to the workshop in addressing issues such as calibration and validation of vadose zone flow and transport models.

3. Martinus Th. van Genuchten

U. S. Salinity Laboratory
4500 Glenwood Drive
Riverside, CA 92501

Dr. van Genuchten is currently research leader at the U. S. Salinity Laboratory and an adjunct professor in soil physics at the University of California, Riverside. His expertise is in the areas of soil physics and hydrology, particularly as pertaining to the unsaturated (vadose) zone. Dr. van Genuchten is internationally known for his development and application of a variety of computer models and related software for predicting water flow and chemical transport in one- and multi-dimensional variably-saturated soil profiles. This work has focused on flow and transport in homogeneous soils, as well as on transport in structured media involving macroporous soils or unsaturated fractured rock. Dr. van Genuchten also developed several popularly used parameter estimation ("inverse") models for estimating the hydraulic and solute transport properties from more easily measured laboratory or field data. Additionally, he proposed a set of quasi-empirical functions to describe the hydraulic properties of unsaturated soils; the "van Genuchten" functions are being widely used in research and management to predict water flow into and through the vadose zone. Dr. van Genuchten has published extensively in peer-reviewed journals such as Water Resources Research, Soil Science Society of America, and Soil Science. He was elected Fellow in the American Geophysical Union, the Soil Science Society of American, and the American Society of Agronomy. His expertise was of special interest to the workshop since the "van Genuchten" functions are extensively used in vadose zone modeling work at Hanford.

WORKSHOP AGENDA

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VADOSE ZONE MODELING WORKSHOP AGENDA

Environmental Risk and Performance Assessment Group
Westinghouse Hanford Company
Richland, WA

March 29, 1993

Location: Richland Tower Inn

8:00 Opening remarks

- o Welcome - John Rawlins, WHC
- o Introduction of Panel members - John Rawlins, WHC (10 min.)
- o Workshop Agenda - John Rawlins, WHC (15 min.)
- o Statement of workshop goals and objectives - Raz Khaleel, WHC (15 min.)

8:40 Performance/Risk Assessment Overview

- o Types of wastes and waste sites - Raz Khaleel, WHC (20 min.)
- o Performance/risk assessment at a CERCLA site at Hanford - Len Collard, WHC (30 min.)

9:30 BREAK (15 min.)

9:45 Vadose zone modeling issues

- o What are the issues? - Raz Khaleel, WHC (30 min.)

10:15 Code Calibration/Validation Issue

- o What constitutes a validation experiment? - Lynn Gelhar, MIT (45 min.)
- o Discussion - Rien van Genuchten, U.S. Salinity Lab., Riverside (30 min.)

11:30 LUNCH BREAK

1:00 Code Calibration/Validation Issue (Cont'd.)

- o Las Cruces Trench Experiment - Peter Wierenga, Univ. of Arizona (40 min.)
- o Injection test site at Hanford - Allen Lu and Raz Khaleel, WHC (30 min.)
- o 241-T-106 Tank Leak - John Smoot, PNL (20 min.)

2:30 BREAK (15 min.)

2:45 Code Calibration/Validation Issue (cont'd.)

- o A calibration/validation proposal - Charley Kincaid, PNL (30 min.)
- o Open Discussion on Calibration and Validation Issue

VADOSE ZONE MODELING WORKSHOP AGENDA

March 30, 1993

Location: Richland Tower Inn

8:00 Modeling Data Requirements

- o Laboratory measurement of hydrologic properties - John Relyea, WHC
(30 min.)
- o Unsaturated hydraulic cond. measurement - Jim Conca, WSU/TC
(30 min.)
- o Use of van Genuchten-Mualem relationships - Raz Khaleel, WHC
(30 min.)
- o Use of Arya-Paris model to generate moisture retention data -
Ben Volk and Raz Khaleel, WHC
(30 min.)

10:00 BREAK (15 min.)

10:15 Modeling Data Requirements(Cont'd.)

- o Dispersivity estimates (Lynn Gelhar, MIT - 45 min.)
- o Open Discussions (1 hr.)

12:00 LUNCH BREAK

1:00 Modeling Data Requirements(Cont'd.)

- o Evaluating uncertainty and spatial variability (Lynn Gelhar, MIT)
(45 min.)

1:45 Open Discussions

- o Wrap-up, Feedback, Summary
- o Other modeling issues: Use of Kd's, Recharge estimates, moisture-dependent anisotropy.

3:00 BREAK (15 min.)

3:15 Executive Session (ER and ERPA personnel, DOE-RL, and regulators).

- o Summary
- o Objectives 2 and 3

COPIES OF VIEWGRAPHS

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TYPES OF WASTES AND WASTE SITES

RAZ KHALEEL
WESTINGHOUSE HANFORD COMPANY

LIQUID WASTES DISCHARGED AND SOLID WASTES BURIED AT HANFORD: 1944-1989

- 1.7 trillion liters (444 billion gallons) of water and liquid wastes discharged to the soil from all sources.
- 625,000 cubic meters (820,000 cubic yards) of solid wastes buried in three general locations over a 429-acre area.
- Liquid wastes discharged through the use of cribs, trenches, ponds, and ditches, as well as through leaks and spills.

LIQUID WASTES DISCHARGED AND SOLID WASTES BURIED AT HANFORD: 1944-1989

- Contaminated sites contain 5.6 million curies of radioactivity. Much higher quantities of radionuclides have actually been discharged, but those with a short half-life are not represented in the 5.6 million curies.
- Radioactive liquid contaminants include cesium, strontium, tritium, iodine, technetium, uranium, and plutonium. Some of the chemical contaminants are nitrates, sodium, phosphate, sulfate, ammonia, fluoride, and carbon tetrachloride.

VADOSE ZONE MODELING WORKSHOP OBJECTIVES

WHY FOCUS ON MODELING ISSUES?

- Predictive reliability is essential because real-time testing to confirm the waste disposal design and to confirm the long-term predictions is impossible.
- Regulatory requirements do indeed provide a major focus for performance assessment. However, it is important to achieve an appropriate level of understanding of the technical basis in predicting isolation potential of a waste site.
- In any predictive effort, in the interest of available resources and time, there must be a compromise between the additional data needed and the loss of predictive reliability when the additional data are not available.

VADOSE ZONE MODELING WORKSHOP OBJECTIVE 1

Develop a consensus position by all "stakeholders" (technologists, end users, and regulators) on the scope of, need for, and results of tasks being conducted or planned as part of the activities identified under TPA milestone M-29-02 document, DOE/RL-91-62. In particular, the following questions need to be answered:

- *Are the data collected to date sufficient to provide a technically defensible performance/risk assessment modeling in support of a CERCLA Record of Decision (ROD)? (Yes or no?)*
- *If the answer is "no", what is the appropriate level of site characterization data and code calibration/validation work necessary to justify technically defensible performance/risk assessment activities?*

**VADOSE ZONE MODELING WORKSHOP
OBJECTIVE 2**

Obtain a commitment from all stakeholders to support (according to each attendee's individual responsibilities) the results, findings, and/or recommendations of the workshop.

- *Will the Environmental Restoration Program (and other funding sources) commit to continued funding in support of resolution of the vadose zone modeling issues?*

**VADOSE ZONE MODELING WORKSHOP
OBJECTIVE 3**

Identify action items that each stakeholder must perform to ensure that the results, findings, and/or recommendations of the workshop are realized.

- *How do we get from where we are to where we need to be?*
- *Who needs to do what by when to assure that the results of the workshop are executed as agreed upon and as planned?*

**VADOSE ZONE MODELING
ISSUES**

**RAZ KHALEEL
WESTINGHOUSE HANFORD COMPANY**

**VADOSE ZONE MODELING ISSUE:
CODE CALIBRATION/VALIDATION**

- Flow and transport codes that are currently being used in performance assessment evaluation of a waste site are not calibrated and validated to have sufficient confidence in their ability to predict contaminant migration.
- Limited data for code calibration/validation are available at Hanford but have not been fully utilized.

**VADOSE ZONE MODELING ISSUE:
EVALUATE APPLICABILITY OF MODELS
TO ESTIMATE UNSATURATED K's**

- Current approach uses a single measurement of saturated hydraulic conductivity, combined with laboratory-measured moisture retention data, to predict the unsaturated K's over the entire range of moisture content.
- Approach untested for unsaturated soils with conductivities varying routinely over several orders of magnitude.

**VADOSE ZONE MODELING ISSUE:
DISPERSIVITY ESTIMATES**

- Literature data for saturated media suggest that dispersivities tend to increase with the scale of experiment. Also, lab measurements on dispersivity are much smaller than those based on field tracer experiments.
- Representing macrodispersion over large distance and time scales in heterogeneous unsaturated media by "constant" values of dispersivity appears to be questionable.
- Under unsaturated conditions, it is reasonable to expect that dispersivities will increase as the scale of the experiment increases as observed in case of the saturated flow.
- Few field-scale dispersivities have been reported for the unsaturated media. Possible use of one of Hanford's "unplanned tracer test" to estimate dispersivities?

**VADOSE ZONE MODELING ISSUE:
UNCERTAINTY AND SPATIAL VARIABILITY**

- Uncertainty refers to lack of knowledge about the variation in input data and in the accuracy of models used. Sources of uncertainty include measurement error, lack of understanding of physical processes of the system, and extrapolation into the distant future.
- Spatial variability refers to variability of sediment properties as characterized by the statistical properties of the spatial distribution such as the mean, variance, and spatial correlation lengths.

**VADOSE ZONE MODELING ISSUE:
EVALUATE APPLICABILITY OF PSD DATA
IN ESTIMATING MOISTURE RETENTION**

- Presence of a significant correlation between the particle size distribution (PSD) and moisture retention can potentially lead to a large cost reduction in site characterization activities aimed at obtaining moisture retention data for various operable units.
- Demonstrate the success (or failure) of using existing models (e.g., Arya-Paris technique) of translating the particle size distribution data to moisture retention curves. Bulk density as well as the particle-size distribution are the only data needed for application of the Arya-Paris model.

**VADOSE ZONE MODELING ISSUE:
 K_d/R_d APPROACH**

- Lack of detailed knowledge about site-specific geochemical conditions, and the difficulty of incorporating detailed geochemical reactions in transport calculations, result in use of K_d/R_d approach.
- Using constant values of K_d in transport calculations for both saturated and unsaturated media.
- Using K_d 's measured under laboratory conditions that are vastly different from those likely under field conditions.

**VADOSE ZONE MODELING ISSUE:
EVALUATE MOISTURE-DEPENDENT
ANISOTROPY**

- Variable, moisture-dependent anisotropy in unsaturated soils is an effective, large-scale (macroscopic) flow property resulting from media textural heterogeneities at a smaller scale.
- For unsaturated media, lateral K to vertical K ratio is enhanced with a decrease in moisture content of the soils; i.e., the anisotropy increases with a decrease in saturation.
- If it is demonstrated that the moisture-dependent anisotropy is a significant process for Hanford soils, appropriate credit can be assigned to account for such a phenomenon in computing groundwater travel times and radionuclide flux rates.

MOISTURE-DEPENDENT ANISOTROPY FOR HANFORD SOILS: INJECTION TEST SITE

RAZ KHALEEL
WESTINGHOUSE HANFORD COMPANY

MACROSCOPIC ANISOTROPY BASED ON STOCHASTIC THEORY

Yeh et al., (1985)

$$\frac{K_{11}}{K_{22}} = \exp \left[\frac{\sigma_f^2 - \sigma_\beta^2 H^2}{1 - \lambda A \cos \gamma} \right]$$

- σ_f^2 = variance of $\ln K$, random field,
- σ_β^2 = variance of the slope of the $\ln K$ vs. ψ relationship
- H = mean value of ψ ,
- λ = correlation length for both $\ln K$, and β random field in the direction perpendicular to stratification,
- A = mean slope of $\ln K$ vs. ψ , and
- γ = angle between the soil layer stratification and the horizontal.

WCPB106-202

FIGURE 6. Well Numbering Scheme.

INJECTION SITE SLUG TEST DATA

INJECTION SITE SLUG TEST DATA: Ksat Histogram Results

INJECTION SITE PERMEAMETER DATA Ksat Histogram Results (N=19)

Injection Site Permeameter Data: K_{sat} Probability Plot

Injection Site Slug Test Data: K_{sat} Probability Plot

INJECTION SITE SLUG TEST DATA

Experimental and Fitted Variograms

INJECTION SITE DATA

INJECTION TEST SITE: Anisotropy vs. Mean Pressure head

K_r vs. Ψ_i - Injection Test Site : Sample 1-1417

**Performance/Risk Assessment
at a CERCLA Site at Hanford**

Len Collard
Westinghouse Hanford Company

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Figure 7-3: Overview of the Remedial Investigation/Feasibility Study Process.

58812 008 002

- I. OVERALL RI/FS PROCESS
- II. DESCRIPTION OF OPERATIONS
- III. SITE SAMPLING - VADOSE ZONE
- IV. LABORATORY TESTING
- V. SELECTION OF SAMPLES FOR TESTING
- VI. MODELING APPROACH
- VII. MODELING DOMAIN
- VIII. RESULTS

WHC-MR-0420

Figure 1-1 Hanford Site Map

4 Acres

B43 - B49 : low-level waste from tributyl phosphate process in 221-U. Sludge from 241-BY tanks transferred to U Plant, dissolved in nitric acid, and extracted with TBP. Acid solution was made alkaline. Wastes were treated with potassium ferrocyanide as a cesium scavenger. Supernatant was decanted to B43 - B49. 11/54 - 12/55

B50 - B57 : In tank heating of 241-BY tanks created evaporates which were condensed and discharges to B50 and B57. 3/65 - 1/74

Estimated Waste Quantities Discharged to Cribbs in the 200-BP-1 Operable Unit

Total Liquid Effluent Discharged		Other Suspected Waste Constituents	
Liters	1.7304x10 ⁹	⁹⁹ Tc	Unknown
Chemical Disposed	Quantity (kg)	Tributyl Phosphate	Trace
Sodium	2,650,500	Paraffin Hydrocarbons	Trace
Nitrate	6,501,500		
Sulfate	469,000		
Phosphate	332,000		
Ferrocyanide	18,900		
Ammonium Nitrate	10,000		
Ammonium Carbonate	21,000		
Radionuclide Inventory (April 1, 1986)		Quantity (Curies)	
³ H		2499	
⁹⁰ Sr		6054	
¹³⁷ Cs		2092	
⁶⁰ Co		0.4490	
²³⁹ Pu		4.0457	
²⁴⁰ Pu		1.0918	
²⁴¹ U		0.1806	
¹⁰⁶ Ru		0.00009	
Total Beta		16,179.2	
Total Alpha		<0.000005	

Sr90 FLUX FOR 200-BP1 CRIBS Excluding B-50 and B-57

LIQUID DISCHARGE TO 200-BP1 CRIBS

200-BP-1 RADIONUCLIDE INVENTORY

from WORK PLAN

WHC-MR-0420

SR-90

CO-60

H-3

3/27/93

U238

PU239/240

CS-137

216B43A.XLS Chart 3

216-43a

Cribs 216-B-43 through 216-B-50 Construction Details

WHC-MR-0420

HB 108010.2F

Not to scale

Source: Hoffman 1992

913 1/64/26682/1 1 43

Figure 2-1. Task 2 and 4 boring locations

200-BP-1 Vadose Zone Crib Borehole Contamination Control Methodology

299-[33]-38 A' South

Preliminary Plume Map - Nitrate (1st Quarter 1991)

WHC-MR-0420

H8106018.BF

200-BP-1 ESTIMATED COSTS (\$Millions)

Total ~ \$20 Million

WHC-MR-0420

RLS Spectral Gamma-Ray Borehole Survey

Project: 200-EP-1

Log Date: Jan 27, 92

Borehole: 299-E33-296 (E-43A)

Anal. Date: Aug 20, 92

RADIONUCLIDE LOGGING SYSTEM

- I. IN SITU CHARACTERIZATION PROBE - 5 INCH DIAMETER PIPE
- II. APPROXIMATELY \$10,000 EACH
- III. CESIUM 137, COBALT 60, AND OTHERS
- IV. QUICK TURNAROUND
- V. STILL DEVELOPING TECHNOLOGY

RLS Spectral Gamma-Ray Borehole Survey

Project: 200-BP-1

Log Date: Jan 27, 92

Borehole: 299-E33-296 (B-43A)

Anal. Date: Aug 20, 92

RLS Spectral Gamma-Ray Borehole Survey

Project: 200-BP-1

Log Date: Sept 5, 92

Borehole: 299-E33-302 (B-49A) Anal. Date: Jul 20, 92

RLS Spectral Gamma-Ray Borehole Survey

Project: 200-BP-1

Log Date: Sept 5, 92

Borehole: 299-E33-302 (B-49A)

Anal. Date: Jul 20, 92

RLS Spectral Gamma-Ray Borehole Survey

Project: 200-3P-1

Log Date: Sept 5, 1972

Borehole: 299-E33-302 (E-49A)

Date: 11/20/82

RADIONUCLIDE LEVELS FOR B49A LABORATORY MEASUREMENTS (pCi/g)

—■— Sr-90 —+— Cs-137 —*— Co-60
 —■— Pu239/240 x— Total U

Table 25. Parameters of Interest, Analytical Methods and Acceptable Detection Limits for the 200-BP-1 Operable Unit Remedial Investigation.

Analyte	Soil		Water	
	Method	Detection	Method	Detection
Radionuclides				
Total alpha	9310 ^a	6 pCi/g	9310 ^a	4 pCi/L
Total beta	9310 ^a	3 pCi/g	9310 ^a	3 pCi/L
Tritium	—	—	906.0 ^b	500 pCi/L
Technetium-99	b	0.5 pCi/g	901.1 ^b	15 pCi/L
Strontium-90	b	0.15 pCi/g	905.0 ^b	3.3 pCi/L
Cesium-137	b	0.6 pCi/g	901.0 ^b	23 pCi/L
Cobalt-60	b	0.02 pCi/g	901.1 ^b	10 pCi/L
Plutonium-238	b	0.0001 pCi/g	901.1 ^b	0.75 pCi/L
Plutonium-239/240	b	0.009 pCi/g	901.1 ^b	0.75 pCi/L
Total uranium	b	0.3 pCi/g	908.3 ^b	0.5 pCi/L
Ruthenium-106	b	0.2 pCi/g	909.1 ^b	3 pCi/L
Nonradionuclides				
Nitrate	300 ^a	1 µg/g	300 ^a	500 µg/L
Total cyanide	9010 ^a	0.5 µg/g	9010 ^a	10 µg/L
Sulfate	300 ^a	1 µg/g	300 ^a	500 µg/L
Selenium	7740 ^a or 7741 ^a	0.5 µg/g	7740 ^a or 7741 ^a	5 µg/L
Ferrocyanide	d	0.5 µg/g	d	10 µg/L
Free cyanide	d	1.0 µg/g	d	10 µg/L
Bismuth	303A ^a	10.0 µg/g	303A ^a	50 µg/L
Phosphate	ASTMD-4327	1.0 µg/kg ^f	ASTMD-4327	500 µg/L

^aMethod from Test Methods for Evaluating Solid Waste (EPA 1986).

