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MEMORANDUM FOR: Malcolm R. Knapp, Chief, WMGT
Division of Waste Management

FROM: Richard Codell, WMGT
Division of Waste Management

SUBJECT: TRIP REPORT - HYDROCOIN MEETING AND SYMPOSIUM ON STATE OF THE ART MODELING OF PERFORMANCE ASSESSMENT

I attended the second meeting of Hydrocoin, which is an international study to compare hydrologic groundwater models, on May 15-18, 1985 in Albuquerque, NM. The agenda for this meeting is attached.

The purpose of this meeting was to present results for the Level I problems dealing with calculations of heads, velocities and trajectories of tracer particles for several problems. Some had analytic solutions, but others did not, and only benchmarking could be performed. Most of the Level I problems have either been written up or I have copies of the slides from the presentations. My general impression was that most models compared favorably with the analytical results or with each other. Some models had difficulty with convergence on some of the unsaturated cases. One of the Level I problems, no. 3, appears to be ill posed, and no one could get a solution without altering the pre-stated conditions for the saturation relationships for K vs. P. The statement of the problem has been altered.

A. Larsson of the Swedish Nuclear Power Inspectorate (SKI) presented a proposed study to follow Hydrocoin known as "Interval." Interval would continue where Intercoin (the comparison of groundwater transport models) left off. It would be a project to evaluate the validity of nuclide transport models, relying mostly on real field data, perhaps natural analogs. There would be an emphasis on the communication between modelers and experimentalists. It would also be a forum for continued international cooperation of the Intercoin and Hydrocoin participants. The subject of Level 2 of Hydrocoin was also discussed. Level 2 is supposed to be a field validation to the extent that this is possible.

On May 16, Tom Nicholson, Tim McCartin, and I spent the day at Sandia Labs, working on the Hydrocoin problems for presentation the next day. There were no scheduled Hydrocoin meetings that day. Most of the other participants stayed at the Convention Center in the morning and watched a slide presentation on research projects at SNL. In the afternoon, they toured Albuquerque, but we did not go along.

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On Friday, May 17, Nancy Hayden and Ralph Peters of SNL (DOE side) presented a proposed Level 2 problem set, based on the Yucca Mountain Site. They presented results of their modeling efforts on the test site. The Hydrocoin Committee later adopted this problem set for the Level 2 Hydrocoin study. The question arose about whether or not it would be appropriate for NRC to participate in this modeling exercise because of our involvement in the licensing of the DOE sites.

Tim Broyd presented a code intercomparison effort for geochemical speciation models which he coordinated at Atkins Labs (UK). This was not part of Hydrocoin. There were 10 test problems run with the models for chemical speciation, some including redox reactions. He reported wide discrepancies between some of the models. In fairness to the codes the thermodynamic data bases differed between codes, and may account for some of the differences.

Dave Hodgkinson of Harwell Labs (UK) presented a proposal for a Level 2 case, which was based on experimental data collected around a granite mine in Cornwall. The granite was highly weathered and fractured. An electrical heater was placed in a drill hole to simulate a waste package. Parallel drill holes were instrumented for temperature. The heater was run more or less continuously for about 5 years. R Thunvik of the Royal Institute of Technology (Sweden) has already performed a code comparison using the Harwell data. This experiment was also adopted by the Hydrocoin Committee.

Tom Nicholson presented a proposal for Level 2 using field data on infiltration in the Panoche soils of central California. This is a well known case and has been used for other validation efforts in unsaturated flow.

Budi Sagar of Rockwell Hanford and Charles Cole of PNL presented a Level 2 proposal on a lab experiment for heat transfer in a cylinder filled with glass beads and heated from below. They are presently validating a 3-d transport model with these data. Several of the participants, including me, criticized this case because it was for a heat transfer regime well outside of that which would be likely for repositories (i.e., high Rayleigh numbers). Also, it would be impossible to use the experimental results for testing 2-d models because the convection cells observed would be strictly a 3-d phenomenon.

Sandia (NRC-side) presented a proposal based on field data in a hard rock quarry in Japan. The Canadian contingent (AECL) presented a proposal for modeling of a gneiss block at the Chalk River site, bounded on one side by a large lake. No decision have been made on adopting any but the Cornish quarry case and the Nevada site case for Level 2.

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Level 3 of Hydrocoin was discussed. This phase of the study will deal with sensitivity and uncertainty in the use of hydrologic models for groundwater investigations. It may also include the effects of coupled processes in modeling. Sensitivity of the models to the knowledge of the data, such as fracture connectivity, disturbances from the construction of the repository, climatic changes, choice of boundary conditions and thermal effects on the flow field are possible topics of study. A low-level or intermediate level radioactive waste site was proposed by Dave Hodgkinson (Harwell, UK). Detailed discussion of Level 3 will be on the agenda at the next Hydrocoin meeting, to be held in Paris this fall.

These are only the highlights of the Hydrocoin meeting. I have a number of reports, handouts, and slides if you are interested.

I attended the "Symposium on Flow and Transport Modeling for Performance Assessment of Deep Geologic Disposal of Radioactive Waste," also held in Albuquerque May 20-21, 1985. This was an international meeting on all aspects of performance assessment for HLW repositories. The agenda is attached. Some of the more interesting presentations are described below.

E. Buetow from the FRG described modeling of a potential waste repository in a Salt dome in Lower Saxony. The initiating scenario was flooding, which could cause a breach of the salt, and migration to the Elbe River. The modeling considered only advective transport without the effects of heat. It was a deterministic study, only because data necessary for a statistical approach were lacking. He calculated a 4000 year travel time to the Elbe. The standards in West Germany appear to relate only to a concentration level rather than an integrated release such as 40 CFR 191.

P. Raimbault described performance assessment practices for HLW repositories in France. The most promising sites for repositories are in granite. Their efforts include the effects of heat and geochemistry, and also sensitivity analyses using LHS with scenario development. This effort seemed more in line with those of the U.S. program.

Tito Bonano presented a rundown of the NRC - sponsored programs at Sandia Labs.

Joe Leiberman described the Performance Assessment National Review Group, which is an independent panel of experts reviewing the progress of DOE and NRC efforts for HLW site investigations.

Brian Goodwin (Canada, AECL) described the SYVAC model, which stands for System Variation and Control. This is an interesting approach to modeling the

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uncertainty of HLW sites. It is basically a Monte Carlo sampling driver for a number of submodels (vault, geosphere, biosphere). The codes use random rather than LHS sampling. The SYVAC program seems to be in wide use in Europe as well as Canada. The code considers up to 540 sampled parameters, and appears to be more comprehensive than efforts such as the NWFT/DWM modeling done by SNL and NRC.

Ralph Peters from Sandia Labs (DOE side) presented an excellent review of performance assessment work in the Yucca Mountain site. The emphasis of his paper was on the calculation of infiltration and groundwater travel time. It does not appear to present anything beyond the studies which NRC has reviewed in the EA.

Joe Devary from PNL presented work on uncertainty analyses of the hydrology in the Palo Duro basin. He described their use of geostatistics (Kriging) for flow model development and sampling plan development, and also their use of the adjoint method for sensitivity. Conditional simulations with a 2-d finite element model were used with good success to calculate groundwater travel time distributions. The travel time distribution was log-normal although he did not present the actual travel times. The data base for the conditional simulations consisted of 85 potentiometric heads and about 2000 permeabilities. The Monte Carlo conditional simulations were compared with a direct, first order simulation for mean travel time and variance with reasonably good results. I do not believe that these results were presented in the EA for salt.

Heather Atwood presented a FE model of the Palo Duro basin which attempted to rationalize observations of groundwater ages. She presented model results which predicted ages of millions of years. One commenter suggested that the uplift in these basins was not that old, so her steady-state model could not be accurate.

I presented an impromptu talk on the interpretation of groundwater travel time (GWTT) as specified in 10 CFR 60. Slides of my presentation are attached. Basically, I described the rationale for the rule on GWTT as an independent measure of the goodness of the repository site. I described the many reasons why GWTT is likely to be a distribution rather then a single value, and how and why we should define GWTT as a fraction of the cumulative distribution for travel times. A lively discussion followed. The audience seemed to favor my approach to GWTT, but many did not like the overall concept of GWTT in the first place. Ivars Neretnieks of the Royal Institute of Technology (Sweden) presented a brief followup talk, demonstrating that for sorbable radionuclides, GWTT was irrelevant to the performance assessment of a repository, although Chen Fu Tsang (LBL) disputed his results. I commented to the speakers that if two such notable experts disagreed, then one could imagine how the layman must

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view the problem, and it was for this reason that a simple criterion such as GWTT was reassuring.

D. Smith from the University of New Mexico, (Dept. of Chemical Engineering) under contract with Sandia thru NRC (A1266) presented a very good dimensional scoping study of the importance of vapor phase and aerosol transport of radionuclides in unsaturated media. He looked at the conditions under which aerosols would be formed, and concluded that it was not likely for the conditions at Yucca Mountain. He also concluded that the flux of vapor would not be significant compared to the liquid pathways.

Tom Pigford (LBL) advocated a transport phenomena approach to releases from waste canisters. He claims that many well-known principles of mass transfer are being ignored by DOE in the definition of release rates from the waste package, and that not enough emphasis is given to the waste package in the particular geologic settings. He sited the Swedish program as having a superior engineered barrier that is reliable. I later discussed with him the bases for his comments on transport phenomena. He referred me to recent presentations in the Material Research Society (MRS) symposia which describe his approach.

D. Metcalfe (Intera) presented the use of adjoint sensitivity in the evaluation of a HLW site in the Paradox basin in Southern Utah. He applied the SWENT code (similar to SWIFT) using an adjoint post processor, GRESS from ORNL to automatically set up an adjointed program. The emphasis of their study was to evaluate the sensitivity of their performance model to regional model parameters and boundary conditions to determine the direction of further field studies.

Chen Fu Tsang (LBL) presented an interesting paper on a validation exercise for coupled flow and heat transfer models. The studies involved history matching of field data, another case where no model adjustments were allowed, and optimization studies on the design of a repository (not actually a validation). The object of the optimization exercise was to show that simple models may be wrongly used beyond their limits of applicability, and that more complicated, physically based models need to be used for some cases.

Ivars Neretnieks described the Swedish HLW project in granite. He directly measured flow through fractures in the Stripa granite mine by collecting the water in plastic sheets placed on the walls and ceilings. Only a small fraction of the visible fractures carried any water. He stated that the equivalent porous medium approach is unsuitable for modeling this case. Matrix diffusion in an important phenomenon in this case.

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Malcolm Segal, from Sandia, described his NRC-funded work in using retardation factors for HLW repository performance assessment. His work recognizes that retardation factors are not an ideal approach, but may be the only practical method for performance assessment because of the high cost of geochemical models. He presented some criteria for the reliability of laboratory data for estimating retardation coefficients.

The meeting ended with a group discussion led by S. Neuman from the University of Arizona.

The Hydrocoin meeting and the conference on Performance Assessment were both worthwhile. I think I got more from the latter. It was a good forum for my discussion of the travel time issue. I have many preprints and copies of slides from the presentation. I would be glad to discuss any of this further at your convenience. The issue of whether or not NRC should be involved in the Yucca Mountain simulation for Level 2 of Hydrocoin should be decided as soon as possible.

Original Signed By

Richard Codell, WMGT
Division of Waste Management

Enclosures:
1. Agenda for Hydrocoin
2. Agenda for Performance Assessment Symposium
3. Copy of Slides for travel time talk

Enclosures available in DCC.