^bMethod from Prescribed Procedures for Measuring Radioactivity in Drinking Water (EPA 1980).

^cMethod development required; detection limits must be at or below minimum concentration in standards for drinking water as defined in 40 CFR 141 (EPA 1986).

^dIon chromatography with amperometric detection.

^eMethod from APHA (1980).

^fFrom current Annual Book of ASTM Standards (ASTM 1989).

200-BP-1 TOP GRAVEL BIN

200-BP-1 TOP GRAVEL BIN

200-BP-1 4 LAYER MODEL

200-BP-1 4 LAYER MODEL

200-BP-1 SAND BIN

200-BP-1 SAND BIN

200-BP-1 SCENARIO A RECHARGE RESULTS FROM T106 STUDY

PHYSICAL PROPERTY TESTS

BULK DENSITY / POROSITY
SPECIFIC GRAVITY FOR PARTICLES

SATURATED HYDRAULIC CONDUCTIVITY
MOISTURE RETENTION (no unsaturated hydraulic conductivity tests were run)

CALCIUM CARBONATE CONTENT
IN SITU MOISTURE CONTENT

PARTICLE SIZE DISTRIBUTION

COLUMN LEACH
SORPTION

OTHER PHYSICAL PROPERTY DATA (from literature)

DISPERSIVITIES

MOLECULAR DIFFUSION

SPECIFIC STORATIVITY

RADIOACTIVE DECAY RATE

UNTESTED DISTRIBUTION COEFFICIENTS

TABLE 1. Summary of K_d Data Specific to Hanford.

Species	Ambient Conditions			High Ionic Strength, Alkaline	High Acid/Organic
	Probable K_d (ml/g)	Range in K_d (ml/g)	Quality of Data (a)	Range in K_d (ml/g)	Range in K_d (ml/g)
$^3\text{H}(\text{HTO})$	0.0	0.0	1	0.0	0.0
$^{137}\text{Cs}^+$	500	500-10,000	2	1-200	1-200
$^{90}\text{Sr}^{2+}$	20	5-100	2	0.3-20	0-20
$^{60}\text{Co}^{2+}$	2000	1000-10,000	2	200-2000	10-200
Bi^{3+}	1	unknown	4	unknown	unknown
UO_2^{2+}	1	0-3	3	0-500	unknown
$\text{Pu}^{(b)}$	100	100-2000	3	100-2000	1-100
$^{99}\text{TcO}_4^-$	0	0-1	2	0-1	0-1
HCN	0.1	unknown	4	unknown	unknown
HPO_4^{2-}	50	20-100	3	20-100	0-10

(a) Quality Rating

- (1) K_d values are very well known, little chance for variation because of chemical changes.
- (2) K_d values are well known, variability caused by competing salts, pH, Eh and organics generally understood.
- (3) K_d values are fairly well known, variability caused by chemical factors (competing salts, redox, organics etc.) not well documented.
- (4) K_d values are not known, probable value is purely an educated guess.

- (b) The Pu oxidation state was not characterized and many forms can co-exist for Hanford ambient conditions $\text{PuO}_2^+ > \text{PuO}_2^{2+} > \text{Pu}^{4+} > \text{Pu}^{3+}$ is likely. Most waste streams at Hanford would produce soluble Pu species with $\text{PuO}_2^+ + \text{PuO}_2^{2+} > \text{Pu}^{4+} + \text{Pu}^{3+}$. Some organic-rich Hanford waste streams could solubilize Pu^{4+} species.

SELECTION OF SAMPLES FOR TESTING

- I. Provide Data for Major Layers to be Modeled
- II. Problems and Difficulties
 - A. Individual Sample Integrity and Representativeness
 - B. Use of Multiple Liners
 - C. Lack of Data in Hot Zone
 - D. Possible Overdriving of Sampler (bulk densities > 2 g/cc)
 - E. True Behavior of Gravels
 - F. Sensitivity of Laboratory Technique
 - 1) Moisture Retention Sample Size
 - 2) Equipment Available

*4. Bulk Density to use with
Moisture Retention Data*

MODELING APPROACH

- I. Conceptual Model - Composite Soils, Single Crib
- II. Computer Program Selection
- III. Contaminants of Concern
 - A. Inventory
 - B. Screening Process
- IV. Scenarios - Conservative, but Not Unrealistic
 - A. Start with Reported Inventory
 - B. Low K_d from range
 - C. Vertical Movement to Groundwater
 - 1. Isotropic
 - D. Lateral Migration
 - 1. Anisotropic
 - 2. "World" Model for Interactions
 - E. Recharge Rates
 - 1. T106 study - average 13 cm/yr. max 22.5 cm/yr (16 cm/yr average precipitation rate)
 - 2. 1 cm/yr
 - 3. 10 cm/yr (preliminary biota barrier)

(2D) || Print || SR_KD10A.PLT ||

MESH AND SELECTED PROPERTY VALUES

3D Model with symmetry in X and Y

Nodes: x=10, y=10, z=50

MESH FOR SINGLE CRIB WITH HORIZONTAL SYMMETRY

sandy Gravel
Ksat=883.01 m/yr

Sand
Ksat=157.68 m/yr

Silt Ksat=0.66 m/yr
silty sandy Gravel
Ksat=1324.5 m/yr

(2D) || Print || Ostart.plt ||

235 m/yr to crib (3 months)

Crib 5 cm/yr initial infiltration

200-BP-1 Crib Fluid Boundary Conditions 3D Model with symmetry in X and Y

Horizontal Distance (m)

APPENDIX 2

Table 5-10. Results of Comparison of Present-Day Predicted Versus Measured Concentrations.

Contaminant	K_d (mL/g)	C_w		Predicted		Measured	
		Units	Units	C_s	Units	$C_{s,med}$	Units
THP	4	1×10^4	$\mu\text{g/L}$	4×10^4	$\mu\text{g/kg}$	1.6×10^4	$\mu\text{g/kg}$
C6-HO	0.5	5×10^4	$\mu\text{C/L}$	2.5	$\mu\text{C/g}$	9.9	$\mu\text{C/g}$
C6-137	500	1×10^6	$\mu\text{C/L}$	5×10^5	$\mu\text{C/g}$	1.2×10^6	$\mu\text{C/g}$
SF-90	20	1×10^6	$\mu\text{C/L}$	2×10^6	$\mu\text{C/g}$	2.4×10^6	$\mu\text{C/g}$
Total U	1	5×10^4	$\mu\text{C/L}$	.50	$\mu\text{C/g}$	.59	$\mu\text{C/g}$

C_w = Concentration in water
 C_s = Concentration in soil = $C_w \times K_d$
 $C_{s,med}$ = (CL soil concentration presented in Table 4-20 for the crib grouping, 216-B-43 through 216-B-50) and (the subsurface infiltration gravel/soil zone).

Uncalibrated Sr90 Model Results Apr, 92

B-45 8/30/92

WHC--MR-0420

Lab values converted by dividing by Kd of 20 ml/g

200-BP-1 TIME HISTORY FOR CO60 IN UNCONFINED AQUIFER

Kd=0.15 mL/g Recharge = 1 cm/yr

\\F:\111\passlum_lab.pl\passlum_rls.plt //

B57 CS-137 LABORATORY AND RLS CONCENTRATIONS (pCi/L)

B57 SIEVE DATA

CRIB BASE AT 16.5 FEET

CS-137 CONC IN SOIL

XY Top Plane - Gravel

B57 $K_r/K_v=2$ 1 cm/yr

CS-137 CONC IN SOIL

XY 2nd Plane - Gravel

B57 $K_r/K_v=2$ 1 cm/yr

CS-137 CONC IN SOIL

XY 3rd Plane - Sand

B57 $K_r/K_v=2$ 1 cm/yr

B57 TRENCH CESIUM 137 - 2D ANALYSIS w/ SYMMETRY

June, 1973 - end of operations

CONC IN SOIL

$K_h/K_v = 2$ all
 $K_d = 2000$ ml/g all

913-1764/27009/12-30-92

Figure 5-9. Finite Difference Mesh for Scenarios A and B.

3.75" I.D. Split Spoon WHC-MR-0420

Physical Samples - Every 10' OR LITHOLOGY CHANGE

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REV 1

FIGURE 11: Sampling scheme for Crib 216-B-43 and 216-B-49.

Table 4-17. Maximum Detected Concentrations of Radionuclides of Potential Concern in each Crib within the Subsurface Infiltration Gravels/Soils (15+ ft.). (Sheet 1 of 2)

CRIB	DEPTH in (ft)	RADIONUCLIDES in $\mu\text{Ci/g}$											Total U	Th-228	Tc-99	Sr-90	Ra-226	Pu-239+240	Pu-239	Pu-238	K-40	Cs-137	Co-60	Sb-125	Cr-51
		Sb-125	Co-60	Cs-137	K-40	Pu-238	Pu-239	Pu-239+240	Ra-226	Sr-90	Th-228	Total U													
216 B-11	566.5 (18.5-24)			3100000		86		105		2000000		308													
	889.6 (29.3-5)				16.9				2.91		0.887														
	171.178 (6.58-9)	1.12								210															
	481.488 (15.8-60)		2					626		6500000		95.3													
216 B-11	627.6 (22-25)																								
	526.1 (17-20)			6300000		109		9950		5900000															
	616.4 (20-21)				15.6				1.81		0.731														56.6
	829.1 (27-30)	23.1	2.72				0.12																		
216 B-16	165.5 (15-18)				11.2			227		350000		35.3													
	586.7 (19-22)		2.2	3600000		6.91																			
	829.1 (27-30)	50.1					0.12		2.11		0.516				120										
	707.9 (23-26)					203		5850		11200000		311		50											
216 B-18	556.1 (18-20)									10700000		223													
	586.7 (19-22)																								
	889.7 (29-32)	13.1	0.028	103			0.022		3.61		0.853														
	526.1 (17-20)			1600000		11		588		2000000		121													
216 B-19	829.1 (27-30)						0.011		3.71																46.3

Table 4-17. Maximum Detected Concentrations of Radionuclides
of Potential Concern in each Cub within the Subsurface Infiltration Gravels/Soils (151 ft.) (Sheet 2 of 2)

CUB	DEPTH in (ft)*	RADIONUCLIDES in pCi/g												Total U	Ct 51
		Sb-125	Co-60	Cs-137	K-40	Po-238	Po-239	Pu-239+240	Ra-226	Sr-90	Tc-99	Th-228			
216-B-49	14.3-14.9 (47.49)	39.9										1.17			
	22.9-23.8 (75.78)		103		16.5					160					
	4.9-5.5 (16.16)			2000000 2		5.06		249	570000						
216-B-50	5.8-6.4 (19.21)		28.6										22.6		
	8.2-8.8 (27.31)	7.6			14.7		0.21		338	132	0.609				
	16.6-1 (15.20)						0.01			67			3		
216-B-57	8.2-10.1 (30.13)			620000		0.086		0.003	892	60	0.875				
	15.1-17.2 (56.86)				16.6										
	Total Number of Data Cts	10	24	30	11	37	8	38	26	58	40	43	92		

* Depths listed are the depth range to which the maximum contaminant concentration was found for a given cub. More than one borehole and/or sample may be required by a given depth range.

* Depths listed are the depth range in which the maximum contaminant concentration was found for a given cub. More than one bandhole and/or sample may be represented by a given depth range.

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CALIBRATION/VALIDATION OF VAM3D MODEL
USING INJECTION TEST DATA AT HANFORD

Allen Lu and Raz Khaleel

- o Injection Test Site (RHO-ST-46; Sisson and Lu, 1984)
- o Graphical Presentation of the Field Data
- o Modeling Scenarios
- o Model Evaluation Criteria
- o Samples of Model Results and Comparisons

FIELD EXPERIMENT

- o The Injection Test Site is in the 200 East Area
- o About 1000 gal of water were delivered for each of ten consecutive weekly injections.
- o A 20-mL solution of the radiological tracers ^{85}Sr and ^{134}Cs were mixed and injected.
- o Field data was obtained by lowering sensors to the desired depths in the observation wells.
- o Soil samples taken from the two monitoring wells during drilling were saved. In situ conductivities were determined in wells adjacent to the test site.

Figure 1. Well Sounding Scheme

Cumulative Volume of Injected Tracer Solution

Field Measurement

Field Measurement

Field Measurement

Field Measurement

Six different model simulation scenarios were evaluated:

- 1) Uniform isotropic soil with soil properties given by averages obtained from soil core data from test site.
- 2) Uniform but anisotropic soil with saturation dependent anisotropy incorporated in the model.
- 3) Non-uniform (10 layers), but isotropic soil.
- 4) As Scenario 3, except that the effect of hysteresis is accounted for in the model simulation.
- 5) Non-uniform, but anisotropic soil with saturation dependent anisotropy incorporated in the model.
- 6) As Scenario 5, but only saturated hydraulic conductivities were allowed to be anisotropic.

MODEL EVALUATION CRITERIA

- o A visual comparison of field data and simulated results in (A) contour plots; and (B) historical plots.
- o A spatial moments (Kool and Wu, 1991) of water content will be computed and compared.
 - o The zero-order moment is used to measure total mass change in the chosen simulation domain.
 - o The first-order moments is used to indicate the change in location of radial and vertical center of mass of the water plume, respectively.
 - o The second-order moments is used to measure the water spreading in the horizontal and vertical directions, respectively.

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VAM2DH FLOW FOR SISSON-LU FIELD SIMULATION (HYTERESIS)
MATERIAL TYPE TABLE

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4
4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4
4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4
4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4
5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7
7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7
7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7
8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8
8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8
9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9
10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10

X POSITION (M)

0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0 8.5 9.0 9.5

Y POSITION (M)

0.0 -2.0 -4.0 -6.0 -8.0 -10.0 -12.0 -14.0 -16.0 -18.0 -20.0

ANISOTROPY (M-I21)

Radius=2m Depth=600cm

ANISOTROPY (M-I21)

Radius=4m Depth=600cm

ANISOTROPY (M-I21)

Radius=1m Depth=600cm

ANISOTROPY (M-I21)

Radius=3m Depth=600cm

$K_h / K_v = 1$

Radius = 2m Depth = 720cm

$K_h / K_v = 1$

Radius = 4m Depth = 720cm

$K_h / K_v = 1$

Radius = 1m Depth = 720cm

$K_h / K_v = 1$

Radius = 3m Depth = 720cm

WHC-MR-0420

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THREE-DIMENSIONAL SIMULATIONS OF CONTAMINANT PLUMES IN THE SANDS AND GRAVELS UNDERLYING THE HANFORD SITE, WASHINGTON

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ABSTRACT

Approximately 450 m³ of liquid containing radioactive and chemical wastes leaked from the 241-T-106 single-shell tank into the vadose zone at the U.S. Department of Energy's Hanford Site in southcentral Washington in 1973. Single-shell tanks at Hanford are buried in generally coarse-grained sediments that overlie Columbia River basalts in the Pasco Basin. The extent of ¹³⁷Cs, ¹⁴⁴Ca, and ¹⁰⁶Ru contaminant plumes in the vadose zone were estimated in 1973 and 1978 by gamma spectrometry in monitoring wells. Moisture retention and radionuclide transport properties were estimated from measurements of soil samples elsewhere at Hanford.

Three-dimensional, transient PORFLO-3 simulations of plume migration were conducted to model the transport of ¹⁰⁶Ru and ¹³⁷Cs from 1973 to 1990. The model domain measures 90 x 88 x 51 m in the x, y, and z directions, respectively. At this scale, each soil layer within the domain is assumed to be of constant thickness. No flow is allowed across the vertical boundaries of the domain. The water table forms the lower boundary, and pressure is assumed to remain fixed at the atmospheric value. A uniform infiltration is applied to the upper surface of the model. The tank itself is represented as an impervious block, allowing infiltrating water to be diverted around the tank.

Simulations for ¹⁰⁶Ru and ¹³⁷Cs approximated the 1973 measured distributions, but the simulated ¹⁰⁶Ru distribution for 1978 extended

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deeper than reported values. The simulated 1978 distribution of ¹³⁷Cs approximated the measured distribution. The 1973 and 1978 distributions are similar due to the long half-life and high sorption coefficient of ¹³⁷Cs.

INTRODUCTION

Hydrologic flow and transport computer codes will be used to develop mathematical models from data collected at U.S. Department of Energy (DOE) sites to evaluate the effects of proposed waste disposal activities and the effectiveness of proposed remediation measures. Of primary interest will be the application of numerical codes for pre- and post-closure high-level nuclear waste repository performance assessment at Yucca Mountain, Nevada, and for performance assessment of several decades of defense wastes housed at several DOE sites across the country. One of the codes recently developed by staff at the Pacific Northwest Laboratory for use at DOE sites is PORFLO-3 (Runcini and Sagar 1983; Sagar and Runcini 1989). PORFLO-3 was designed to analyze flow and transport in complex, variably saturated three-dimensional hydrogeologic settings. Availability of data on contaminant plumes in the vadose zone is rare. The present work is an initial benchmarking of the code using data on a leak of liquid radioactive wastes into the vadose zone at DOE's Hanford Site.

The Hanford Site, located in southcentral Washington State, has been dedicated to nuclear projects since the early 1940s. Chemical processing of spent nuclear fuel has resulted in the accumulation of large inventories of chemical, nuclear, and mixed wastes at the site. From 1949 to 1984 most of the liquid waste was stored in 49 underground tanks. Single-shell tanks are so named because their concrete structure houses a single layer of carbon-steel lining. In contrast, more recently constructed tanks (1970s) have two carbon-steel linings and are called double-shell tanks.

The first leak of a single-shell tank was detected in 1983. Since then 16 single-shell tanks have been reported to have leaked. One of the

biggest leaks was detected in June of 1973 in the 241-T-108 single-shell tank located in the T Tank Farm in the 200 West Area. Based on the monitoring of liquid levels inside the tank, it was estimated that approximately 435 m³ (115,000 gallons) of liquid containing radioactive and chemical wastes was discharged to the soil (AEC-RL 1973; ARHCO 1973; Gillette 1973). Observation holes were drilled around the leak site to delineate the contaminant plume. Concentrations of radionuclide species were estimated from total gamma energy in the observation holes in 1973 (ARHCO 1973) and 1978 (Routson et al. 1979). The objective of the present study is to use this field data with the PORFLO-3 code to calibrate a complex numerical model of the T-108 tank site.