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DATE	85/06/11	85/06/11					

SECOND HYDROCOIN WORKSHOP

MAY 15-18, 1985

Regent Hotel, Albuquerque, New Mexico

May 15	ISLETA/JEMEZ ROOMS
8:00 a.m.	REGISTRATION
9:00 a.m.	C. Cole and A. Larsson Opening of meeting
9:15	K. Andersson Status report
9:30	B. Grundfelt Introduction to level 1 cases
10:00	Ph. Raimbault (C.E.A.), Ph. Jacquier, M. J. Mejon Results of HYDROCOIN level 1, cases 2, 6, and 7
10:30	Coffee break
	CHAIRMAN E. BUETOW
10:50	P. Goblet (Ecole des Mines), Ph. Raimbault, M. J. Mejon Results on cases 1, 2, and 4 obtained with the METIS code
11:20	N. Hayden (NNWSI) Level 1 results from NNWSI
11:50	P. Clifton (BWIP) Level 1 results from BWIP
12:10	Lunch
	CHAIRMAN T. BROYD
1:45 p.m.	David D. Noy (BCS) Level 1 results from level 1, 2, 3, and 6
2:15	R. Thunvik (SKB/KTH) SKB/KTH results on cases 1, 2, 3, and 4
2:45	E. Buetow (GSF), L. Heredia (GSF) and E. Holzbecher (TUB) Level 1 calculations with the SWIFT code

3:15	Coffee break
	CHAIRMAN P. GLASBERGEN
3:40	C. Cole (PNL) Level 1 results from PNL
4:10	B. Gureghian (OCRD) Level 1 results from OCRD
4:40 - 5:10	T. Broyd (Atkins) New results on level 1 cases 6 and 7

May 16	NAMBE/NAVAJO ROOMS
9:00 a.m.	Surrogate WIPP Tour
12:00	Lunch
1:30 p.m.	HISTORICAL TOUR BY BUS PICK UP IN FRONT OF REGENT HOTEL
5:30	Return to Hotel
7:00	Hosted Dinner/Social hour ACOMA ROOM

May 17	TESUQUE ROOM
	Continued Presentation of Level 1 cases
	CHAIRMAN
9:00 a.m.	A. W. Herbert (AERE) Further results on level 1 cases 2, 3, 5, and 7
9:30	T. McCartin (U.S. NRC) USNRC results on level 1 cases 1, 2, and 7
10:00	Coffee break
	CHAIRMAN
10:20	P. Davis and D. Updegraff (Sandia) Level 1, cases 6 and 4 results for the SWIFT II, USGS3D and TOUGH Computer Codes
10:50	H. Kimura, A. Nakagoshi, H. Nakamura (JAERI) JAERI results on level 1 cases with the code 3D SEEP
11:20	S. K. Gupta (ONWI) Level 1 results from ONWI (one or two contributions)

12:10	Lunch
	CHAIRMAN
1:45 p.m.	K. Meling and S. Vuori (VTT) Preliminary results of HYDROCOIN - level 1 cases and a description of a modified procedure to calculate streamlines
2:15	T. Leijsne, F. Sauter, P. Glasbergen, N. Praayman (RIVM) Preliminary results of cases 1, 2, and 5 calculated with the METROPOL-code
2:45	Further level 1 results
3:15	Coffee break
	CHAIRMAN
	Preliminary Level 2 Results
3:40	D.P. Hodgkinson and A.W. Herbert (AERE) Preliminary results for the heat transfer validation exercise
4:10	R. Thunvik (SKB/KTH) SKB/KTH preliminary results on the heat transfer case
5:00	Break
	INTRAVAL
	CHAIRMAN
6:30	K. Andersson (SKI) and B. Grundfelt (KEMAKTA) Information on plans for a new project concerning validation of nuclide transport models (INTRAVAL)
	PROPOSALS FOR HYDROCOIN LEVEL 2
7:00	U.S. NRC proposals
8:00	U.S. DOE proposals (C. Cole)
8:30 - 9:00	Short discussion

May 18	APACHE ROOM
	CONCLUSIONS FROM LEVEL 1
	CHAIRMAN
9:30 a.m.	Summary of level 1 results (B. Grundfelt and D. Hodgkinson)
10:00	Introduction to contents of level 1 report (B. Grundfelt)
10:30	Coffee break
	CHAIRMAN
10:50	General discussion on level 1
12:00	Lunch
	LEVEL 2 PROPOSALS AND DISCUSSION
	CHAIRMAN
1:30 p.m.	SKB proposal (C. Thegerstroem)
2:00	AECL proposal
3:00	Introduction to level 2 discussion (B. Grundfelt)
3:15	Coffee break
3:30	General discussion on level 2
	IDEAS FOR LEVEL 3 WORK
	CHAIRMAN
4:30	HYDROCOIN Secretariat
4:45	U.S. DOE proposals (C. Cole)
5:15	U.S. NRC proposals (T. Nicholosn)
5:30	Break
	CHAIRMAN
5:45	Sensitivity and uncertainty analysis for shallow land burial (D.P. Hodgkinson)
6:15 - 7:00	Discussion on level 3.

REVISED AGENDA - MAY 20, 1985

Symposium on Groundwater Flow and Transport Modeling For Performance Assessment of Deep Geologic Disposal of Radioactive Waste A Critical Evaluation of the State of the Art

LOCATION: REGENT HOTEL, ALBUQUERQUE, NEW MEXICO

DATE: MAY 20-21, 1985

SPONSORS: Jointly by U. S. Department of Energy and the U. S. Nuclear Regulatory Commission

PURPOSE

The purpose of this symposium is to provide for an exchange of ideas on current and developing performance assessment approaches in the field of groundwater flow and transport modeling, associated with geologic disposal of radioactive waste. The location, timing, and participation is designed to take advantage of the collective presence of the scientists attending the second HYDROCOIN Workshop and Coordinating Group Meeting being held just before and after this symposium at the same location.

Joint Technical Program Chairmen

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TWX: 710-824-0412 NRC BHD WSH

Fee -- U.S. $10

ORGANIZATION

The two day symposium will be organized into three sessions, one session for each of the three subject areas each day with an overall discussion period at the end of each day. At the close of each day S. P. Neuman will lead a discussion of the material presented and its implications for future research.

Minutes of these discussions will be taken. The proceedings of the symposium including the minutes of the discussions will be published jointly edited by the DOE and NRC or their designees.