SITE HYDROGEOLOGY AND MODEL INPUT

Single-shell tanks at Hanford are buried in generally coarse-grained sediments that overlie Columbia River basalts in the Pasco Basin. The sediments are divided into the Miocene-Pliocene Ringold Formation and overlying Pleistocene Hanford formation, separated by a distinct layer known as the Plio-Pleistocene unit. The Ringold Formation is generally coarse-grained but with occasional thin layers of fine sand or silt with small amounts of clay. Caliche is observed in both the basal Ringold Formation and Plio-Pleistocene unit. The Hanford formation contains a very coarse-grained flood facies called the Pasco Gravel and a finer-grained facies known as the Touchet Beds.

Leakage from the T-108 tank appears to have been contained within the 51-m vadose zone; therefore, the modeling analysis will focus on transport through the vadose zone. The vadose zone in the vicinity of the tank can be divided into five major layers. The single-shell tanks at the T Tank Farm were backfilled with a 12-m-thick layer of silty, sandy gravel that includes a 2- to 3-m layer over the tank. This disturbed zone is underlain by about 8 m of pebbly, very coarse-to-medium sand, 4 m of coarse-to-medium sand, 14 m of calcareous silt and fine sand, and 23 m of sandy gravel. The fourth layer of calcareous silt and fine sand may contain a well-developed caliche horizon of

sufficiently low permeability to significantly inhibit the downward movement of moisture.

In the horizontal plane, the model domain extends to about four or five tank diameters ($d = 22$ m) beyond the tank. At this scale, each soil layer within the domain is assumed to be of constant thickness. No flow is allowed across the vertical boundaries of the domain. Thus, on the scale of the model domain (~ 20 m), the flow is vertical. However in the vicinity of the leak, it is fully three-dimensional in nature. The water table forms the lower boundary for the model. The pressure at this boundary is assumed to remain fixed at the atmospheric value. A uniform infiltration is applied to the upper surface of the model. The tank itself is represented as an impervious block. This allows the infiltrating water to be diverted around the tank. Thus, in a local zone around the perimeter of the tank, the volumetric flux may be significantly enhanced.

The flow and transport properties of the soil through which the plume migrates constitute critical input data for the model. Such properties specific to the T-108 tank site are not available. However, several small catalogs of properties for Hanford soils exist. The textural descriptions from a catalog of six Hanford soil moisture characteristic curves (Sewart et al. 1987) were compared with the textural description of the five soil layers identified at the T Tank Farm. The saturated hydraulic conductivities of the soils in the catalog range between 1 and 40×10^{-2} m/day. The selection of soil moisture characteristics from this catalog is very qualitative and biased by the small range of selection in the catalog. Consequently the absence of T-108 site-specific data introduces an undetermined amount of uncertainty into the modeling.

The transport coefficients are estimated for each of the five major soil horizons. For all model layers the Fickian molecular diffusion coefficient D is held constant at 1×10^{-5} m²/s, and longitudinal and transverse dispersivity is held constant at 1 and 0.1 m, respectively.

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For those model simulations incorporating retardation, a distribution coefficient (K_d) of 5×10^{-7} m³/g (0.5 mL/g) was used for ¹⁰⁶Ru and 1×10^{-4} m³/g (100.0 mL/g) for ¹³⁷Cs.

At or near the base of the southeast side of the T-106 tank, approximately 435 m³ of supernate containing various radionuclides leaked into this soil column during an approximately 50-day period in the late spring of 1973 (Routson et al. 1979). The most mobile constituent in the tank was ¹⁰⁶Ru; by the summer of 1973 it had migrated about 15-20 m laterally and about 20 m vertically below the southeast base of the tank (ARHCO 1973). For purposes of modeling, release was assumed to occur at an uniform rate over the leak duration. The tank was assumed to be an impermeable zone within the flow field; the contaminants were introduced into the soil column along a portion of the southeast base of the tank where data indicates the leak originated.

SIMULATIONS

Model calibration started with a final simulation incorporating all of the collected data. The initial simulated ¹⁰⁶Ru plume appeared to be bigger than the actual plume. When the generic saturated soil vertical hydraulic conductivities in all five model layers were reduced by a factor of two, the 1973 ¹⁰⁶Ru simulated plume was approximately similar to the measured plume. A smaller saturated hydraulic conductivity is justifiable due to the higher viscosity of the leaked fluid compared with that of water assumed for the simulation.

Using the modified hydraulic conductivity, the ¹⁰⁶Ru plume migration was then simulated from 1973 to 1989. Following the reasonable approximation of the 1973 plume, the 1978 measured plume for ¹⁰⁶Ru could not be matched. The measured plume for 1978 indicates little migration of the ¹⁰⁶Ru plume from 1973. The modeling results, however, indicate that the plume expands significantly in 1978. The simulations indicate that by the early 1980s, the plume extends through the low-permeability model layer 4. Because ¹⁰⁶Ru may exhibit

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a small sorption on Hanford soil, an alternate calibration using a K_d was also performed. The resulting retardation factor produced a reasonable calibration to the 1973 ¹⁰⁶Ru plume but was again insufficient to keep the calculated ¹⁰⁶Ru plume stationary in 1978 and beyond. Recession of the plume due to radioactive decay is evident by the early 1980s for both cases but is most pronounced in the K_d simulation.

Both simulations, however, indicated a significant widening of the plume by 1978. This result appears to be the consequence of high initial inventory of ¹⁰⁶Ru. Adjustment of the inventory may produce a matching 1978 plume; however, this adjustment was not tried. There may also be other explanations, such as use of non-site-specific soil properties in the model and errors in measured data. Further investigation of these input parameters may be warranted.

The 1973 simulated plume for ¹³⁷Cs was similar to the measured values using the standard input with the K_d for ¹³⁷Cs sorption. Due to sorption, the calculated ¹³⁷Cs plume was found to be static not only in 1973 but also in 1980. Consequently, the model results indicate that the plume would only penetrate several meters below the base of the tank and would become essentially stationary within about a month after the tank was pumped out, stopping the leak.

SUMMARY

Availability of data on plumes in the vadose zone is rare. The T-106 tank leak data provide a good opportunity to test the applicability of numerical models to contaminant transport in the vadose zone. The ARHCO code used for this analysis incorporates a complex set of equations for water flow, heat transfer, and mass transport. Application to the T-106 tank leak data produced a good approximation of the plume's behavior in the vadose zone. The model indicates the plume's behavior in the vadose zone is complex and that the plume's behavior is not predictable from other sources.

Despite the discrepancy between the calculated and measured 1978 ^{106}Ru plume, there is sufficient evidence that the numerical model can successfully simulate the transient behavior of a three-dimensional plume in the vadose zone. The modeling results indicate that ^{106}Ru will be at measurable levels for several more years. Additional work is needed to reconcile differences between the simulations and the measured data.

In summary:

- In the absence of soil properties at the T-106 tank site, generic soil properties were input to the model.
- Minor adjustments of the generic soil properties in the model allowed for approximation of measured ^{106}Ru and ^{137}Cs plumes with the model.
- For long-term performance assessment, it would be preferable to obtain measured soil properties from the T-106 tank site.
- Preliminary calibration results indicate that for the first 150 days, convection is the dominant phenomena and the plume migration is dominated by the large leak volume rather than the recharge rate.
- At later simulation times, reduction in the ^{106}Ru plume by radioactive decay is very evident.

ACKNOWLEDGEMENT

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FIGURE 1 LOCATION OF HANFORD AREA AND T TANK FARM

FIGURE 2 STRATIGRAPHY OF T TANK FARM

FIGURE 5 SIMULATED ^{106}Ru DISTRIBUTIONS THROUGH 150 DAYS

FIGURE 6 SIMULATED ^{106}Ru DISTRIBUTIONS THROUGH 150 DAYS WITH ADJUSTED K_d

FIGURE 2 SIMULATED ^{106}Ru DISTRIBUTIONS AT 2, 5, 13, AND 17 YEARS WITH ADJUSTED K_2

FIGURE 3 SIMULATED ^{137}Cs DISTRIBUTIONS THROUGH 180 DAYS WITH ADJUSTED K_2

CALIBRATION/VALIDATION

A PROPOSAL

Charley Kincaid

Pacific Northwest Laboratory

March 29, 1993

PURPOSE

- TO ESTABLISH DOE, EPA, WASHINGTON-DOE DIALOGUE ON CODES, MODELS, VALIDATION
- TO ESTABLISH MODELING CAPABILITIES FOR RODs
 - Remedial Investigations
 - Feasibility Studies
 - Remediation Decisions
 - Remediation Design Monitoring Evaluation
- TO DETERMINE THE FEASIBILITY OF TRANSFERRING VALID MODELS
 - Neighboring Sites: Similar Geology Hydrology
 - Similar Releases: Ponds, Dams, Ditches

WHC-MR-0420

BACKGROUND

- MODELING CAPABILITIES FOR WHAT ??
 - STATUS AND EXPECTATIONS
 - Current - Unvalidated Models - Low Reliance in RODs
 - Future - Validated Models - Medium to High Reliance
 - POTENTIAL COMPLEXITY
 - No-Action Alternative - the Baseline
 - contaminant release
 - potential of interference among releases
 - geohydrology
 - Alternate Remediations
 - physics, chemistry, microbiology of treatment
 - WHY ?
 - Credible Input to Risk Assessment
 - Support for less costly remediations

SCOPE

- AGREE ON NEEDED MODELING CAPABILITIES FOR
 - Process Models
 - Liquid Water and Conservative Solute
 - Other Fluids and Phases
 - Reactive Contaminants
 - Time Frame and Spatial Scale
 - Long-term and Far-Field (Aquifer) Forecasts
 - Short-term and Near-Field (Vadose) Predictions
- AGREE ON ACCEPTABLE LEVELS OF MODEL UNCERTAINTY/CONFIDENCE, ACCURACY ... VALIDITY
 - Parameters - Field Measurable and Modelable
 - Definition of Uncertainty, Confidence, Accuracy to be Used
- DESIGN AND COMPLETE FIELD EXPERIMENTS - FIELD STUDIES OF PRIOR DISPOSALS
 - Constraints: Cost of New Experiment versus Use of Releases
 - Demonstrated Level of Certainty in Characterization and Response
- DESIGN AND ESTABLISH FIELD SITES - MODELS
 - Demonstrated Level of Validation in Model Prediction and Forecasts

#5

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APPROACH

- DETERMINE NEEDS OF DOE, EPA, W-DOE, (OTHER STAKEHOLDERS)
 - Processes
 - Time and Spatial Scales
 - Measures of Accuracy, Confidence, Uncertainty
- IDENTIFY AND/OR DEVELOP CODES AND MODELS FOR REGULATORY APPLICATION
 - Expected Documentation
 - Software Availability, Maintenance, and Support
- IDENTIFY AND/OR CONDUCT APPROPRIATE FIELD EXPERIMENTS OR STUDIES FOR REGULATORY APPLICATION
- DOCUMENT MODEL PERFORMANCE
 - Analysis of Experiments
 - Comparison of Model Predictions to Observations
 - Assessment of Model Validity
 - Assessment of Model Transferability

#6

CONSTRAINT: TYPICAL DOCUMENTATION FOR CODES & MODELS

- SOFTWARE DEVELOPMENT OR ADAPTATION REQUIREMENTS
- SOFTWARE DESIGN
- SOFTWARE USER GUIDANCE
- SOFTWARE INSTALLATION GUIDANCE & BENCHMARK CASES
- SOFTWARE APPLICATIONS

CONSTRAINT: TYPICAL DOCUMENTATION FOR FIELD STUDIES

- DESIGN OF FIELD EXPERIMENTS / STUDIES
 - Objective and Plan for the Experiment / Study
 - Measurement Techniques, Accuracy, and Error for Characterization and Monitoring
- NEPA DOCUMENTATION
- REPORTS ON EXPERIMENTAL RESULTS
 - Site Characterization and Analysis of Properties and Initial Conditions
 - 1st Phase, 2nd Phase, Reports
 - Post-Mortem Characterization and Complete Analysis

THIS REVIEW: ADVICE AND INPUT

- SCOPE OF A SUCCESSFUL "VALIDATION" EFFORT
 - Physics, Chemistry, Microbiology
 - Long-term, far-field and/or short-term, near-field
 - Dimensionality
- ALTERNATE MEASURES OF ACCURACY, CONFIDENCE, UNCERTAINTY
 - Level of "Validation" Achievable
- FEASIBILITY OF TRANSFERRING VALIDATED MODELS
 - Similar Geomorphology and Release

What Constitutes a Validation Experiment?

Lynn Gelhar
Massachusetts Institute of Technology

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Figure 1
FLOW CHART ILLUSTRATING THE MODELLING PROCESS

POSSIBLE MODELING APPROACHES

A. Deterministic Numerical Models

- (i) Classical - homogeneous layers or zones
 - ignores spatial variability
 - no error measure
 - *model parameters not directly measurable*
- (ii) Detailed w/"actual" heterogeneity
 - measurements impractical 3D!!
 - computationally infeasible? 10^9 nodes

B. Stochastic Models

Intraformational heterogeneity represented by spatial random fields characterized with a small number of statistical parameters

mean $\Rightarrow$ form of large scale p.d.e. + effective properties (a method for determining model parameters from direct small-scale measurements)

variance $\Rightarrow$ model error provides a systematic basis for model validation (and calibration)

STOCHASTIC UNSATURATED FLOW THEORY

re Yeh....WRR (1985) ; Mantoglou... WRR (1987)

Polmann (1990)

$$K = K_s e^{-\alpha\psi}, \quad \ln K = \ln K_s - \alpha\psi$$

$$\ln K_s = \ln K_g + f, \quad E[f] = 0, \quad \sigma_f^2 = E[f^2]$$

$$\alpha = A + a, \quad E[a] = 0, \quad \sigma_a^2 = E[a^2] \uparrow$$

$\ln K_s$ & α random fields w/ variances
& correlation scales λ_i

MADDOCK SOIL sites 1 and 2

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(5)

Data from Las Cruces Trench Site

preliminary data from P. Vieringer

STOCHASTIC FLOW ANALYSIS

(6)

re Yeh et al, 1985; Mantoglou ... 1987

conservation of mass

$$\frac{\partial \theta}{\partial t} + \frac{\partial q_i}{\partial x_i} = 0$$

Darcy equation

$$q_i = -K(\psi, x_i) \frac{\partial (\underbrace{z - \psi}_{\text{head}})}{\partial x_i}$$

$$\frac{C}{K} \frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x_i^2} + \frac{\partial \ln K}{\partial x_i} \left(\frac{\partial \psi}{\partial x_i} - \frac{\partial z}{\partial x_i} \right)$$

$\downarrow \frac{d\theta}{d\psi}$
 $\frac{C}{K} \frac{\partial \psi}{\partial t}$
 $\frac{d\theta}{d\psi}$

$$\ln K = \ln K_s - \alpha \psi \quad \text{random inputs}$$

Let $\psi = H + h$, $E[h] = 0$
 $\ln K_s = F + f$, $E[f] = 0$
 $\alpha = A + a$, $E[a] = 0$
 $C = \Gamma + \gamma$, $E[\gamma] = 0$

Solve for $h \Rightarrow \sigma_h^2 \equiv E[h^2]$, ..., $E[ah]$, etc
 (assuming small perturbations & local stationarity)

Mean equation: (mixed form)

$$\frac{\partial \Theta(H, \frac{\partial H}{\partial t}; \sigma_f^2 \dots)}{\partial t} = \frac{\partial}{\partial x_i} \left[\hat{K}_{ij} \cdot (H, \frac{\partial H}{\partial t}, \frac{\partial H}{\partial x_i}; \sigma_f^2 \dots) \frac{\partial (z - H)}{\partial x_i} \right]$$

mean moisture
content

effective hydraulic
tensor

TENSION VARIANCE

⑦

Steady flow / layered soil / unit gradient

$$\sigma_h^2 = \frac{(\sigma_f^2 + \sigma_a^2 H^2) \lambda_1}{A (1 + A \lambda_1)}$$

for $\ln k_s \neq \alpha$
uncorrelatednote strong dependence on mean tension H large $H \Rightarrow \sigma_h / H \rightarrow \text{constant}$

$$A \lambda_1 \ll 1$$

$$\sigma_h^2 \propto \lambda_1 / A$$

$$A \lambda_1 \gg 1$$

$$\sigma_h^2 \propto A^{-2} \text{ independent of } \lambda_1$$

If $\ln k_s \neq \alpha$ are ^{perfectly} correlated, i.e.,

$$\alpha = \gamma f, \quad (\sigma_f^2 + \sigma_a^2 H^2) \rightarrow \sigma_f^2 (1 - \gamma H)^2$$

$$\text{or } \gamma = \frac{\sigma_a}{\sigma_f}$$

$$H = 1/\gamma \Rightarrow \sigma_h^2 = 0$$

see Yeh (1989) WRR 25(10) p2149

EFFECTIVE CONDUCTIVITY

Steady Flow Results:

$$H = E[\Psi]$$

$$\left. \begin{aligned} \ln \hat{K}_{11} &= \ln K_g - \hat{A}H - \frac{\sigma_f^2 + \sigma_a^2 H^2}{2(1 + A\lambda_1)} \\ \ln \hat{K}_{22} &= \ln K_g - \hat{A}H + \frac{\sigma_f^2 + \sigma_a^2 H^2}{2(1 + A\lambda_1)} \end{aligned} \right\} \begin{array}{l} \text{vertical} \\ \ln \frac{\hat{K}_{22}}{\hat{K}_{11}} = \frac{\sigma_f^2 + \sigma_a^2 H^2}{1 + A\lambda_1} \\ \text{horizontal} \end{array}$$

$$\hat{A} = A \left(1 - \frac{\sigma_a^2 \lambda_1}{A(1 + \lambda_1 A)} \right), \quad \lambda_1 = \text{correlation scale}$$

135
H mean tension

Note: $\sigma_\Psi^2 = \frac{(\sigma_f^2 + \sigma_a^2 H^2) \lambda_1}{A(1 + A\lambda_1)}$

UNSATURATED FLOW

EFFECTIVE HYDRAULIC CONDUCTIVITY

UNSTEADY FLOW - STRATIFIED SOIL

MADDOCK SOIL

Stochastic Mean Simulations

re Polmann et al (1990) were

Large-scale model w/ effective parameters

$$\frac{\partial \Theta}{\partial t} = \frac{\partial}{\partial x_1} \left(\hat{K}_{11} \frac{\partial (H+x_1)}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(\hat{K}_{22} \frac{\partial H}{\partial x_2} \right)$$

$$\Theta = \Theta \left(H, \frac{\partial H}{\partial t}, \frac{\partial H}{\partial x_i}; \sigma_i^2, \lambda_i, A, \dots \right)$$

assumed small ≈ 0

$$\hat{K}_{ii} = K_{ii} \left(H, \frac{\partial H}{\partial t}, \frac{\partial H}{\partial x_i}; \sigma_i^2, \dots \right)$$

Numerical approximation:

→ Galerkin finite element discretization

→ modified Picard iteration

→ mass conserving "mixed" formulation (Θ, H)

(11)

Stochastic Modeling of Large-Scale Flow in Heterogeneous Unsaturated Soils

DONALD J. POLMANN,¹ DENNIS McLAUGHLIN STEVE LUTS,²
LYNN W. GELHAR, AND RACHID ABABOU³

3D
heterogeneous
model
(Ababou)

Figure x-xa. Schematic representation of the Ababou flow domain.