MAY 20, 1985

DAY 1

1.	8:00 - 8:15	OPENING REMARKS
		SESSION I -- PERFORMANCE ASSESSMENT I

CHAIRMAN: MR. ALF LARSSON - SWEDISH NUCLEAR POWER INSPECTORATE

2.	8:15 - 8:45	E. BUETOW, L. HEREDIA, S. LUTKEMEIER-HOSSEINPOUR, S. S. STRUCK (TUB)--APPROACHES TO MODEL GROUNDWATER FLOW AND RADIONUCLIDE TRNASPORT AT A GERMAN SALT DOME
3.	8:45 - 9:15	M. RAIMBAULT, J. LEWI (CEA/IPSN) METHODOLOGIE FOR LONG-TERM PERFORMANCE ASSESSMENT OF NUCLEAR WASTE REPOSITORIES IN GEOLOGICAL FORMATION DEVELOPED AT THE CEA/IPSN
4.	9:15 - 9:45	E. BONANO (SNL)--DEVELOPMENT OF PERFORMANCE ASSESSMENT METHODOLOGY FOR NUCLEAR WASTE ISOLATION IN GEOLOGIC MEDIA
	9:45 - 10:00	COFFEE BREAK
5.	10:00 - 10:30	J. LIEBERMAN (OTHA, INC.) W.-L. LEE (R. F. WESTON, INC.) PREDICTIVE RELIABILITY FOR PERFORMANCE ASSESSMENT: A PEER REVIEW
6.	10:30 - 11:00	T. NARASHIMHAN, M. ALAVI (LBL)--CHAMP--A COMPUTER CODE FOR MODELING TRANSIENT FLUID FLOW AND CHEMICAL TRANSPORT WITH HYDRODYNAMIC DISPERSION IN VARIABLY SATURATED SYSTEMS
7.	11:00 - 11:30	B. GOODWIN (AECL)--SYVAC APPROACH FOR LONG-TERM ENVIRONMENTAL ASSESSMENT
8.	11:30 - 12:00	T. RASMUSSEN (U OF ARIZONA)--SITE CHARACTERIZATION USING MULTI-APPROACHES
		LUNCH

MAY 21, 1985

DAY 2

----------MORNING----------

SESSION III -- TRANSPORT

CHAIRMAN: MR. KJELL ANDERSSON - SWEDISH NUCLEAR POWER INSPECTORATE

17.	8:00 - 8:30	A. MULLER (NEA/OECD), P. TASKER (HARWELL)--THE USE OF THE PHREEQUE CODE IN MODELING ENVIRONMENTAL GEOCHEMICAL PROBLEMS ENCOUNTERED IN PERFORMANCE ASSESSMENT MODELING
18.	8:30 - 9:00	D. SMITH (UNM), C. UPDEGRAFF (SAIC), E. BONANO (SNL)--A PRELIMINARY ASSESSMENT OF RADIONUCLIDE VAPOR PHASE TRANSPORT IN UNSATURATED TUFF

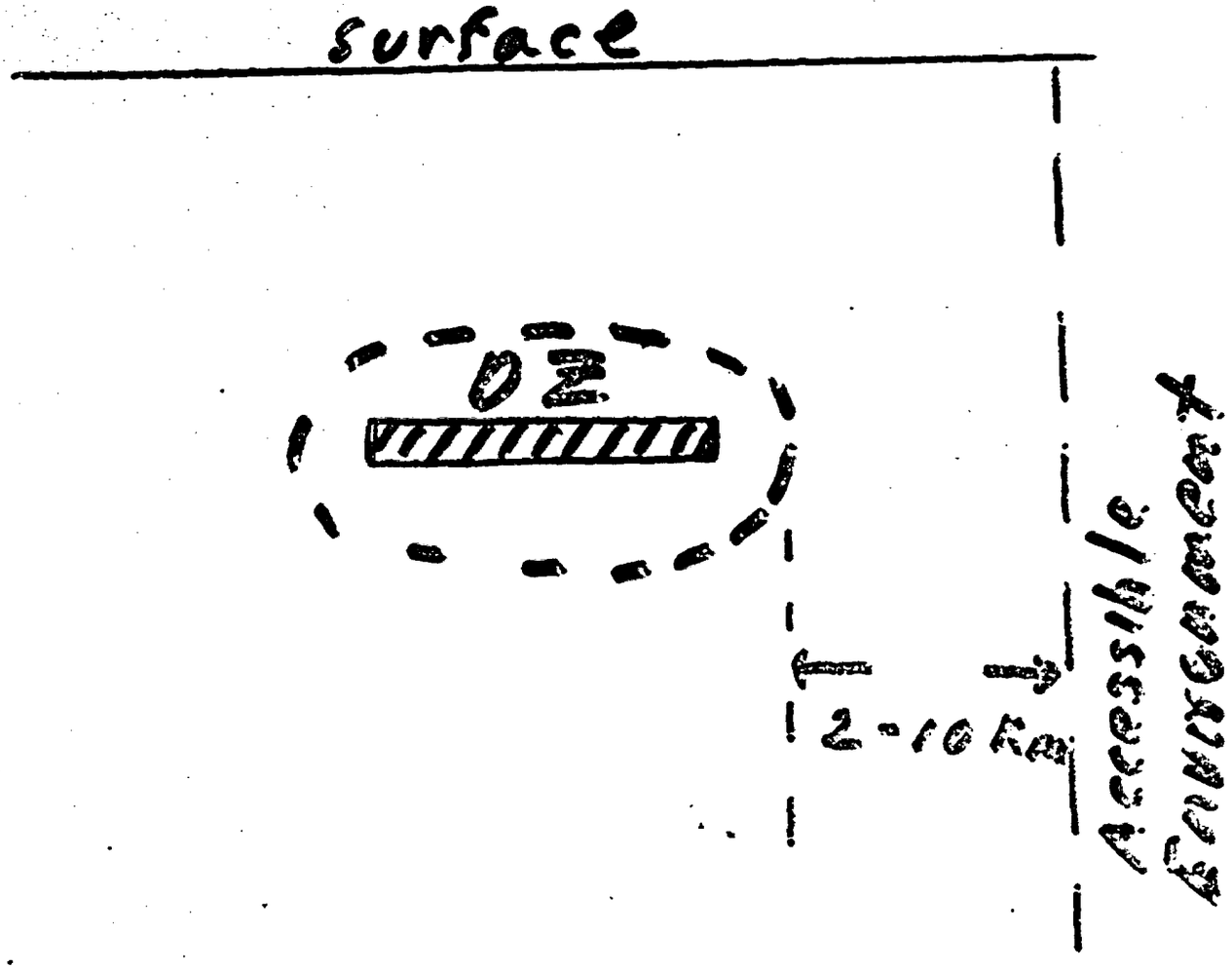
SESSION IV -- PERFORMANCE ASSESSMENT II

CHAIRMAN: MR. BERTIL GRUNDFELT - KEMAKTA CONSULTANTS CO.

19.	9:00 - 9:30	T. PIGFORD (LBL)--PREDICTIVE RELIABILITY FOR PERFORMANCE ASSESSMENT
20.	9:30 - 10:))	D. METCALFE (INTERRA), W. HARPER, S. GUPTA (ONWI)--APPLICATION OF ADJOINT TECHNIQUE TO PERFORM ASSESSMENT OF HYDROGEOLOGIC CONCERNS
	10:00 - 10:15	COFFEE BREAK
21.	10:15 - 10:45	R. NELSON, E. JACOBSON, W. CONBERE (PNL)--UNCERTAINTY ASSESSMENT FOR FLUID FLOW AND CONTAMINANT TRANSPORT MODELING IN HETEROGENEOUS GROUNDWATER SYSTEMS
22.	10:45 - 11:15	A. HERBERT, D. HODGKINSON, C. JACKSON, D. LEVER, J. RAE, P. ROBINSON, S. SHARLAND, P. TASKER (AERE)--SOME CURRENT PROBLEMS IN GROUNDWATER FLOW AND RADIONUCLIDE TRANSPORT MODELING
23.	11:15 - 11:45	C. TSANG (LBL)--LESSONS LEARNED IN THE VERIFICATION AND VALIDATION STUDIES OF A COUPLED HEAT AND FLUID FLOW CODE
		LUNCH

Groundwater Travel Time

"The geologic repository shall be located so that the pre-waste emplacement groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1000 years or such other time as may be approved by the commission."


surface
DZ
2-10 km
Accessible
groundwater

Rationale for 1000 Yr GWTT

1. Independent Measure of Geologic Barrier

2. Period of Decay of most hazardous fission products

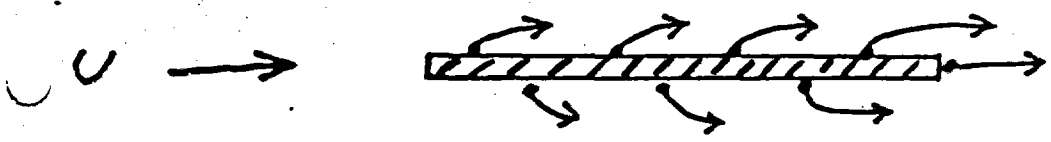
3. Easily Understood

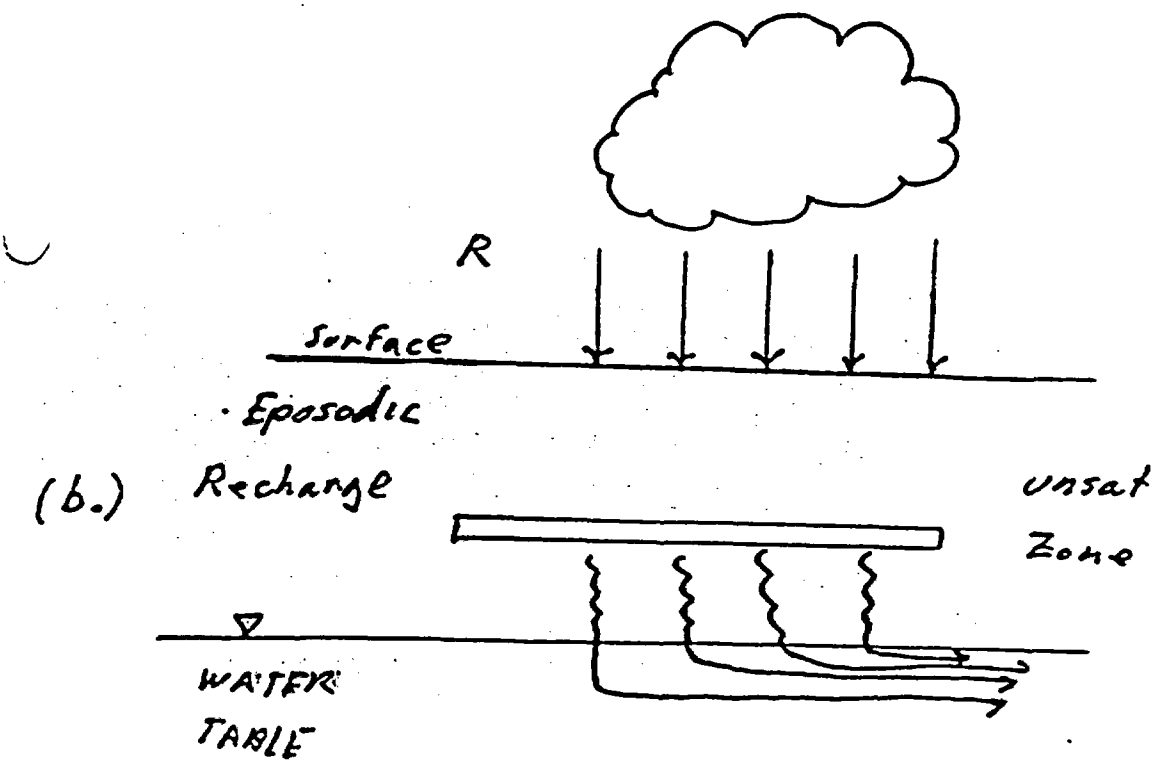
4. Part of rule which has undergone public rulemaking