2D
stochastic
mean
flow
model

Figure x-xb. Schematic representation of the mean model flow domain.

71

Figure x-x: Moisture content distributions for two-dimensional deterministic and stochastic models at 5, 10 and 15 days.

15 days

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(13)

re Palmann et al. (1991)

Figure x-x. Tension distributions for Ababou and mean stochastic models at 15 days.

140
WRR. 7c

101

Figure x-x. Vertical tension profiles under wetted strip centerline for Ababou and mean model simulations (profile numbers refer to Figure x-x).

See Luis & McLaughlin (1992), Adv. W.R. 15, 15-32 for
WRR.3 hypothesis testing framework

hysteresis effect
 @ 0.5 m deep

Figure x-x. Hysteresis and anisotropy of effective conductivity at 0.5m depth below centerline of wetted strip.

other simulations:

Keel et al. (1990)

WRR. 5 Jäntti et al (1990) WRR

UNSATURATED FLOW EXPERIMENT

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(14)

re Stephens & Heerman (1988), WRR 24(5), 770-779
NEW MEXICO TECH lab experiment

<u>Slide</u>	<u>Flow rate ml/hr</u>	<u>time-hr</u>	} ~ same volume
1	1	24	
2	20	1	
3	100	4	
4	100	12	
5	100	12

**LABORATORY MEASUREMENT OF
HYDROLOGIC PROPERTIES**

J.F. Relyea, H.L. Benny and R.T. McIntosh

**GEOTECHNICAL ENGINEERING
LABORATORY**

PARTICLE SIZE DISTRIBUTION

Sieves (10 cm to .0075 cm)

Hydrometer (.0034 cm to .0001 cm)

**Calcium Carbonate (AVG = 0.7%;
STDEV = 1.2%)**

Cementation by CaCO_3 is found in the fine fraction (less than 0.2 cm) of nearly all samples. Particle size data is probably not useful for estimating moisture retention curve without removal of carbonate.

POROSITY

Bulk Density

Measured on oven dry soil and volume of sample sleeve filled by sample.

**Specific Gravity / Grain Density
Measured on fine and course fraction. Average used for calculation of porosity.**

MOISTURE CONTENT

Moisture content is measured on samples as received from the field. Some are stored in the field for several weeks to months before testing and dry substantially. Others are soaked by melting ice before reaching the lab.

SATURATED HYDRAULIC CONDUCTIVITY

- o Saturated hydraulic conductivity data are measured on both intact (as received) and recompact samples (specified bulk density if required).
- o Samples range from 1" to 4" diameter. Length is limited by length of all thread-available
- o Head is usually supplied by a water column or by air pressure over water for more impermeable samples

SATURATED HYDRAULIC CONDUCTIVITY

- o Tests methods are (1) Falling head, (2) Constant head and (3) Falling head - Rising tail.
- o Falling head used for more permeable samples: down to $1\text{E-}4$ cm/sec.
- o Constant head from $1\text{E-}4$ down to $1\text{E-}8$ cm/sec.
- o Falling head - Rising tail used for least permeable samples: $1\text{E-}8$ down to $1\text{E-}10$ cm/sec.
- o Ranges overlap an order of magnitude or more.

SATURATED HYDRAULIC CONDUCTIVITY

- o Pressure must be controlled to prevent channeling
- o Filter paper or screen needed to prevent small particle movement..
- o Conductivity measured on empty apparatus to determine head loss of equipment. Needed to correct values for high permeability samples.
- o Have flexible wall permeameter capability

MOISTURE RETENTION CURVE

- o Moisture retention curves (soil water content versus matric potential) are measured on the fine fraction (less than 0.2 cm).
- o Data generated is on an oven dry weight basis and converted to volumetric by multiplying by the sample bulk density.
- o Kettle and CX-2 drying curves are matched to the Tempe drying curve by multiplying the curves by the Tempe Cell bulk density.

MOISTURE RETENTION CURVE

TEMPE CELL

- o Wetting and drying curves are measured between 0 and 1 bar.
- o Empty cells are weighed (1 before filling; 2 after removing the sample and (3 after cleaning the cell for reuse.
- o Moisture content is measured on sample (1 after filling the cell and (2 after the run is terminated.
- o The moisture content of the final sample is matched to that of the sample at the last measured data point.

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SAMPLE NO.	2-3069
Contact	Jim Roberts
Well No.	199-K-37
Operable Unit	100-KB-4
HEIS No.	DOEN19
Depth	40.5' - 41.5'

TEMPE CELLS	Sample #	2-3069 1 Bar Drying Curve									
tension in cm	N/A	N/A	0	2.5	1	11	24.5	27.5	14	70.5	
error in tension value +/-			0	2.5	1	11	24.5	27.5	14	70.5	
container number	MC-10	TC-10	TC-10	TC-10	TC-10	TC-10	TC-10	TC-10	TC-10	TC-10	
weight of container/ring, wet sample	151.01	548.96	575.28	573.73	573.09	573.02	572.71	572.48	570.00	567.87	
weight of container/ring, dry sample	150.91	548.82	548.50	548.50	548.50	548.50	548.50	548.50	548.50	548.50	
weight of moisture	0.10	0.14	26.78	25.23	24.59	24.52	24.21	23.98	21.50	19.37	
weight of container and ring	50.58	426.44	426.20	426.20	426.20	426.20	426.20	426.20	426.20	426.20	
weight of dry sample	10.43	122.38	122.30	122.30	122.30	122.30	122.30	122.30	122.30	122.30	
moisture content % by wt.	9.11%		21.90%	20.63%	20.11%	20.05%	19.80%	19.61%	17.58%	15.84%	
moisture content % by vol.			19.23%	18.96%	18.02%	15.92%	15.47%	15.13%	11.50%	10.38%	
date measured			12/22/92	12/23/92	12/29/92	12/30/92	12/31/92	1/4/93	1/5/93		
temperature deg. C			25	25	22	22	22	23	23	24	
volume of brass ring, cm ³	58.26		25	25	22	22	22	23	23	24	

TEMPE CELLS	Sample #	2-3069 1 Bar Drying Curve									
tension in cm	102	201.5	100	500	700	1000	N/A	N/A			
error in tension value +/-	5	2	20	20	20	20					
container number	TC-10	TC-10	TC-10	TC-10	TC-10	TC-10	TC-10	TC-10	MC-11		
weight of container/ring, wet sample	562.88	557.61	555.51	554.28	553.68	553.00	552.97	552.97	552.97		
weight of container/ring, dry sample	548.50	548.50	548.50	548.50	548.50	548.50	548.50	548.50	548.50		
weight of moisture	14.38	9.11	7.01	5.76	5.18	4.50	4.47	4.47	4.47		
weight of container and ring	426.20	426.20	426.20	426.20	426.20	426.20	426.20	426.20	426.20		
weight of dry sample	122.30	122.30	122.30	122.30	122.30	122.30	122.30	122.30	122.30		
moisture content % by wt.	11.76%	7.45%	5.73%	4.71%	4.24%	3.68%	3.65%	3.65%	3.65%		
moisture content % by vol.	21.07%	13.35%	10.27%	8.44%	7.59%	6.59%	6.55%	6.55%	6.55%		
date measured	11/5/92	11/6/92	11/9/92	11/10/92	11/11/92	11/12/92	11/13/92	11/14/92			
temperature deg. C	24	24	23	25	24	24					
volume of brass ring, cm ³	58.26		25	25	24	24					

Cell wt. before cleanup = 426.08 grams
Cell wt. after cleanup = 426.5 grams
426.34 Average of all 3

1 BAR DRYING CURVE

TEMPE CELLS

tension in cm

error in tension value +/-

container number

weight of container/ring, wet sample

weight of container/ring, dry sample

weight of moisture

weight of container and ring

weight of dry sample

moisture content % by wt.

moisture content % by vol.

date measured

temperature deg. C

volume of brass ring, cm³

SAMPLE # 2-3069

N/A N/A

0 0.5

0 0.5

MC-10 TC-10 TC-10 TC-10

151.01 548.96 575.28 573.73

150.91 548.82 548.50 548.50

0.10 0.14 26.78 25.23

50.58 426.44 426.20 426.20

10.43 122.38 122.30 122.30

9.11% 21.90% 20.63%

19.23% 18.96% 18.02%

12/22/92 12/23/92

25 25

58.26

1 BAR DRYING CURVE

TEMPE CELLS

tension in cm

error in tension value +/-

container number

weight of container/ring, wet sample

weight of container/ring, dry sample

weight of moisture

weight of container and ring

weight of dry sample

moisture content % by wt.

moisture content % by vol.

date measured

temperature deg. C

volume of brass ring, cm³

SAMPLE # 2-3069

700 1000 N/A N/A

20 20

TC-10 TC-10 TC-10 MC-11

553.68 553.00 552.97 552.97

548.50 548.50 548.50 548.50

5.18 4.50 4.47 4.47

426.20 426.20 426.20 426.20

122.30 122.30 122.30 122.30

9.2% 3.7% 3.7% 3.6%

18.5% 6.5% 6.5% 6.5%

11/12/92 11/12/92 11/13/92 11/14/92

24 24

Cell wt. 425.08 grams

Cell wt. 425.5 grams

425.21 Average

BULK DENSITY 1.79

PRESSURE KETTLE

- o Data points are measured from 0.5 to 10 bars in kettles.
- o Volumetric moisture contents are obtained by multiplying the moisture content (weight %) by Tempe cell bulk density.
- o Data points are measured in duplicate.

MOISTURE RETENTION CURVE

CX-2

- o The CX-2 measures the water activity (relative humidity) of a sample to 0.1%. This corresponds to matric potentials from 5 to >1000 bars.
- o The water activity is the total of matric and osmotic potentials. Salts must be leached from the sample before testing to measure the matric potential.
- o Osmotic effects are not significant on well samples. Grout samples; however, are dominated by osmotic effects.

UNSATURATED HYDRAULIC CONDUCTIVITY

- o Unsaturated hydraulic conductivity data are gathered on both intact and recompact samples (usually 10 cm diameter by 15 cm long).
- o Samples are brought to specified matric potential using air pressure first. Then vacuum is applied to the top and bottom plates.

UNSATURATED HYDRAULIC CONDUCTIVITY

- o Mariotte flask is used at low matric potential (0 to -100 cm) to maintain constant head. Large reservoir is used at higher matric potential, falling head not significant.
- o Leaks in vacuum/pressure system are the biggest problem. Mariotte flasks at higher tensions are not practical. Any small leak leads to water entering the vacuum system.

2-1306 (1) 2-1306 (2) 2-1306 (3) 2-1306 (4)

SAMPLE 2-1306

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Centrifuge Technology for Vadose Zone Transport Measurements

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TRI-CITIES

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ENVIRONMENTAL MANAGEMENT
OPERATIONS
PACIFIC NORTHWEST LABORATORY

The Primary Transport Parameters

K - Hydraulic Conductivity (water permeability)

$$q = K \cdot \nabla \psi$$

water flux = conductivity x pressure gradient

D - Diffusion Coefficient (static diffusion of single ions)

$$J = D \cdot \nabla \psi$$

ion flux = diffusion coefficient x concentration gradient

R_f - Retardation Factor (Chemical sorption and exchanges)

$$R_f = V_{gw} \div V_c$$

Limitations of Traditional Methods

- Traditional methods require months to years to conduct experiments at the low water contents characteristic of arid sites.
- Estimations derived from data obtained under saturated conditions are difficult to support without sufficient unsaturated data.
- Traditional laboratory methods cannot test remediation strategies under low water contents and field conditions prior to field testing.

UNSATURATED FLOW APPARATUS (UFA)

- combines ultracentrifugation with precision fluid flow through a rotating seal
- attains hydraulic steady-state in hours instead of weeks to years at low water contents
- acceleration is a whole body force analogous to gravity (no physical changes in sample - no compaction, no density changes, no induced fracturing or grain rearrangements)

Some Advantages of the UFATM

- Determines the transport behavior of soils and sediments for aqueous and non-aqueous phase fluids. These data can be used to develop remediation strategies and predict contaminant migration.
- Soil and sediment samples in the UFATM reach hydraulic steady-state with any fluid in 1 to 10 hours over a range of saturated to highly unsaturated conditions.

Figure 1. The UFATM Rotor and Seal Assembly.

UNSATURATED FLOW APPARATUS (UFA)

- multiphase/multicomponent capabilities
- 0° to 150° C
- flow rates to 0.1 ml/hour
- accelerations up to 20,000 g

After the water content is fixed in the sample and the material is at hydraulic steady-state, transport parameters can be determined from a variety of associated methods.

- Hydraulic conductivity can be determined from the driving force and flux.
- The electrical conductivity can be measured for determination of diffusion coefficients using the Nernst-Einstein equation.
- The effluent can be monitored/collected/analyzed for chemical changes, retardation effects, and determination of partitioning.

Under a centripetal acceleration in which the water is driven by both the matric potential and the centrifugal force per unit volume, $\rho\omega^2 r$, Darcy's Law is given by:

$$q = -K(\psi) [d\psi/dr - \rho\omega^2 r]$$

where:

q = flux density

K = hydraulic conductivity

ψ = matric potential

ρ = bulk density

ω = rotation speed

r = radial distance from axis of rotation

At speeds above about 300 rpm, provided that a sufficient flux density exists,

$$d\psi/dr \ll \rho\omega^2 r$$

and Darcy's Law reduces to:

$$K(\psi) = q / \rho\omega^2 r$$

As an example, a 45-gram sample of a silt accelerated to 2,000 rpm with a flow rate into the silt of 3 ml/hr achieved hydraulic steady state in two hours at the target volumetric water content of 22.4% and an unsaturated hydraulic conductivity of 2.5×10^{-7} cm/s.

Darcy's Law is a bulk property and does not depend upon the type of driving force

- Positive Pressure Gradient (High Pressure Cells)
- Negative Matric Potential (Weirenga Cell)
- Gravitational Acceleration (Soil Columns)
- Centripetal Acceleration (UFA™)
- Magnetic/Electric Potentials (Magstream)

The following figure compares the UFA centrifuge method with three traditional techniques for determining hydraulic conductivity for soil from the Buried waste Test Facility at Hanford. Open squares are direct measurements of hydraulic conductivity using the UFA under unit-gradient conditions obtained in a three-day period. Open triangles are direct measurements of hydraulic conductivity using a traditional column flow experiment under unit-gradient conditions, requiring a total experimental time of more than a year. The closed circle is the 13-year field lysimeter data obtained under unit-gradient conditions at water contents in the field, a point which ties the laboratory data to the field conditions. The solid line is an estimation derived by curve-fitting to water retention data using a Mualem relationship.

The agreement of the UFA data with all three methods is excellent and demonstrates the validity and rapidity of the UFA method relative to traditional methods.

FIGURE A.3. Measured Hydraulic Conductivity Data and van Genuchten Function Fit for FLTF Soil

Figure 12

Figure 2

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Figure 6

Figure 7

Figure 8

Figure 9

Figure 10

Figure 11

USE OF VAN GENUCHTEN-MUALEM RELATIONSHIPS TO PREDICT UNSATURATED HYDRAULIC CONDUCTIVITY

RAZ KHALEEL
WESTINGHOUSE HANFORD COMPANY

VAN GENUCHTEN-MUALEM RELATIONSHIPS

$$\theta = \theta_r + \frac{(\theta_s - \theta_r)}{[1 + (\alpha \psi)^N]^M}$$

$$\frac{k(\theta)}{k_s} = \left[\frac{\theta - \theta_r}{\theta_s - \theta_r} \right]^2 \left\{ 1 - \left[1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{1/M} \right]^m \right\}^2$$

OBJECTIVE

VALIDATE VAN GENUCHTEN-MUALEM
RELATIONSHIPS TO ESTIMATE
UNSATURATED HYDRAULIC
CONDUCTIVITY FOR HANFORD SOILS,
ESPECIALLY AT LOW MOISTURE CONTENTS

**PENALTY FOR USING INCORRECT
ESTIMATES FOR UNSATURATED
HYDRAULIC CONDUCTIVITY AT LOW
MOISTURE CONTENTS**

By not having accurate estimates of hydraulic conductivities at low moisture contents, we will be forced to use conservative estimates and this can potentially lead to overdesigns for various waste disposal sites at Hanford.

ANALYSIS OF MOISTURE RETENTION AND UNSATURATED CONDUCTIVITY DATA

Three different parameter estimation procedures were used to analyze the data:

- o Predictive Method,**
- o Simultaneous Fitting with Five Parameters, and**
- o Simultaneous Fitting with Six Parameters.**

ANALYSIS OF MOISTURE RETENTION AND UNSATURATED CONDUCTIVITY DATA

- o For the predictive method, the laboratory-measured K_s , was fixed at its measured value and the pore parameter ι was fixed at 0.5; θ_r , θ_s , α , n , with $m = 1-1/n$, were fitted to the moisture retention data.
- o For simultaneous fitting with five parameters, the laboratory-measured K_s , was fixed at its measured value and θ_r , θ_s , α , n , and ι , with $m = 1-1/n$, were fitted to the moisture retention and conductivity data.
- o For simultaneous fitting with six parameters, all six unknown parameters θ_r , θ_s , α , n , ι , and K_s , with $m = 1-1/n$, were fitted to the data.

0-085D.vgp

ETGTEC100582-RETG

9-0465D.vgg

ETGTEC100592-RETC

0-1040.vgd

ETG7EC:00592.VETC

0-1040-000

ETGTTC100592-RETC

2-16360.vgp

ETGTEC102792-RET.C

2-1636A.vgp

ETGTEC110592-RETG

2-1625A.vgp

ETGTEC110392-RETG

2-2225D.vgp

ETGTEC102792-RET.C

Injection Test Site : Sample 2-2225 : Drying
Well 299-E24-92, 32 ft., Loamy Sand

W-05 Predicted Method

W-05 Simultaneous Fit - 5 Parameter

W-05 Simultaneous Fit - 6 Parameter

Injection Test Site Predicted Method

Injection Test Site Simultaneous Method - 5 Parameters

Injection Test Site Simultaneous Fit - 6 Parameters

PREDICTIVE METHOD

- o The unsaturated K data, using the predictive method, shows considerable scatter suggesting that the moisture retention parameters may not adequately describe the unsaturated conductivity curves.
- o Except for a few outliers, most of the values fall within approximately one order of magnitude in the wet region and two orders of magnitude in the dry range.
- o No bias is apparent in the predicted K's; there appears to be almost an equal number of points above and below the regression line

SIMULTANEOUS FITTING

- o The simultaneous method with five or six parameters produces soil hydraulic parameters that most accurately describe both the water-retention and hydraulic-conductivity relationships.
- o The simultaneous method using six parameters was found to produce the best fit overall, but differences from using either five or six parameters are slight.
- o Provided enough measured data are available, keeping parameter I variable in the parameter estimation process will likely improve the analysis of data.