CAUSES for TRAVEL TIME DISTRIBUTION

a. Distributed Source

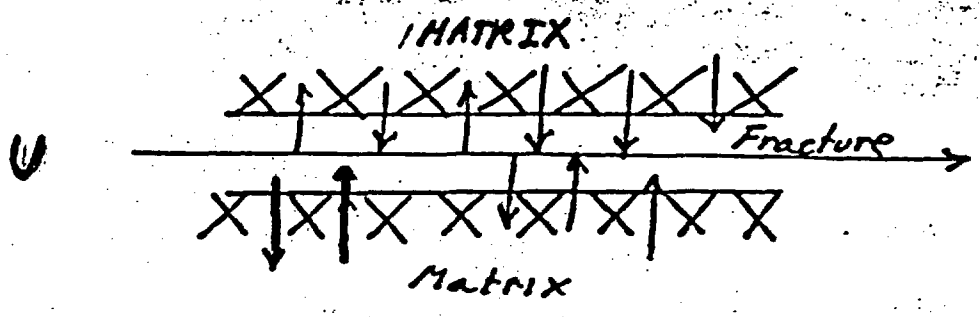
Accessible Environment



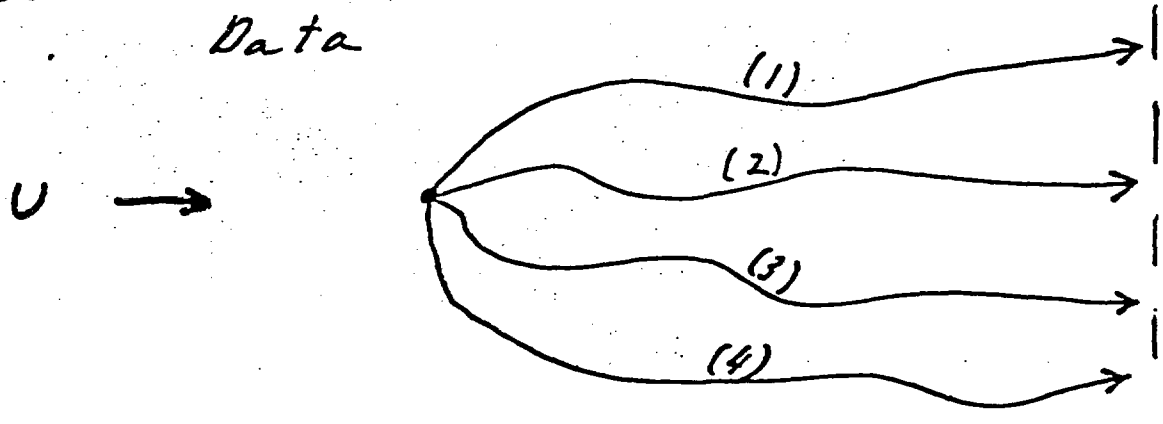


Accessible Environment

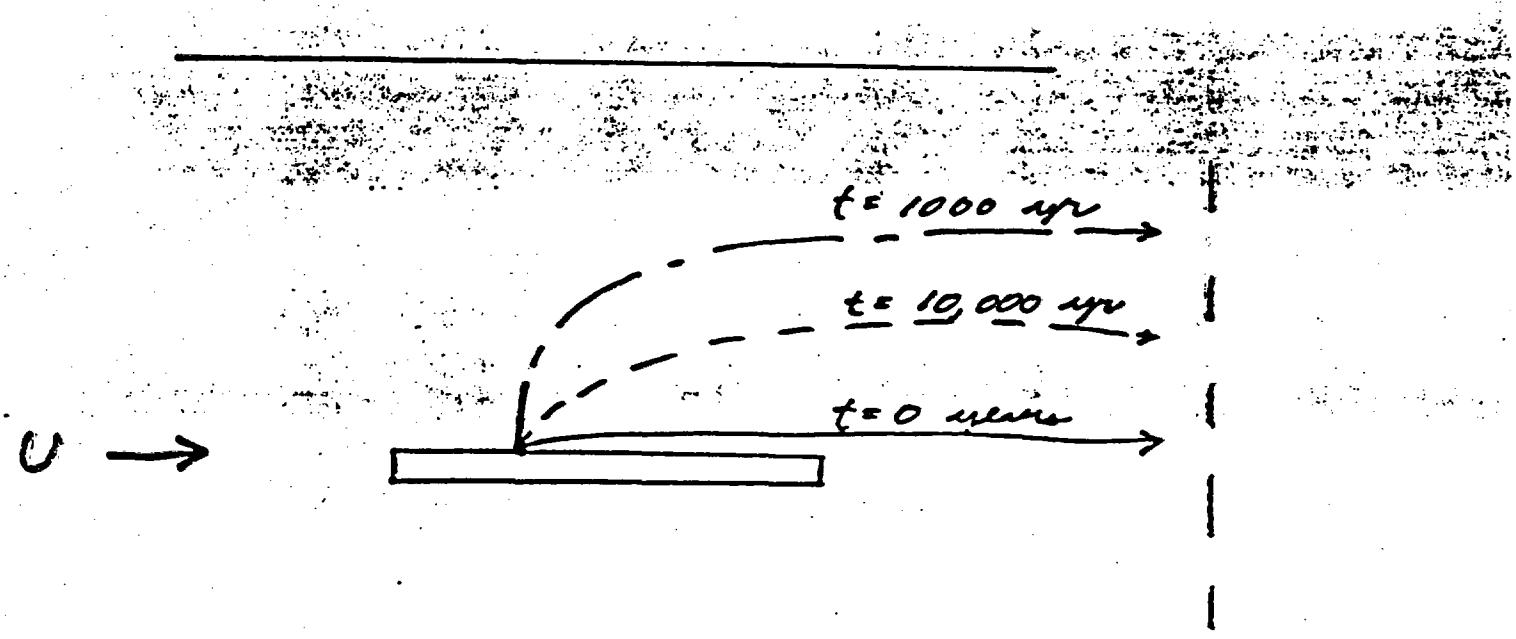
c. MATRIX DIFFUSION



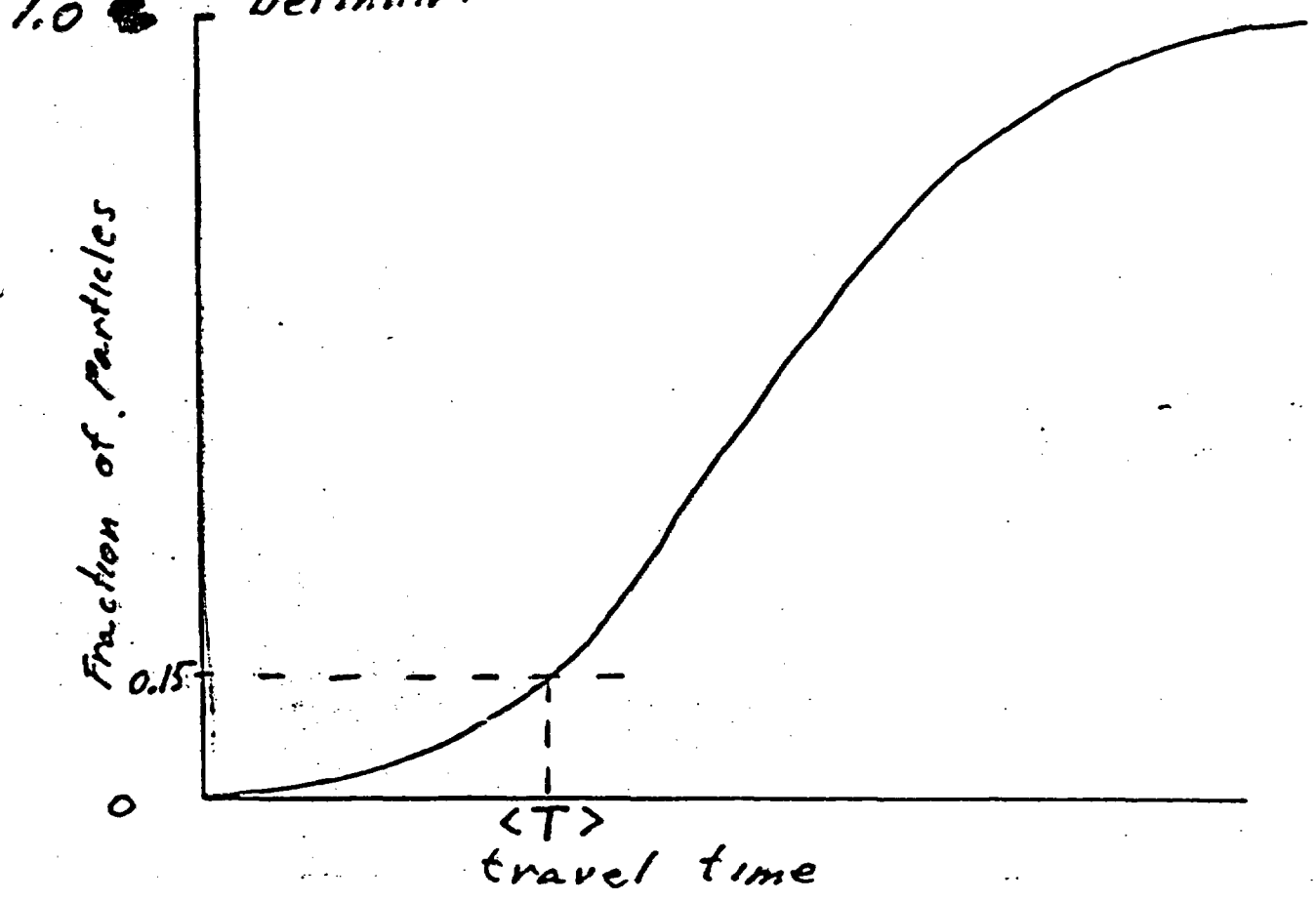
d. Multiple Realizations of Data



e. Thermal Effects on Flow (Buoyancy)
(also drying)