USE OF ARYA-PARIS MODEL TO ESTIMATE MOISTURE RETENTION DATA

BEN VOLK AND RAZ KHALEEL

Why is MRC versus PSD Correlation Necessary?

- Inability to collect moisture retention data on every operable unit
- Cost of Moisture Retention Curve
\$2200 per sample as compared to \$200 for Sieve Analysis
- Time to Perform Moisture Retention Analysis
27 hours per sample as compared to 1 hour for sieve analysis
- Accuracy of laboratory derived data
- Accuracy of in situ field tests
- Reduce number of characterization wells that must be drilled
- Use locally measured soil data (ie/ 200E, 200W, and 300 Areas) to predict contamination movement across the site

Arya and Paris Model (1981)

- An empirical model with constant, α .
- Underlying assumptions:
 - Soil particle size related to a corresponding pore diameter
 - Model treats the soil as a bundle of capillary tubes
 - Capillary tube volume is a function of
 - a) particle size
 - b) weight fraction of the particle size
 - c) empirically determined constant, α
- Input data needed: Particle Size Distribution, Bulk Density, and Particle Density.
- Step 1. Divide the PSD data into M size fractions where the solid mass in the i th particle class is equated to the mass of N_i spherical particles of radius R_i . Volume of the particles, $V_{p,i}$ is:

$$V_{p,i} = 4/3 \pi R_i^3 N_i \quad (1)$$

The volume of the voids, $V_{v,i}$, can be represented by a single capillary tube of radius r_i :

$$V_{v,i} = \pi r_i^2 h_i \quad (2)$$

where h_i is the capillary tube length. The length of the tube is determined by multiplying the diameters of the particles ($2R_i$) by the number of particles:

$$h_i = 2R_i N_i^\alpha \quad (3)$$

where α is an empirical constant between 1 and 2. The α term is required to account for the non-spherical nature of some of the particles

Arya and Paris Model - Continued

By combining equations (1), (2), and (3), Arya and Paris arrived at the expression for capillary tube radius, r_i :

$$r_i = R_i (2/3eN_i)^{1/(2+\alpha)} \quad (4)$$

where e is the void ratio. The tube radius is then related to the capillary pressure, ψ_i , via the equation for rise of water in a capillary tube:

$$\psi_i = 2\gamma \cos \theta / r_i \quad (5)$$

where ψ_i is the soil water pressure, γ is the surface tension of water, θ is the contact angle, ρ_w is the density of water, g is gravity, and r_i is the pore radius.

- Arya-Paris found that α ranged from 1.35 to 1.39.

Arya and Paris - Determining Alpha

- Perform iterative analysis of measured capillary pressures versus predicted capillary pressures by assuming an alpha and minimizing the root mean squared error (Fortran Program).

ARYA AND PARIS MODEL
Computational Procedure

B. W. Volk
7-29-92

Input												
Particle Diam.	Av. Radius	Weight	Pore Vol.	Sum	Vol. Water	Average VWC	Number of		Mean Pore	Soil Water		
Interval (um)	R _i (cm)	W (g)	V _{vi}	V _{vi}	(Thetavi)	(Thetaparvi)	Part. n _i	n _i ^{1/3} (1-alpha)	Radius, r _i	PS _{ii}		
0	1	2.50E-05	0.140	0.03001	0.03001	0.051	-	-	-	-	-	-
1	2	7.50E-05	0.030	0.00643	0.03644	0.062	0.056	6.41E+09	1.88E-04	6.32E-07	2.32E+05	
2	5	1.75E-04	0.074	0.01586	0.05230	0.088	0.075	1.24E+09	3.50E-04	2.01E-06	7.29E+04	
5	10	3.75E-04	0.076	0.01629	0.06859	0.116	0.102	1.30E+08	8.26E-04	6.63E-06	2.22E+04	
10	20	7.50E-04	0.115	0.02465	0.09325	0.158	0.137	2.46E+07	1.56E-03	1.82E-05	8.07E+03	
20	30	1.25E-03	0.120	0.02572	0.11897	0.201	0.179	5.53E+06	2.74E-03	4.03E-05	3.65E+03	
30	50	2.00E-03	0.160	0.03430	0.15327	0.259	0.230	1.80E+06	4.20E-03	7.97E-05	1.84E+03	
50	100	3.75E-03	0.100	0.02144	0.17470	0.295	0.277	1.71E+05	1.03E-02	2.34E-04	6.28E+02	
100	200	7.50E-03	0.065	0.01393	0.18863	0.319	0.307	1.39E+04	2.67E-02	7.54E-04	1.95E+02	
200	500	1.75E-02	0.070	0.01501	0.20364	0.344	0.331	1.18E+03	6.81E-02	2.81E-03	5.23E+01	
500	700	3.00E-02	0.020	0.00429	0.20793	0.351	0.348	6.67E+01	2.03E-01	8.31E-03	1.77E+01	
700	1000	4.25E-02	0.015	0.00322	0.21114	0.357	0.354	1.76E+01	3.36E-01	1.52E-02	9.69E+00	
1000	2000	7.50E-02	0.015	0.00322	0.21436	0.362	0.360	3.20E+00	6.43E-01	3.70E-02	3.97E+00	
			1.000									

Bulk Volume= 0.5917 cm³ (1 gram sample)
Bulk Density= 1.69 g/cm³
Surface Tension= 72 dynes/cm
Contact Angle= 0 degrees
Water Density= 1 g/cm³
Gravity= 980 cm/s²
Alpha constant= 1.38 unitless
Part. Density= 2.65 g/cm³

Table 1

ARYA-PARIS MODEL
CE702

3 MAY 1991 01:51 ARYACAL.CHT
FROM A-P FORTRAN MODEL ARYACAL.FOR)
ALPHA = 1.24

WHC-MR-0420

Calibration Data - Arya-Paris and Tyler-Wheatscraft Model

B. W. Voik

Site	Sample #	Depth (Feet)	Formation Type	Soil Type	Q	Alpha
FLTF	D02-10	1	< 20 Hanford-Upper Sand	Silt Loam	2.63	1.17
"	D02-16	2	< 20 Hanford-Upper Sand	Silt Loam	2.60	1.19
"	D04-04	3	< 20 Hanford-Upper Sand	Silt Loam	2.62	1.20
"	D04-10	4	< 20 Hanford-Upper Sand	Silt Loam	2.61	1.19
"	D05-03	5	< 20 Hanford-Upper Sand	Silt Loam	2.60	1.22
"	D07-04	6	< 20 Hanford-Upper Sand	Silt Loam	2.61	1.20
"	D08-15	7	< 20 Hanford-Upper Sand	Silt Loam	2.61	1.16
"	D09-01	8	< 20 Hanford-Upper Sand	Silt Loam	2.61	1.16
"	D09-02	9	< 20 Hanford-Upper Sand	Silt Loam	2.61	1.18
"	D09-05	10	< 20 Hanford-Upper Sand	Silt Loam	2.55	1.24
"	D10-04	11	< 20 Hanford-Upper Sand	Silt Loam	2.56	1.23
"	D11-06	12	< 20 Hanford-Upper Sand	Silt Loam	2.61	1.20
"	D11-08	13	< 20 Hanford-Upper Sand	Silt Loam	2.57	1.21
"	D12-14	14	< 20 Hanford-Upper Sand	Silt Loam	2.64	1.16
"	D13-08	15	< 20 Hanford-Upper Sand	Silt Loam	2.61	1.17
"	D14-04	16	< 20 Hanford-Upper Sand	Silt Loam	2.61	1.18
U. S. Ecology MW-5	@ 50	17	50 Hanford-Upper Sand	Sand	2.20	1.25
"	@ 70	18	70 Hanford-Upper Sand	Sand	2.49	1.25
"	@ 90	19	90 Hanford-Upper Sand	Sand	2.10	1.24
"	@ 130	20	130 Hanford-Upper Sand	Sand	2.17	1.23
"	@ 170	21	170 Hanford-Upper Sand	Sand	2.19	1.24
"	@ 190	22	190 Hanford-Lower Sand	Sand	2.05	1.31
"	@ 210	23	210 Hanford-Lower Sand	Sand	2.04	1.21
"	@ 230	24	230 Hanford-Lower Sand	Sand	2.01	1.21
"	@ 270	25	270 Hanford-Lower Sand	Loamy Sand	2.48	1.39
U. S. Ecology MW-8	@ 14	26	14 Hanford-Upper Sand	Sand	1.99	1.23
"	@ 145	27	145 Hanford-Upper Sand	Sandy Loam	2.72	1.08
"	@ 185	28	185 Hanford-Middle Sand	Sand	2.01	1.73
U. S. Ecology MW-10	@ 45	29	45 Hanford-Upper Sand	Sand	2.34	1.35
"	@ 86	30	86 Hanford-Upper Sand	Sand	2.32	1.28
"	@ 105	31	105 Hanford-Upper Sand	Sand	2.44	1.41
"	@ 125	32	125 Hanford-Upper Sand	Sand	2.40	1.35
"	@ 165	33	165 Hanford-Upper Sand	Sand	2.28	1.30
"	@ 195	34	195 Hanford-Middle Sand	Sand	2.26	1.82
"	@ 205	35	205 Hanford-Lower Sand	Sand	2.27	1.60
"	@ 245	36	245 Hanford-Lower Sand	Sand	2.34	1.28
"	@ 265	37	265 Hanford-Lower Sand	Sand	2.39	1.27
"	@ 285	38	285 Hanford-Lower Sand	Sand	2.36	1.22
"	@ 305	39	305 Hanford-Lower Sand	Sand	2.25	1.27
259-W7-99	W-069	40	10 Hanford-Upper Sand	Sandy Loam	2.63	1.30
"	W-077	41	65 Hanford-Upper Sand	Sandy Loam	2.60	1.19
"	W-079	42	69 Hanford-Upper Sand	Silt Loam	2.42	1.06
"	W-080	43	71 Hanford-Upper Sand	Sandy Loam	2.51	1.13
"	W-082	44	82 Hanford-Upper Sand	Sandy Loam	2.58	1.55
"	W-085	45	88 Hanford-Upper Sand	Loamy Sand	2.55	1.47
"	W-099	46	99 Hanford-Upper Sand	Loamy Sand	2.54	1.56
"	W-101	47	104 Hanford-Upper Sand	Sand	2.52	1.21
"	W-104	48	118 Hanford-Upper Sand	Sand	2.40	1.19
"	W-107	49	132 Hanford-Upper Sand	Sand	2.45	1.15
"	W-113	50	142 Hanford-Upper Sand	Sand	2.23	1.10
Arithmetic Mean =					2.43	1.27
Standard Deviation =					0.20	0.15
Calibration Parameters						
Sand Prediction =	Alpha	SDev	Q	Loamy Sand Pred. =	Alpha	SDev
Number of Samples =	1.33	0.16	2.27	Number of Samples =	1.47	0.07
Silt Loam Pred. =	25		25	Sandy Loam Pred. =	3	
Number of Samples =	1.18	0.03	2.59	Number of Samples =	1.25	0.17
	17		17		5	

ARYA PARIS FITTING PARAMETERS: 50 SAMPLES

Calibration Parameters	Alpha	SDev.	Q	Alpha	SDev.	Q
Sand Prediction =	1.33	0.16	2.27	Loamy Sand Pred. =	1.47	0.07
Number of Samples =	25			Number of Samples =	3	
Silt Loam Pred. =	1.18	0.03	2.59	Sandy Loam Pred. =	1.25	0.17
Number of Samples =	17			Number of Samples =	5

From Tyler and Wheatcraft, 1992

Alpha Vs D

S. W. Volk 03-24-93

ARYA-PARIS MODEL Inj. Test Site, Sample 2-1636

BWV 03-14-93, SAND
From Adfit.for, Alpha = 1.33, Rsq = .979
Calc Alpha = 1.34, Rsq = .980

ARYA-PARIS MODEL inj. Test Site, Sample 2-1639

BWV 03-14-93, SAND
From Adfit.for, Alpha = 1.33, Rsq = .966
Calc Alpha = 1.23, Rsq = .961

ARYA-PARIS MODEL Inj Test Site, Sample 1-1417

BWV 03-11-93, SANDY LOAM
From Adfit for, Alpha = 1.25, Rsq = .978
Calc Alpha = 1.46, Rsq = .983

ARYA-PARIS MODEL Inj Test Site, Sample 2-2230

BWV 03-11-93, LOAMY SAND
From Adfit for, Alpha = 1.47, Rsq = .947
Calc Alpha = 1.35, Rsq = .97

ARYA-PARIS MODEL 200-BP-1, Sample 1-0531

BWV 02-11-93, SILT LOAM
From Actit. for, Alpha = 1.18, Rsq = .986
Calc Alpha = 1.16, Rsq = .977

ARYA-PARIS MODEL 200-BP-1, Sample 1-0531

BWV 02-11-93, SILT LOAM
From Actit. for, Alpha = 1.18, Rsq = .986
Calc Alpha = 1.34, RMS = .105

Sensitivity to ρ_b
Used $\rho_b = 2.06 \text{ g/cc}$
Actual $\rho_b = 1.36 \text{ g/cc}$

ARYA-PARIS MODEL AP Tank Farm, Sample 241-AP-2

BWV 03-19-93, SAND
From Adfit for, Alpha = 1.03, Rsq = .870
Calc Alpha = 1.50, Rsq = .926

ARYA-PARIS MODEL AP Tank Farm, Sample 241-AP-3

BWV 03-19-93, SAND
From Adfit for, Alpha = 1.33, Rsq = .574
Calc Alpha = 1.58, Rsq = .991

ARYA-PARIS MODEL AP Tank Farm, Sample 241-AP-4

BWV 03-19-93, SAND
From Apfit.for, Alpha = 1.33, Res = 816
Calc Alpha = 1.68, Res = .958

ARYA-PARIS MODEL New Jersey Soil, Sample S58NJ-12

BWV 03-21-93, SILT LOAM
From Apfit.for, Alpha = 1.18, Res = 922
Calc Alpha = 1.38, Res = 996

ARYA-PARIS MODEL

New Jersey Soil, Sample S58NJ-12
Sensitivity to Bulk Density

BWV 3-24-93, SILT LOAM
Calc Alpha = 1.38 • RHOB = 1.69
(1.23 • 1.25, 1.30 • 1.50, 1.41 • 1.75)

ARYA-PARIS MODEL ISSUES

- Sensitivity to bulk density
- Sensitivity to Alpha
 - Reduce by using Arya-Dierolf improved model
- Full sieve analysis
 - Dry sieve and hydrometer
 - Correct moisture retention curves for >2 mm size
- Hysteresis
 - Model can be based on drying or wetting curve
- Empirical model
 - No physical significance of alpha parameter
 - Physical significance with alpha
- Spatial variability
 - Geology may be difficult to predict
- Calcium carbonate cementing

ARYA-PARIS MODEL CONCLUSIONS

- Accurate correlation is obtainable provided:
 - Number of samples in database is increased
- Significant cost reduction:
 - less cost per sample
 - less wells drilled
- Significant time savings:
 - Expedite Hanford Site characterization and remediation

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Dispersivity Estimates

Lynn Gelhar
Massachusetts Institute of Technology

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DISPERSIVITY ?

- a measure of contaminant spreading and dilution ?
- an unpredictable fudge factor ?
- depends on scale ?
- determined by small-scale heterogeneity ?

STOCHASTIC METHODOLOGY

re Gelhar & Axness (1983), WRR 19(1)

Gelhar (1984) NATO ASI # E82

Gelhar (1987) NATO ASI # E128

Gelhar (1993) Stochastic Subsurface Hydrology, PH.

* $\Rightarrow$ lnK variability represented by 3D covariance/spectra
with spatial correlation scales λ_i , $i = 1, 2, 3$ *

$\Rightarrow$ flow equations with random parameters
 $\rightarrow$ stochastic p.d.e.

$\Rightarrow$ perturbation solution using spectral technique
assuming local statistical homogeneity

$\Rightarrow$ generic analytical results

- large scale mean behavior (effective properties)

K_{ij} effective conductivity

$\rightarrow A_{ij}$ macrodispersivity $\leftarrow$

- variance of dependent variables

σ_h^2 , σ_c^2
head conc.

covariance

CAPE COD SITE

VERTICALLY AVERAGED B_F CONCENTRATION - 32 days

mg/L
10-50
50-100
>100

15 port
multi level samplers ↗

Figure 3 - Vertically averaged bromide concentration distribution, in milligrams per liter, after 32 days travel time.

Injection wells

data from USGS
D. LeBlanc, S. Garabedian

CCAF

173 AAYS

北平

Concentration contours of Br (mg/L), 173 days after injection

Dr concentration (mg/L)

25-50

50-75

571

data from S. Garabedian
D. LeBlanc

10-25

see also WAB (1990) 77(5) 895-924

Spatial moments + conc

Fl

CAPE COD

From borehole flowmeter logging
2 inch dia fully-screened wells

data by K. Hess, USGS $F = \log K$

(7)

27/10

EXPLANATION
(HYDRAU > CONDUCTIVITY)-- (cm/s)

10 wells

>0.14 cm/s <0.08

Figure 4.-- Vertical section of natural logarithm of hydraulic conductivity.
Location of section line shown in figure 2

from K. Hess, USGS
borehole flowmeter

(100)

3620

9

ln K variogram

borehole flowmeter data, K. Hess (1990) USGS

STOCHASTIC THEORY:

$$A_{11} = \frac{\sigma_f^2 \lambda_1}{\gamma^2} \quad \text{longitudinal dispersivity}$$

$$= \underline{\underline{0.98 \text{ m}}}$$

$$\gamma\left(\frac{\sigma_f^2 \lambda_1}{\lambda_3}\right) = 1.12$$

lab batch K_d data by
Warren Wood, USGS

preliminary
data

K data by
S. Wolf (1985)
MIT Engr. Thesis

STOCHASTIC THEORY (MIT Parsons Lab Rpt 315, Garabedian...)

$$\text{effective } K_d = E[K_d] \Rightarrow R_{\text{eff}} = 1 + \frac{\rho_b \bar{K}_d}{n} \approx 9$$

long. dispersivity

non-retardational dispersivity

$$A = \underbrace{\frac{\sigma_y^2 \lambda_1}{\gamma^2} \left(1 - \frac{\gamma \rho_b \beta}{n \bar{R}}\right)^2}_{\text{correlated.}} + \underbrace{\frac{\rho_b^2 \sigma_y^2 \lambda_1}{n^2 \bar{R}^2}}_{\text{uncorrelated.}} \approx 7 A_0$$

retardation

$$R = \frac{V_{ar}}{V_{Li}} = 8.3$$

long. dispersivity

$$\frac{A_{Li}}{A_{gr}} \approx 10$$

Figure 55. Contours of maximum lithium concentration in mg/L in
220
comparison to those for bromide

from

Gelhar, L.W., C. Welty and K.R. Rehfeldt, "A Critical Review of Data on Field Scale Dispersion in Aquifers", Water Resources Research, ~~submitted April, 1991~~, 28(F), 1992.

see also

Gelhar, L.W., A. Mantoglou, C. Welty and K.R. Rehfeldt, "A Review Of Field Scale Physical Solute Transport Processes In Saturated And Unsaturated Porous Media," Final Rpt. RP2485-5, Elec. Power Res. Inst., Palo Alto, CA, EPRI EA-4190, August 1985.