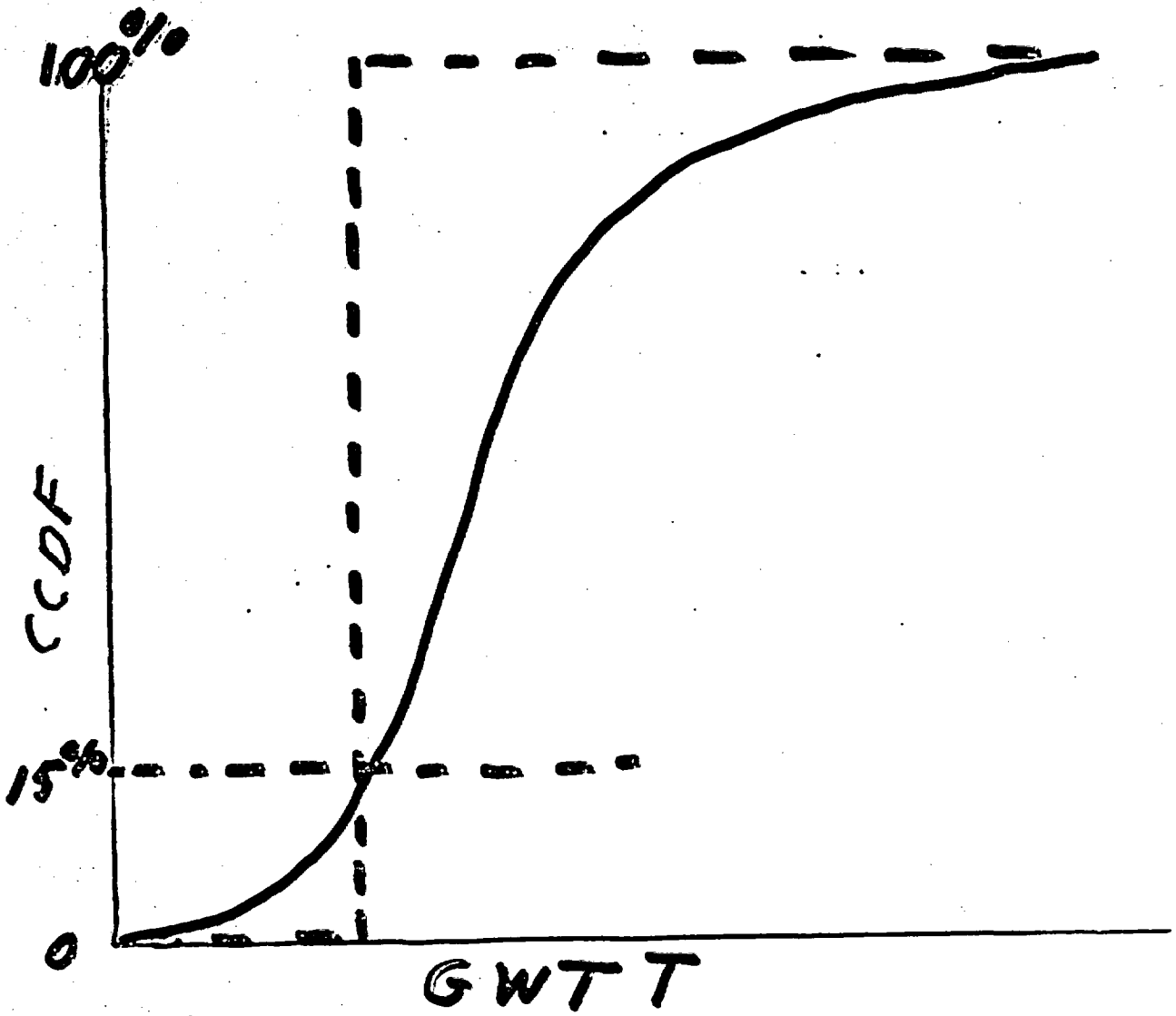


Definition of Groundwater Travel time



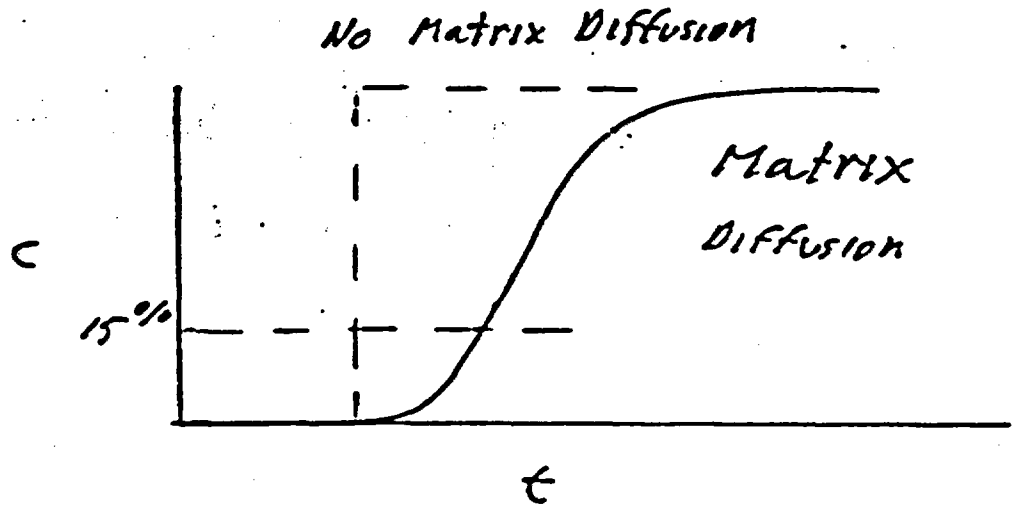
GROUND-WATER TRAVEL TIME IS DEFINED AS:

" THE X-PERCENTILE OF THE COMPLIMENTARY CUMULATIVE DISTRIBUTION FUNCTION (CCDF) OF ALL TRAVEL TIMES FROM THE LOCUS OF THE DISTURBED ZONE TO THE ACCESSIBLE ENVIRONMENT AVERAGED OVER 10,000 YEARS AFTER THE CLOSURE OF THE REPOSITORY. EACH TRAVEL TIME INCORPORATED INTO THE CCDF SHALL BE APPROPRIATELY WEIGHTED BY ITS VOLUMETRIC FLOW RATE AND ITS QUANTIFIABLE UNCERTAINTY DEFINED BY THE AVAILABILITY OF DATA. UNQUANTIFIABLE UNCERTAINTY SHALL BE INCORPORATED AS CONSERVATISM USED IN THE DEFINITION OF THE FLOW PATHS CONSIDERED IN THE CCDF."

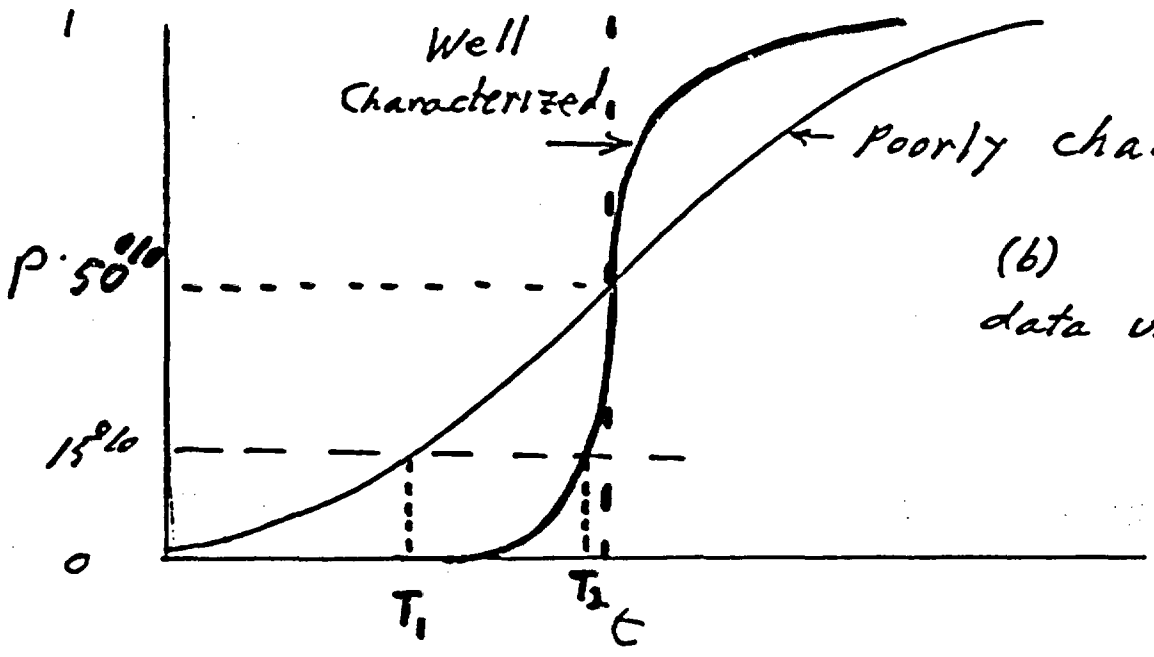

100%
CCDF
15%
0
GWTT

Rationale

for 15% of CCDF



(a)
Matrix diffusion



(b)
data uncertainty

Conclusions

1. Independent Measure of Goodness of site

2. Distributed nature of quantity

3. Incentive for good siting practices and characterization

4. Position only a framework.