(13)

UNSATURATED DISPERSION

(14)

3D Stochastic Heterogeneity

- 3D statistically anisotropic random fields represent spatial structure of hydraulic properties
- perturbation solutions to evaluate effective (large-scale) parameters showing micro-anisotropy, -hysteresis, -dispersivity

Comments:

- seemingly realistic 3D heterogeneity
- variance also predicted
- unfamiliar & untested
- soil statistical parameters difficult to obtain
- potentially predictive & testable
- works for saturated flow

3D STOCHASTIC MODEL

D. Polmann, Ph.D. ⁽¹⁵⁾ ₁₉₇₅ - sis

—○—"Real" Soil (partial correlation)

Imperfectly Stratified

$$\lambda_1 = \lambda_{b1} = 25\text{cm} \text{ \& } \lambda_{b2} = 100\text{cm} = \lambda_2$$

Steady-state flow with uniform mean tension

Maddock soil

Figure 5.28. Longitudinal dispersivities for unsaturated soils as related to displacement scale (based on Gelhar et al., 1985, Table 3-4).

Figure 6.5. Standard deviation and correlation scales of hydraulic conductivity or transmissivity versus overall scale.

Using Lysimeters to Predict Recharge at an Arid Site

G.W. Gee, M.D. Campbell, M.J. Fayer,
H.D. Freeman and M.L. Rockhold,

Pacific Northwest Laboratory
Richland, Washington

Work performed for the U.S. Department of Energy under
Contract Df AC06-76RLO 1830

Hanford Site Water Balance (mm/yr)

WHC-MR-0420

LIQUID EFFLUENTS CHARGE

MANFORD SITE

Recharge Around Leaking Tanks

RECHARGE ESTIMATES

Facility*	Soil/Vegetation	Irrig.	Time	Recharge Estimate	
				(mm/yr)	(% of Precip.)
200-East	Sand/Tumbleweed	No	1971-1985	<2	<1
200-East	Sand/Bare	No	1988-1989	90	43
BWTF	Sand/Bare	No	1985-1986	111	48
BWTF	Sand/Bare	No	1986-1987	102	55
BWTF	Sand/Bare	No	1987-1988	40	29
BWTF	Sand/Bare	No	1988-1989	42	24
BWTF	Sand/Bare	No	1984-1986	62	35
BWTF	Sand/Cheatgrass	No	1986-1987	1	5
BWTF	Sand/Tumbleweed	No	1987-1988	0*	0
BWTF	Sand/Tumbleweed	No	1988-1989	10	6
BWTF	Sand/Tumbleweed	No			
ALE	Silt Loam/Sagebrush	No	1986-1990	0*	0
ALE	Silt Loam/Bunchgrass	No	1986-1990	0*	0
FLTF	Silt Loam/Bare	Yes	1987-1990	0*	0
FLTF	Silt Loam/Bare	No	1987-1990	0*	0
FLTF	Silt Loam/Sagebrush	Yes	1987-1990	0*	0
FLTF	Silt Loam/Sagebrush	No	1987-1990	0*	0
STLF	Gravel over Silt/Bare	Yes	1988-1989	204	59
STLF	Gravel over Silt/Bare	No	1988-1989	74	48

Figure 1. Hanford Site map. Numbered circles represent lysimeter locations. Shaded area represents extent of August 1984 wildfire.

HANFORD SITE LYSIMETER FACILITIES

① 200-East Lysimeters

② Buried Waste Test Facility

③ Lysimeter Facility at ALE

④ Field Lysimeter Test Facility

⑤ Small Tube Lysimeter Facility

MODEL VALIDATION ?

200 E, DEEP LYSIMETER

Schematic of the Field Lysimeter Test Facility

Field Lysimeter Test Facility

Treatment	Precipitation			Surface			Soil	Thickness			Lysimeter #		
	A ^(a)	2A ^(b)	B ^(c)	Bare	Veg	Admix		Gravel	Texture	1.0 m		1.5 m	3.0 m
1	X				X			SIL		X		W01-1, D04-1, D07-1, C03-1	
2	X			X				SIL		X		W02-2, D01-2, D08-2	
3		X			X			SIL		X		W03-3, D13-3, D14-3, C06-3	
4		X		X				SIL		X		W04-4, D10-4, D12-4	
5	X				X	X		SIL		X		D02-5, D05-5	
6	X				X			SIL	X			D03-6, D06-6	
7			X					SIL		X		D09-7, D11-7	
8	X						X	S			X	C01-8	
9	X				X			S			X	C02-9	
10		X				X	X	S			X	C04-10	
11		X			X			S			X	C05-11	
(a) Ambient precipitation										SIL = Silt Loam			
(b) 2X, 3X annual average										S = Sand			
(c) Breakthrough +2X, 3X annual average													

LYSIMETER WATER STORAGE

FIG. 4 Water Storage and precipitation for seven treatments at FTF from Nov. 1987 through Oct. 1992

Fig. 11. Measured and simulated storage for the 2 × -average precipitation treatment, lysimeter W4. Shown is the simulation with 1.43 times the saturated conductivity (K_s), the pore interaction term, $\ell = 0$, a snow cover, and 0.7 times potential evaporation (PE).

FIGURE 2.1. Measured and Simulated Storage in Lysimeter WL-4

FIGURE 2.2. Measured and Simulated Storage in Lysimeter WL-2

FLTF CLEAR-TUBE LYSIMETER DRAINAGE

Chart2

LYSIMETER DRAINAGE

Flt Drainage - Bare Lysimeters

01-Nov-90 Thru 15-Mar-93

Table 2. Parameters describing the hydraulic properties of materials in the lysimeters with the van Genuchten and Mualem functions.

Material	Parameter†				
	θ_r	θ_s	α	n	K_s
	cm ³ /cm ³	cm ³ /cm ³	1/cm		cm/h
Silt loam					
Laboratory desorption	0.00	0.496	0.0178	1.34	4.03‡
Field sorption	0.00	0.411	0.0419	1.29	3.24§
Sand	0.010	0.445	0.0726	2.80	394.0
Gravel	0.005	0.419	4.93	2.19	1260.0

† θ_r = residual volumetric water content, θ_s = saturated volumetric water content, α and n = curve-fitting parameters, and K_s = saturated hydraulic conductivity.

‡ Fitted value of saturated conductivity.

§ Average of values determined in the field with a Guelph permeameter (Rockhold et al., 1988).

HYDRAULIC PROPERTIES FOR COVER MATERIALS

Fig. 2. (a) Water retention and (b) hydraulic conductivity of the materials in the lysimeters. The values of vapor conductivity relative to a suction-head gradient for the silt loam at 15.3°C are included for comparison.

FIGURE 3.1 Hysteresis Effect on Water Retention

FIGURE 3.5. Measured and Simulated Water Contents at a Depth of 60 cm in Lysimeter D)

FIGURE 3.4. Measured and Simulated Water Contents at a Depth of 15 cm in Lysimeter 19

FIGURE 3.3. Measured and Simulated Drainage from Lysimeter 19

TABLE 2.1. Water Balance Parameters (mm) During March 6-8, 1989. Precipitation and drainage were zero. Measured evaporation was determined as the change in storage. The simulations used the calibrated parameters.

	March 1989			Total
<u>Lysimeter WL-2</u>	<u>6</u>	<u>7</u>	<u>8</u>	
Measured Evaporation	0.8	1.4	1.5	3.7
Simulated Evaporation	0.0	1.3	2.1	3.4
<u>Lysimeter WL-4</u>				
Measured Evaporation	0.8	1.3	1.5	3.6
Simulated Evaporation	0.0	1.3	2.1	3.4
Potential Evaporation	2.2	1.9	3.0	7.1
0.7*PE (calibrated PE)	1.5	1.3	2.1	4.9

WATER BALANCE (LYSIMETERS)

SUMMARY

1. Lysimeters - only way to Directly Measure Drainage.
2. Arid Site Predictions of Drainage Require Lysimeters (Computer Models of ET and Drainage Require Calibration Data).
3. Waste Site Recharge - Inferred by Lysimeter Drainage Data.
 - Drainage Affected by Variation in Annual Precipitation (P) - Lags Noted
 - Gravel - Covered Soil - Recharge $> 70\% P$
 - Bare, Coarse Sands - Recharge $> 50\% P$
 - Grass - Covered Sands - Recharge $> 30\% P$
 - Summer Annual (Tumbleweed) - Recharge $< 30\% P$
 - Fine Soil (Vegetated or Bare) - Recharge $\rightarrow 0$
4. Climate, Vegetation, Soil Variables Key to Water Balance.
5. Drainage Data Base Available for Model Calibration (Additional 5 to 7 yrs Continuous Record needed for Model Validation).

WORKSHOP MINUTES

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VADOSE ZONE MODELING WORKSHOP MINUTES

March 29, 1993

= > workshop attendee

* workshop presenter

* John Rawlins - Opening Remarks

introduction

Lynn Gelhar - MIT

Peter Wierenga - University of Arizona

Rien van Genuchten - U.S. Salinity Lab., Riverside

covered workshop agenda

* Raz Khaleel - Statement of Workshop Goals and Objectives

Overview of previous workshop

history

-had similar workshop 3 1/2 years ago

previous workshop recommendations:

1) site characterization data base

2) code calibration/validation

a) document existing database

b) some Hanford Sites aren't fully utilized

process identification:

1) validation of Van Genuchten-Mualem relationships

2) saturation-dependent anisotropy for vadose zone

Why focus on modeling issues?

1) predictive reliability

2) regulatory requirements

3) compromise between data requirements and loss of predictive reliability

Objectives

A) Objective 1

Following codes used on site:

1.) PORFLO

2.) VAM2D-CG (HydroGeologic)

3.) UNSATH (PNL)

Develop a consensus position by all "stakeholders"

B) Objective 2

Obtain a commitment from all stakeholders to support the results, findings, and/or recommendations.

C) Objective 3

Identify action items

=> Ward Staubit

There is great concern in the 200 Area Waste Sites. We can not spend big dollars on all Hanford sites. We need to keep a perspective on the modeling strategy and apply model on a site specific basis.

* Raz Khaleel - Statement of Workshop Goals and Objectives (continued)

=> Peter Wierenga
Questioned previous workshop

=> Rien van Genuchten
Need to make reports available to panel members for review.

* Raz Khaleel - Types of Wastes and Waste Sites

Showed overall Hanford site map

- 1) 200 plateau
- 2) 100 & 300 Area along river
- 3) 400 Area-FFTF

Hanford Waste Sites

- 1) Over 1400 waste sites have been identified, including both active TSD facilities and inactive sites.
- 2) Four aggregate areas are subdivided into 21 waste areas based on facility and type of operation.
- 3) Looked at 78 sites.

Waste Site Distribution @ Hanford pie chart

Liquid Wastes Discharged & Solid Waste Buried @ Hanford (1944-1989)

- 1) 5.6 million curies of radioactivity

=> Rien van Genuchten
Clarification of pie chart - 20% of total radioactive waste.

Viewgraphs of tank farms, cribs, & trenches

Hydrogeology of Hanford Site

- fence diagram of 200 West Area
- groundwater is at 150-250 ft. depth
- Mike Connelly's viewgraphs

How much data collection will be enough for a 560 square mile site?
This will hopefully be resolved from panel members.

=> Rien Van Genuchten
What type of data is collected?
Bulk density, etc.

* Len Collard - Performance/Risk Assessment at a CERCLA site at Hanford

200-BP-1 Cribs

- 1) overall RI/FS (Remedial Investigation/Feasibility Study) process
- 2) description of operations
- 3) site sampling
- 4) lab testing
- 5) selection of samples

6) modeling approach

* Len Collard - Performance/Risk Assessment at a CERCLA site at Hanford

200-BP-1 Cribs (continued)

7) modeling domain

8) results

1) RI/FS

- conduct baseline risk assessment
- provide additional site characterization

2) operations

- 200-BP-1 site consists of 4 acres and contains 8 cribs
- 2 types of discharges
 - 1) supernatant
 - cribs B43-B49
 - 2) evaporation
 - cribs B50 and B57
 - operating time 3/65 - 1974
- waste quantities discharged to cribs in 200-BP-1

crib construction viewgraph

earth backfill

sisalkraft paper

washed gravel

=> Rien van Genuchten

Concerned about crib operation and contaminants trickling out of washed gravel.

=> Peter Wierenga

What is your philosophy of discharge?

* Len Collard

To hold contaminants in the soil column and if it did reach the groundwater, the concentration would be small.

=> Peter Wierenga

How do you keep track of what was discharged - the only to correctly determine the discharge is to compare what was pumped in vs. what was pumped out.

=> Doug Sherwood

Gave input on 200-BP-1 crib operations.

=> Allen Lu

Concentrated on radionuclides not chemical solvents.

=> Mark I. Wood

200-BP-1 input.

=> Scott Kindred

Questioned 200-BP-1 values.

200-BP-1 radionuclides inventory viewgraph

* Len Collard - Performance/Risk Assessment at a CERCLA site at Hanford
(continued)

=> Lynn Gelhar

Questioned radionuclides values? Where did they come from?

liquid discharge to 200-BP-1 cribs viewgraph

Sr90 flux for 200-BP-1 cribs viewgraph

3) site sampling activities

total of 28 boreholes

a) groundwater well - depth > 200 ft.

b) most wells had a depth of 50 ft.

c) surface sampling

=> Peter Wierenga

When did sampling take place?

* Len Collard

Sampling took place in recent years.

=> Peter Wierenga

Who is doing the drilling/testing?

* Len Collard

KEH is responsible for the well drilling and testing is done both on and off site.

=> Lynn Gelhar

Is there a site characterization report?

=> Ward Staubitz

There will be a site characterization report this Thursday.

=> Peter Wierenga

Questioned both the physical and chemical sampling.

=> Rien van Genuchten

Please give panel members a list of the physical and chemical properties and lab results.

=> Ward Staubitz

Chemical sample and physical property sample techniques:

- only scanned part of the sample so they could keep moisture in
- have gravimetric moisture content results

3) site sampling activities (continued)

borehole schematic of material type

=> Rien van Genuchten

Question concerning silt layer over 200-BP-1 site.

=> Doug Sherwood

There are about 11 deep bore wells for the 200-BP-1 site.

* Len Collard - Performance/Risk Assessment at a CERCLA site at Hanford
(continued)

=> Rien van Genuchten

What was the physical and chemical data collected? A database of this information is needed.

* Len Collard

I have a list of what physical property tests were ran, but I do not have data values.

=> Rien van Genuchten

Were you able to keep gravels compact for moisture retention test?
Was the unsaturated hydraulic conductivity overestimated?

* Len Collard

The dryer regions are correct.

=> John Relyea

Throwing our larger rocks creates more voids that are filled, thus the unsaturated hydraulic conductivity will be overestimated. The unsaturated hydraulic conductivity value will be higher in model than in the field.

=> Peter Wierenga

The 200-BP-1 data looks very conservative - low conductivities.

=> Ward Staubit

The unsaturated hydraulic conductivity is non-conservative on a flow and transport contaminant modeling philosophy.

=> Lynn Gelhar

Speculating on curves - can you do larger field testing by using pipes, thus have a larger test sample.

=> John Relyea

I will address this tomorrow in my presentation - we currently use 20 points per curve.

=> Rien van Genuchten

What kind of "n" values did you get?

=> Ward Staubit

We need to make copies of the RI report and distribute them to the panel members. Did you need a model for the risk assessment of this site?

=> Rien van Genuchten

How did you handle absorption? Where did you get Kd values?

* Len Collard

Kd values were obtained by Hanford studies.

* Len Collard - Performance/Risk Assessment at a CERCLA site at Hanford
(continued)

=> Rien van Genuchten
How did results come out for the unsaturated zones? Where were
measurements taken?

* Len Collard
Borehole.

=> Rien van Genuchten
Can you reconstruct the measurements taken vs. sample depth?

***** BREAK *****

* Len Collard - Performance/Risk Assessment at a CERCLA site at Hanford
(continued)

Fluid boundary conditions - geometric layout of grid viewgraph.

=> Rien van Genuchten
Do you have reasonable estimates of source?

* Len Collard
Yes.

samples were only taken at discreet points
RLS Spectral Gamma-Ray Borehole survey viewgraphs

=> Rien van Genuchten
Have you looked at geochemical controls?

=> Ward Staubitz
Straight absorption was assumed.

=> Lynn Gelhar
Are you going to be showing Kd data?

=> Rien Van Genuchten
What was the maximum Cesium concentration in 200-BP-1 layers?

* Len Collard
600K pCi/gram

=> John Relyea
Do you have anything on the history of cribs and why did they cease
operations?

* Len Collard
No.

Radionuclides levels for 349A Lab Measurements viewgraph
Sampling scheme for deep boreholes B43-B49 viewgraph

- * Len Collard - Performance/Risk Assessment at a CERCLA site at Hanford
(continued)

=> Ward Staubitz

What was the interval of physical properties taken?

- * Len Collard

Moisture content, particle size distribution and cobalt content were taken at 5 ft. intervals. Unsaturated hydraulic conductivity was not taken at 5 ft. intervals though.

5) selection of samples for testing

- 1) provide data for major layers
- 2) problems
 - a) individual sample integrity and representativeness
 - b) use of multiple liners
 - c) lack of data in hot zone
 - d) possible overdriving of sampler
 - bulk density > 2g/cc
 - e) true behavior of gravels
 - f) sensitivity of lab technique
 - g) bulk density to use with moisture retention data
 - field bulk density

=> John Relyea

Two liners are currently being used.

6) modeling approach

- 1) conceptual model
- 2) computer program selection
- 3) contaminants of concern
 - a) inventory
 - b) screening process
- 4) scenarios are conservative, but not unrealistic
 - a) start with reported inventory
 - b) low Kd from range
 - c) vertical movement to groundwater - isotropic
 - d) later migration
 - 1) anisotropic
 - 2) world model for interactions
 - e) recharge rates
 - 1) T106 Study
 - average 13 cm/yr
 - precipitation rate 16 cm/yr
 - 2) 1 cm/yr
 - 3) 10 cm/yr (preliminary biota barrier)

=> Rien van Genuchten

No vegetation.

mesh for single crib with horizontal symmetry viewgraph

* Len Collard - Performance/Risk Assessment at a CERCLA site at Hanford
(continued)

=> Ward Staubitz
Where did you get saturated hydraulic conductivity values?

* Len Collard
Top gravel layer had a number of different samples in which the highest saturated hydraulic conductivity was picked. The silt layer had only one sample taken thus that saturated hydraulic conductivity was used.

=> Rien van Genuchten
Did you correct initial moisture content for gravel?

* Len Collard
No.

=> Rien van Genuchten
Then you are not being consistent.

=> Peter Wierenga
It does not matter what the initial saturated hydraulic conductivity values were for a small time scale.

=> Rien van Genuchten
I am concerned with your mechanics. I agree with your steady state calculations, however, if you overestimate your moisture content and fix boundary conditions at the top, then the velocity will be underestimated (pore velocity is smaller), thus what Len did was not the worst case scenario, but best case scenario.

=> Mark Rockhold
Questioned recharge rates.

=> Niall Kline
Below crib velocity.

=> Rien van Genuchten
Did you fix the amount of liquid or did you let the soil determine?
Should determine total amount - the flux conditions throughout the crib operation and then after operation, apply just rainfall.

Chose ambient conditions of Kd value.
Sr-90 concentration plots

=> Lynn Gelhar
Kd=20 for strontium.

=> Rick Healy

Do you have results for a conservative Kd?

=> Ward Staubitz

Why does biota barrier accelerate?

* Len Collard - Performance/Risk Assessment at a CERCLA site at Hanford
(continued)

* Len Collard

I did a world model with all cribs - 3D model.

=> Rick Healy

What were the dispersivity values and "x" and "y" increments?

=> Mark Rockhold

Did you calculate Peclet numbers?

world model viewgraph

surface boundary conditions independent of moisture content

=> Scott Kindred

How did the 1992 results compare with field measurements?

* Len Collard

They were not compared.

=> Lynn Gelhar

What is the horizontal and vertical distance in world map 1974 to 1992?

What is the volume of major infiltration?

* Len Collard

B50 crib dominates.

=> Doug Sherwood

There was 40 million liters released to the B50 crib.

=> Mark Wood

What happens when you lower the Kd value?

* Len Collard

The concentration in water increases.

=> Peter Wierenga

Did you look at nitrates and tritium?

* Len Collard

There is no information on the duration of operation.

* Raz Khaleel - What Are The Issues?

A) Calibration/Validation

1) flow and transport codes calibrated/validated

2) database

B) Evaluate estimates of unsaturated hydraulic conductivity (viewgraph)

- C) Dispersivity estimates
- D) Uncertainty and spatial variability
- E) Evaluate applicability of PSD data in estimating moisture retention (Arya-Paris model)
- F) Kd/Rd approach
- G) Evaluate moisture-dependent anisotropy

* Raz Khaleel - What Are The Issues? (continued)

Stochastic Theory - macroscopic anisotropy

Injection Test Site

- 1980 & 1981 time frame
- water was injected at 15 ft. depth

saturated hydraulic conductivity histogram results

=> Lynn Gelhar

Do they have an open borehole above groundwater?

=> Rien van Genuchten

Are you concerned about the two methods? Your method gives you 1000 times the results.

=> Mark Rockhold

Question defining slug test.

=> Peter Wierenga

Three orders of magnitude is severe.

experimental and fitted variograms viewgraph

Injection Test Site data flowchart viewgraph

Kr vs Psi viewgraph

=> Rien van Genuchten

Questioned data on Kr vs. Psi viewgraph.

RETC viewgraph

=> Mark Rockhold

What is your procedure for combining a centrifuge sample to that of a lab sample? There are porosity problems and inconsistencies.

=> Lynn Gelhar

I suggest using the data directly instead of fitting it first.

Kr/Kz anisotropy vs. mean pressure head viewgraph

Injection Test Site borehole layout viewgraph

Kr/Kz anisotropy based on turn ratios

=> Lynn Gelhar

Did not understand how above values were calculated.

=> Rien van Genuchten

What gradient did you assume in Darcy's Law?

=> Rick Healy

Did you have lab data? Did you use vertical hydraulic conductivity or horizontal hydraulic conductivity?

* Raz Khaleel - What Are The Issues? (continued)

=> Mark Rockhold

What retention curves did you choose?

=> Peter Wierenga

Do you have water content distributions?

***** BREAK FOR LUNCH *****

* Peter Wierenga - Las Cruces Trench Experiment

Objectives

- 1) test deterministic and stochastic models for water flow and solute transport
- 2) test site characterization and monitoring techniques

must have good control over boundary conditions

borehole parameter test

- see how long it takes a known amount of water to seep into ground

groundwater = 300 ft.

Sampling

- 9 soil layers
- 50 cores - saturated hydraulic conductivity per layer
- 0.50 m horizontal spacing
- 0.65 m vertical spacing average

Hydraulic properties

- 1) in-situ saturated hydraulic conductivity
- 2) core soil water retention data
- 3) van Genuchten parameters.

2D model to predict infiltration/evaporation

0.50 cm/day

how to determine hydraulic properties?

wet end of water retention curve

one step outflow method

- problems with this method in determining unsaturated hydraulic conductivity values.

Conclusions

- 1) transient experiments provide good estimates of the soil

hydraulic property relationships

- a) transient tension measurements measured flux boundary conditions
- 2) gamma is an important parameter

=> Raz Khaleel

It looks like data is close to saturation.

* Peter Wierenga - Las Cruces Trench Experiment (continued)

* Peter Wierenga

We had data to 500 cm. In the prediction mode, it is important to know the dry end. One must also take into account vapor flow. I believe the best method is in the "in between range", less confidence in dry end and saturation end.

=> Scott Kindred

Importance of vapor flow in unsaturated zone, i.e. Philip and Reese.

=> Glendon Gee

There needs to be a concurrence with the importance of vapor flow.

* Allen Lu - Injection Test Site at Hanford

- Injection Test Site (RHO-ST-46; Sisson + Lu, 1984)
- graphical presentation of the field data
- modeling scenarios
- model evaluation criteria
- samples of model results and comparisons

Field Experiment

- 1) 200 East area
- 2) approximately 1000 gallons of water were delivered for ten consecutive weeks to each well
- 3) a 20 mL solution of the radiological tracers ^{85}Sr and ^{134}Cs were mixed and injected
- 4) field data was obtained by lowering sensors to the desired depths in the observation wells
- 5) soil samples were taken from two monitoring wells

Injection Test Site viewgraphs

=> Peter Wierenga

Do you have an initial moisture content contour?

6 different model simulation scenarios

- 1) uniform isotropic soil
- 2) uniform but anisotropic soil
- 3) non-uniform (10 layers) but isotropic soil
- 4) same as scenario 3, but hysteresis is accounted for
- 5) nonuniform but anisotropic soil
- 6) same as scenario 5, but only saturated hydraulic conductivity were allowed to be anisotropic soil

Model Evaluation Criteria
contour plots and time history plots

Injection Test Site viewgraphs

=> Rien van Genuchten
What was the anisotropy ratio?

* Allen Lu - Injection Test Site at Hanford (continued)

* Allen Lu
It was varied.

=> Lynn Gelhar
Where is the water distributed?

showed zero moment and first moment viewgraphs

=> Lynn Gelhar
Why not do a complete circle?

=> Mark Rockhold
Do you have to interpolate water content values that relate with time?

=> Peter Wierenga
Did you get good mass balance? Need to apply this over the full model -
make a complete circle.

* Allen Lu
Averaging over the range - get close to full mass balance.

=> John Relyea
How long did it take to get all the probe measurements?

=> Peter Wierenga
How many probes did you have?

* Allen Lu
There is a total of 32 wells.

* John Smoot - 241-T-106 Tank Leak

- occurred 4 years ago
- took place in the north central part of the 200 West area
- volume of liquid = 2000 m³
- single shell tank constructed in 1943 leaked
- tank diameter = 75 ft.
- bottom of tank = 11 m below surface
- top of tank = 2.1 m below surface
- tank contains wide variety of radioactive components
- leak occurred in 1973
- leak duration = 2 months
- 1978 deepened some of the boreholes

- 5 soil layers

=> Ward Staubitz
Did you have particle size distribution data?

3D mesh - PORFLOW 3 simulation results

=> Rien van Genuchten
Are those relative saturations?

* John Smoot - 241-T-106 Tank Leak (continued)

* John Smoot
Yes.

=> Scott Kindred
Estimate on numerical dispersion?

* John Smoot
Small retardation factor.

Conclusions

- 1) PORFLOW 3 results looked good
- 2) good match for 1973 Ru-106 plume
- 3) discrepancies for 1978 Ru-106 plume
- 4) good match for Cs-137 plume
- 5) more site specific data is needed

=> John Relyea
High ionic strength?

* John Smoot
Did not take into account the bulk density and Kd from tank contaminants.

=> Frank Schmittroth
Are you sensitive to the inventories?

=> Peter Wierenga
After the leak stopped, what was the driving force? Rainfall?

=> Scott Kindred
Was 5 cm/yr the infiltration rate used?

***** BREAK *****

* Charley Kincaid - A Calibration/Validation Proposal

put together activity data sheet (ADS)

Purpose

- 1) gaining consensus from all players

=> Rien van Genuchten
What and who defines a validated model?

- => Peter Wierenga
Who developed all the nonsense of constraints? It looks as if time and efforts are wasted on doing documentation, instead of real life work.
- * Charley Kincaid
This is needed for Quality Assurance and for traceability.
- => Rien van Genuchten
Question concerning validating computer code.
- * Charley Kincaid - A Calibration/Validation Proposal (continued)
- => Fred Mann
Personally feels that constraint documentation is driven by Microsoft, Borland, etc., and not by the nuclear field.
- => Scott Kindred
Finds a disconnect between the RI/FS process and modeling aspect, i.e. 200-BP-1.
- => Peter Wierenga
What is the consensus?
- * Charley Kincaid
Must have enough confidence in model to go to his superiors/public with it. DOE and DOE contractors can not make that decision. Feel that a consensus needs to be made with the scientific community.
- => Chuck Cline
Tried to standardize four models, i.e. several models of PORFLO on site. This is a problem on site.
- => Ward Staubit
What are these models going to be used for? What is too much? Need to collect less data and rely more on models.
- => Lynn Gelhar
Did not feel that 200-BP-1 was a good model.
- => Ward Staubit
Agrees with Lynn Gelhar - also has samples stored that can be resampled and new curves collected. Do you feel expense is justified?
- => Doug Sherwood
Lynn Gelhar has not been given detailed information, i.e. # of samples, etc., concerning 200-BP-1. Felt that Lynn Gelhar did not get a full enough picture to make a decision.
- => Rien van Genuchten
We were not given information. We should go back to the earlier question concerning validation/calibration of 200-BP-1.
- => Scott Kindred
Concerning risk assessment, there was plenty of data on 200-BP-1, but

did not have enough information for validation though.

- => Ward Staubit
Would you be comfortable in applying 200-BP-1 data to another site as a data set?
- => Scott Kindred
Depends on site itself. For sites where contaminants reach groundwater, we would want better characterization. We do however, want to use 200-BP-1 data.
- * Charley Kincaid - A Calibration/Validation Proposal (continued)
- => Doug Sherwood
200-BP-1 is similar, as far as operation and length, to other sites in 200 East area.
- => Charley Kincaid
The 200 East fence is an arbitrary line - sites vary in the same areas.
- => Doug Sherwood
Money can not be spent at other sites as it was spent at 200-BP-1.
- => Rien van Genuchten
Given these complexities - do you feel that there will be a validated code for the Hanford site? You are putting a number of criteria that is desirable, but may not obtainable.
- => Ward Staubit
This does bring up the fundamental question - can we validate a model? One way or another, a decision will have to be made using input from this panel.
- => Chuck Cline
T106 is as close to validation as we have. It is closing in to \$2 million for 1 borehole to 180 ft..
- => Lynn Gelhar
Aren't you talking about \$50 billion in cost to clean the Hanford site?

* Lynn Gelhar - What Constitutes a Validation Experiment?

Does the model really predict? <= This is the key question.

Do not see calibration/validation as same process?

Possible Modeling Approaches

A. Deterministic Numerical Model

i. Classical

- ignore spatial variable
- no error measure
- model parameters not directly measurable

ii. Detailed with "actual" heterogeneity

- measurements impractical

- computationally infeasible
- B. Stochastic
 - Represented by spatial random fields
 - characterized with a small number of parameters
 - mean
 - variance

Add geologic information to data sets
Solve for average and variations about mean
Important to capture variation in K vs. Sat curves
Large scale model with variable parameters

* Lynn Gelhar - What Constitutes a Validation Experiment? (continued)

Degree of spread with 20 of mean solution
New Mexico Technical lab experiment (Stephens 1988)

=> Rien van Genuchten
Has this been tried in determination sense?

* Lynn Gelhar
Yes - Mualem took ratio of harmonic mean to arithmetic mean.

* Rien Van Genuchten - Issues of Model Testing

Mathematical verification
- accuracy of numerical solution (algorithm)

Experimental validation

- simplified representation of system or process
- validation of process - not a code
- validation applies only to specific set of conditions
 - space, time
 - initial/boundary conditions
- models are tools

Calibration

- history matching
- parameter estimation (inverse problem)
- parameter uniqueness problems (in case of good fit)
- conceptual problems
- parameters are model/real specific

Predictions/Extrapolation

- space
- other boundary conditions
- other initial conditions
- times

=> Fred Schmittroth
How far into future extrapolate?

* Rien van Genuchten

Length of data collection depends on site specific problems. Changing conditions - no way to appreciate long term changes based on short time of data collection.

=> Scott Kindred
Comparing physical properties with recharge - what parameters are important?

=> Glendon Gee
How do you incorporate man-made effects?

* Rien Van Genuchten - Issues of Model Testing (continued)

=> Peter Wierenga
Implying a need to stabilize - do you assume non-changing of condition?

=> Scott Kindred
Baseline RI - things remain same.

=> Doug Sherwood
Regulations have not reviewed/read report - we do not endure conclusions we want help to judge modeling.

=> Charley Kincaid
Like turn away from validation to history matching. How to build program/confidence?

* Rien van Genuchten
Use models only as management tool?

=> Charley Kincaid
Models used as tools gain acceptance. First step to gain consensus of model use, ask - What is achievable? What is needed?. All this is part of consensus building. Proposal is that, not funded now or next year.

=> Ward Staubitz
No sitewide support for modeling everything on site specific scale.

* Rien van Genuchten
Why not?

=> Ward Staubitz
Tri-Party Agreement - DOE's ability to get things done. No binding agreement/no funding.

=> Doug Sherwood
Technical building development tied to sites.

=> Ward Staubitz
Proposal put umbrella over modeling coordination/funding. Strategy of models/unofficial sharing.

- => Peter Wierenga
Is there approach to models/unofficial sharing?
- => Ward Staubitz
No sitewide effort/coordination.
- * Rien van Genuchten
A global problem is that outside agencies must go and ask.
- => Peter Wierenga
Ideally, have a small group in charge.
- * Rien Van Genuchten - Issues of Model Testing (continued)
- => Charley Kincaid
Group got together 4 years ago to address question. DOE ought to see this as a sitewide problem, but DOE decided it was too much trouble. Nothing happened.
- => Al Law
Some work along this line - Groundwater Management Protection Plan. DOE-RL will implement soon. This is oriented toward characterization and modeling is mentioned.
- * Rien van Genuchten
Advantages of this is huge, need much more information and find weaknesses.
- => Al Law
ERMC oriented toward site specific.
- => Ward Staubitz
Energy modeler on own, depends on individual effort to contact colleagues. Ought to be meeting to tie efforts together.
- Meeting Adjourned

VADOSE ZONE MODELING WORKSHOP MINUTES

March 30, 1993

= > workshop

attendee

* workshop presenter

* John Rawlins - Introduction

* John Relyea - Laboratory Measurement of Hydrologic Properties

Physical property test on site:

- 1) particle size distribution
 - never know what we are going to get
 - Hanford history includes volcanoes, wind, flood, glaciers
- 2) porosity & bulk density
- 3) specific gravity & grain density
- 4) moisture content
 - liners do not hold moisture in soil when temperatures exceed 140 degrees Fahrenheit
- 5) saturated hydraulic conductivity methods
 - 1) falling head
 - 2) constant head
 - 3) falling head-rising tail

=> Rien van Genuchten

How do you control pressure to control channeling?

* John Relyea

Do not over pressurize.

- 6) moisture retention curve
 - CX-2 measures relative humidity

=> Rien van Genuchten

Do you deair the water to get complete saturation?

Do you use the first drying curve or the main drying curve?

* John Relyea

We measure first drying curve for saturation.

=> Raz Khaleel

What is the main drying curve?

=> Rien Van Genuchten

The drying curve that is done after completing wetting curve.

- 7) unsaturated hydraulic conductivity

=> Lynn Gelhar

Do you have good hydraulic contact?

* John Relyea

Yes

hydraulic conductivity values

* Jim Conca - Unsaturated Hydraulic Conductivity Measurement (continued)

=> Rien van Genuchten

Do you have equal confidence in wet range as in dry range?

* Jim Conca

We are concentrating on the unsaturated hydraulic conductivity part of the curve, but traditional methods allow for a good calculation of saturated hydraulic conductivity.

=> Rien van Genuchten

Could you go up to saturation if you wanted?

* Jim Conca

Yes

there is not a great effect on the hydraulic conductivity from the packing method used. Example: W7-9 #0-072

=> Lynn Gelhar

Do you have a report that discusses your findings?

* Jim Conca

Yes

=> Peter Wierenga

Does the flow come from one point?

* Jim Conca

The flow hits the front and then gets dispersed.

=> Ward Staubitz

This is an important piece of information into guiding us on site characterization.

we are currently running samples for Z-Plant

* Raz Khaleel - Use of van Genuchten-Mualem Relationships to Predict Unsaturated Hydraulic Conductivity

covered van Genuchten-Mualem equation

Objective

-validate van Genuchten-Mualem relationship to estimate unsaturated hydraulic conductivity for Hanford soils, especially at low moisture contents

Current approach

-library of moisture retention curves of the Hanford site is very limited
-moisture retention curve + van Genuchten-Mualem relations +

=> Peter Wierenga
Is it all stainless steel?

* John Relyea - Laboratory Measurement of Hydrologic Properties (continued)

* John Relyea
No

=> Lynn Gelhar
How high of a potential do you go?

* John Relyea
1/2 bar

=> Ward Staubitz
How many samples do you process?

* John Relyea
For retention curves - approximately 3000 samples overall.
We do more saturated hydraulic conductivity (>500) than unsaturated hydraulic conductivity. Geotechnical Engineering Laboratory started doing unsaturated hydraulic conductivity in January

=> Rien van Genuchten
Can you run samples simultaneously?

* John Relyea
Yes - can run 6 samples at the same time.

* Jim Conca - Unsaturated Hydraulic Conductivity Measurement

Unsaturated Flow Apparatus (UFA)
-developed by Jim Conca and Judith Wright
-attains hydraulic steady-state in hours, instead of weeks to years
-acceleration is a whole body force

=> Lynn Gelhar
What is the dispersion cap made out of?

* Jim Conca
Neuroplastic or aluminum - depends on sample material.

reach hydraulic steady state
-where moisture in = moisture out
-hydraulic conductivity can be determined from the driving force and flux

-use Darcy's relationship under centripetal acceleration
-Darcy's Law is a bulk property and provides no mechanistic information
thus it doesn't matter what the driving force is - just that it follows Darcy's Law

UFA
- is fast and can obtain information at low water contents and low

saturated hydraulic conductivity = unsaturated hydraulic
conductivity curves

- * Raz Khaleel - Use of van Genuchten-Mualem Relationships to Predict
Unsaturated Hydraulic Conductivity (continued)

acquire data from 3 labs

- 1) Ksat measurement data
- 2) Jim Conca's Lab
- 3) John Relyea's Lab

parameter estimation

- 1) predicted
- 2) simultaneous - 5 parameter Ksat = fixed
- 3) simultaneous - 6 parameter all float

Example:

compare moisture retention curves generated by above methods
simultaneous - 6 parameter method proves to be best fit

=> Rien van Genuchten

Most of your data points are in the dry end not the wet range. I would
be nervous about the fitting.

=> John Relyea

We realize we are not getting enough points in the wet range, but that
has changed because we are getting more points now.

=> Rien van Genuchten

Definitely need more points in wet range.

=> Raz Khaleel

How many data points would you consider enough?

=> Rien van Genuchten

Whatever it takes to define the curve.

=> Allen Lu

Importance here is that the simultaneous - 6 parameter is best.

=> Jim Conca

It is hard to get the wet end in Hanford soils.

=> Ward Staubitz

We are mostly concerned in dry end.

=> John Relyea

We see moisture contents down to 4% - it depends on soil texture and
pressure. The 10% moisture content that is stated is an old value.
Hanford sand is less than 10%.

=> Ward Staubitz

Mainly looking at drainage curve at the sites we are interested.

- => Len Collard
Volumetric moisture content for the 200BP1 site is 4%-7%.
- * Raz Khaleel - Use of van Genuchten-Mualem Relationships to Predict Unsaturated Hydraulic Conductivity (continued)
- => Rick Healy
What is the matric potential that corresponds with that?
- => Len Collard
It is low - I'm not exactly sure of the specific value.
- => Rien van Genuchten
If you are interested in $K(\theta)$ at low moisture content, why are you using the saturated hydraulic conductivity to measure or predict the curve.
- => John Relyea
We can not measure the unsaturated hydraulic conductivity at 10%.
- => Peter Wierenga
Match hydraulic conductivity at 50 millibar would be more realistic and safer.
- => John Relyea
Referenced last page of his presentation handout.
- => Ward Staubitz
Since the lower end of curve is what we are interested in, it would be more realistic to not fit to the saturated hydraulic conductivity.
- => Peter Wierenga
I feel much better fitting to the unsaturated hydraulic conductivity.
- => John Relyea
The problem with that is that it is time consuming.

viewgraph - fitted hydraulic conductivity vs. measured hydraulic conductivity with regression line
- => Lynn Gelhar
The current approach of fitting to saturated hydraulic conductivity in reference to the predictive method shows a lot of errors.

viewgraph - Injection Test Site plots

This is on going - more data needs to be analyzed before a conclusion can be made.

Simultaneous fitting considerable improves fitting.
- => Rien van Genuchten
Remember $\lambda = 0.5$ is an average, it can range between -10 and 10. Do not trust fitted λ .

***** BREAK *****

* Ben Volk - Use of Arya-Paris Model to Estimate Moisture Retention Data

passed out presentation handout

Only the drying curve was used for this model, but the wetting could also be done.

=> Lynn Gelhar

Why is your contact angle = 0 ?

* Ben Volk

Not sure what it is.

=> Lynn Gelhar

To set it to 0 is not justifiable then.

fractal dimension

=> Rien van Genuchten

Did you adjust for entrapped air?

* Ben Volk

Fully saturated porosity was used.

=> Rien van Genuchten

Using 90% of saturated water content might improve data considerable.

=> Rien van Genuchten

What is the calculated value?

* Ben Volk

Ran calculations on lab samples

What is the predicted value?

* Ben Volk

Plug in alpha and generate curve.

Hydrometer would give more points in smaller sieve ranges.

=> Rick Healy

I'm concerned with moisture retention curves being run on a percentage of sample, but other hydrogeologic properties are being measured on entire sample? There are inconsistencies.

=> John Relyea

There are papers on both side of the fence. Concerned with % > 2 mm of the moisture retention curves we generate, even though they are not corrected by our lab - they should be corrected. Sieve data is included as part of lab package. Moisture contents are done on all of sample in liners.

* Ben Volk - Use of Arya-Paris Model to Estimate Moisture Retention Data
(continued)

=> John Relyea

Samples need a radiological release before transportation can be done, thus they do sit in liners. The best would be to have the liners come in after lab sample is taken.

=> Peter Wierenga

Neutron probe measurement in borehole in the field would be useful.

=> Ward Staubitz

Problems are encountered with neutron probe due to borehole diameters which are large, have different casings, etc.. We do have problems with field moisture content and water retention curves.

=> Peter Wierenga

You also have problem with field measured tension. Have you tried filter paper?

=> Ward Staubitz

We did try filter paper for awhile.

=> John Relyea

We are trying to consolidate the entire lab group to one location.

=> Peter Wierenga

Is there a protocol to a lab sample?

=> Ward Staubitz

The procedure can be found in the EIIs and should be followed. The EIIs can be changed if need to be.

=> Rien van Genuchten

Experience with fractal scaling - it is a useful tool, but not sure how it is going to help. What about relating tension to % silt, % clay, etc.?

* Ben Volk

We have a large enough database, thus we might be able to utilize this.

=> Rick Healy

You said your results are sensitive to bulk density, did you account for larger fraction in regards to particle size distribution > 2mm?

* Ben Volk

Yes - should adjust moisture retention curve.

* Lynn Gelhar - Dispersivity Estimates

dispersivity

- a measure of contaminant spreading & dilution
- an unpredictable fudge factor
- depends on scale
- determined by small scale heterogeneity?

Stochastic Methodology

- ln K variability represented by 3D.....
- macrodispersivity

Cape Cod Experiments

- depth of aquifer = 100 ft
- mass sampling
 - 15 samples per borehole
- truly illustrates dispersion
 - not smooth as in a model
- dilution
 - concentration values aren't as high as before
- a negative correlation between retardation and conductivities
- it is not right to use the same dispersivity for reactive and nonreactive cases
- need different dispersivities for retarded and non-retarded cases
- a lot of spreading and dilution occur with higher longitudinal dispersivity values
- this is all saturated data

=> Scott Kindred

The problem with upper end at Hanford is due to large formation changes.

dispersivity also depends on size of plume

unsaturated dispersion

- macro anisotropy
- macro hysteresis
- macro dispersivity

people are just beginning to see the light - give them 5 years

saturation dependence on dispersivity is a question - there is no confirmation on relationship

viewgraph - scales of variability vs. overall scale

- increase in correlation scale as overall scale increases

=> Raz Khaleel

Do not have a lot of spatial data - there is a relation to correlate the spatial and temporal variances?

* Lynn Gelhar

Skeptical - more unsaturated hydraulic conductivity work is done here at Hanford than any other places I have seen.

* Lynn Gelhar - Dispersivity Estimates (continued)

=> Rien van Genuchten

Does it depend on a steady state system?

* Lynn Gelhar

Transverse dispersion.... have not gotten that far yet to answer.

=> John Relyea

Small dispersion vertically - could it really be a 2D problem?

* Lynn Gelhar

No - even though it is small it is important to have.

=> Scott Kindred

In saturated zone, we are trying to make predictions in regard to plumes 15 miles up gradient from Columbia River. We get bad results in regards to dispersivity.

* Lynn Gelhar

Select dispersivity in regards to 15 miles not 1 mile.
Naff result is more...

just superimpose it...

there are theories that deal w/dispersivity over a long range

=> Len Collard

Should we be looking at different dispersivities for each break or part of model?

* Lynn Gelhar

Look at overall model and choose a dispersivity over a range that increases linearly.

***** LUNCH BREAK *****

* Glendon Gee - Hanford Recharge

viewgraph - Hanford Site Water Balance

=> Rien van Genuchten

Why is it allowed to go on like this?

* Glendon Gee

DOE

for the past 4 years they have been looking at interim covers

=> Doug Sherwood

What are you talking about as far as area?

* Glendon Gee

West side of river.

* Glendon Gee - Hanford Recharge (continued)

viewgraph - Groundwater Recharge

-recharge $L \times 10^{10}/\text{yr}$

studies

natural recharge

cold creek, dry creek, etc.

0.5

USGS

1.25

PNL

3.5

recharge is significant on Hanford site

-liquid effluents are decreasing

Past Hanford Site Recharge Studies were done in 1970s and 1980s.

Can we model recharge into the future?

Conclusions

- 1) Lysimeters-only way to directly measure drainage
- 2) arid site predictions of drainage require lysimeters
- 3) waste site recharge
- 4)
- 5)

=> Len Collard

What do you feel are appropriate recharge rates to use? Do you have any documentation for defense?

* Glendon Gee

It changes all over site and climate.

=> Ward Staubitz

Look at current soil cover for modeling site.

* Glendon Gee

Model is deterministic - we shouldn't average a recharge rate. If you know precipitation rates then use that. Have to take a look at events and get a response from the system.

=> Peter Wierenga

Not only depends on moisture falling, but also how it falls, i.e. if soil is dry or wet, etc..

* Glendon Gee

It is a fairly confident model - it is as good as we got.

=> Rien van Genuchten

Does the soil freeze?

* Glendon Gee

Yes

Is there a preferential flow?

* Glendon Gee

Hard to answer that.

* Glendon Gee - Hanford Recharge (continued)

=> Peter Wierenga

May be should calibrate it over a period of both wet and dry events.
How is your vegetation by lysimeters?

* Glendon Gee

We had roots 10 ft. - 15 ft. when we dug trenches.

=> Scott Kindred

Talking of 2 things

- 1) natural vegetation
- 2) engineered design

Sagebrush roots in one lysimeter went 3 ft..

=> Scott Kindred

Maybe we want to look at 15 ft. of sandy loam.

=> Mel Piepho

If it drains over 100 years, it is not significant.
I agree if it only happened every 100 yrs, but I am not convinced. We had the same amount of precipitation this last winter as 5 winters ago. The difference is there was more snow this past winter.

=> Rien van Genuchten

Getting back to calibrating - Question, if you need to continue to recalibrate?
Use the model as a tool and continue.

Tracer studies are good for a natural site condition, but problems exist in terms of waste management.

=> Rien van Genuchten

Why not spray chloride on it and sample periodically?

* John Rawlins - Should summarize about workshop.

=> Raz Khaleel

Started with 3 objectives, only 1 of which was technical.
-provide audience update of some of the issues
-get feedback

Hopefully in executive session we can speak about future and speak later of funding aspects.

=> Ward Staubitz

-get an update of site characterization in vadose zone
(state of the art)
-get independent comment
-gain some confidence in that we are taking a reasonable approach and that there is not a quick and easy way to do the work
-met most of my expectations

=> Lynn Gelhar

- borehole injection experiment with transport simulations are great
- see more of the real database, have not seen enough of the guts
- unsaturated property characterization is important and progress is good. Need to see more screening type measurements.
- always interested in surrogate type measurements to tell you about detail

=> Raz Khaleel

Do you see an opportunity in using CERCLA type work in model validation/calibration?

=> Lynn Gelhar

Like to see more on the parameters before being convinced on validation. Problems are the base of data - calculations are relatively simple.

=> Ward Staubitz

Is model validation do-able? Is detail testing of a model necessary to increase confidence in that model? In next investigation - can you use less data?

=> Lynn Gelhar

It has to be done.

=> Doug Sherwood

- agree with Lynn Gelhar
- we can not do it for unit to unit
- we can not characterize each site and get a risk for the whole site
- need to learn to get better

=> Chuck Cline

It is critical that we know at a minimum what data is needed for a performance data.

=> John Smoot

Agree and feel that this is definitely critical.

=> Lynn Gelhar

Useful to speak about specific problems. Is tank leak a problem and what can we do to solve it?

=> Chuck Cline

Even to use a tank leak as a tracer - how much is enough data to make it sufficient?

=> Lynn Gelhar

Right now fudging a factor into T106 study - anisotropy.

=> Rick Healy

How is this model to be used to help us solve the system?

- => Peter Wierenga
A model is nothing more than a formalization of thoughts. Need model to make predictions or generalizations.
- => Glendon Gee
All of the waste is stored relatively close to surface and is not at the groundwater. It probably will not surface until our grandkids are dead. Personal feel that drilling wells is useless spending.
- => Ward Staubitz
Not an issue of well drilling vs. modeling.
Does modeling really tell us much?
- => Lynn Gelhar
If you can put it in to context the nature of the problems, how the sites are similar, etc., then see if you can put an answer to it.
- => Ward Staubitz
We do it by operable unit - should we model site wide? Right now it is hap hazard and there is no continuity?
- => Scott Kindred
We have actually only done vadose zone modeling on one site.
- => Peter Wierenga
Use steady state model, average recharge, and less emphasis on saturated hydraulic conductivity.
- => Peter Wierenga
If I had to choose between unsaturated hydraulic conductivity and recharge - it would be "recharge".
- => Doug Sherwood
The panel only heard about Kd, not solubility processes. Not all contaminants at 200BP1 were not Kd controlled. Did not here enough about chemistry?
- => Peter Wierenga
Should look at nitrate data.
- => Doug Sherwood
Good suggestion - we should look at it. We have 30 year old boreholes for the objective of studying contaminants.
- => Len Collard
Problem - arrival time of data vs. when to embark on modeling aspect.
Problem - try to use a recharge that was realistic.
Problem - taking gravel into account.

=> Rien van Genuchten

Good work is going on.
Extremely useful to sit down and have this workshop.
A lot of sitewide coordination is needed, i.e. database.
This database should be a centralized effort.
Look into other methods, i.e. Arya-Paris.
Coordination will pay off.
Recharge efforts should be supported.
Model calibration/validation - still somewhat confused, work needs to be done.
Do not only work with Kd

=> Len Collard

Do you feel in a risk assessment environment, what degree of calibration should be done and what is defensible?

=> Rien van Genuchten

Try to calibrate as best as I could. Whatever model is chosen, calibrate using Richards calculations and use Jim Conca's data. Round off what ever gives you a higher velocity and use that as risk assessment. Have to play with model and it takes time. Look into chemistry too. Look at programs that will couple with current codes. Need a team to do it.

=> Allen Lu

Calibration/validation - feel that Injection Test Site data is still the best data.

=> Lynn Gelhar

Have not seen enough of Injection Test Site to judge it or make comments on the results. How do you actually use field data?

=> Chuck Cline

What do you tell the borehole people?

=> Lynn Gelhar

Have not used correlation between α and $\ln K_s$ for Injection Test Site. It is difficult for me to comment because I have not seen the data.

=> Rien van Genuchten

Get as much information as you can without drilling new borehole. Then there is a modeling equation. Try to improve things as time goes on.

=> Doug Sherwood

Come to Len Collard's defense. Drilling was 7 months behind schedule.

=> Ward Staubitz

Len Collard was alone for funding of 200BP1. How does database address this problem?

=> Rien van Genuchten

Spend a million for these issues of database. Instead of drilling new borehole, put funds toward developing database - this is the key.

- => Ward Staubitz
Good recommendation.
- => Peter Wierenga
-should be more effort in coordinating
-look at nitrate data
-drill borehole downstream of tank
-do not make modeling so complex
-do not need all unsaturated hydraulic conductivity models
-go about it in a simplified approach
-continue with seminars : suggest vadose zone seminars
-speak to politicians
- => Rick Healy
Agree with stressing simplified modeling approach.
- => Peter Wierenga
In terms of model simulation/validation, I would be inclined to set up a new experiment. Bring group together and do a detailed design - hard to do mass balance on existing crib.
- => Scott Kindred
Do simple calculations and keep model simple. I feel that spending money on a detail field experiment is a good idea.
- => Rien Van Genuchten
Research is very important.
- => Scott Kindred
Do we have enough information to make these kind of decisions.
- => Ward Staubitz
There is no support for research right now.
- => John Rawlins
Concentrate on CERCLA issues.
- => Chuck Cline
Defend what we have to do to DOE to get funding.
- => John Rawlins
We have a couple months to get together to develop a proposal for funding.
- => Chuck Cline
Keep in mind that funding is for 2 years away.
- => Doug Sherwood
We have not looked into other sites - grout, etc..
DOE keeps those out of CERCLA realm for some reason.
- => Raz Khaleel
We need to get copies made from all the presentations and a report will be done.

=> Ward Staubitz

Where do we go from here? Are semi-monthly meetings agreeable?

=> Raz Khaleel

We need to talk about that. A lot of work is being done by several individuals in different groups. We need to see if we can get everyone involved and get upper management support.

=> Ward Staubitz

Bob Stewart is the new technical branch chief - DOE contact.

Meeting Closed

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LIST OF WORKSHOP ATTENDEES

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VADOSE ZONE MODELING WORKSHOP
Richland, WA

LIST OF ATTENDEES

Chuck Cline	Washington Dept. of ECOLOGY
Len Collard	WHC
James Conca	Washington State University, Tri-Cities
Jerry Davis	WHC
Truc De Lorenzo	WHC
David Duranceau	WHC
Eugene Freeman	WHC
Glendon Gee	PNL
Lynn Gelhar	MIT
Rien van Genuchten	USDA, ARS
Dori Harris	WHC
Rick Healy	USGS-Denver
Paula Heller	WHC
Raz Khaleel	WHC
Charley Kincaid	PNL
Scott Kindred	Golder Associates
Niall Kline	WHC
Al Law	WHC
Allen Lu	WHC
Fred Mann	WHC
William McMahon	WHC
Clarence Oster	BCSR
Mel Piepho	WHC
John Rawlins	WHC
John Relyea	WHC
Mark Rockhold	PNL
Frank Schmittroth	WHC
Doug Sherwood	EPA
John Smoot	PNL
Ward Staubit	USGS-Tacoma
Howard Sutherland	WHC
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1	<u>U.S. Geological Survey</u> District Office Building 53, Denver Federal Center MS 415, Box 25046 Lakewood, Colorado 80225 Dr. R. W. Healy
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