CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

SUBJECT: NRC Meeting and Seminar by Prof. Shlomo P. Neuman on "Validation of Repository Assessment Models and the Role of Research"

DATE AND PLACE: November 9, 1990
U.S.NRC White Flint offices
Washington D.C.

AUTHOR: Rachid Ababou

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TRIP REPORT

SUBJECT: NRC Meeting and Seminar by Prof. Shlomo P. Neuman on "Validation of Repository Assessment Models and the Role of Research"

AUTHOR: Rachid Ababou

DATE AND PLACE: November 9, 1990
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Washington D.C.

PERSON PRESENT: CNWRA

Rachid Ababou

BACKGROUND, PURPOSE, AND SUMMARY OF MEETING:

This one-day meeting was held at the White Flint Building offices of NRC, November 9, 1990. The NRC contact was Thomas J. Nicholson (Office of Research). Prof. Shlomo P. Neuman (Department of Hydrology, University of Arizona, Tucson) was invited to expose his views on the "Validation of Repository Assessment Models and the Role of Research", previously submitted to NRC in the form of a draft essay dated July 5, 1990. This draft essay was prepared in the wake of the GEOVAL-90 conference. The meeting was lively and well attended, by NRC management and NMSS/RES staff. Gerry Stirewalt and I represented the Center. In particular, Budhi Sagar had delegated me to speak for the Center's performance assessment group.

The following is a summary of the exchange of ideas that went on at the meeting, assembled from scattered notes. For convenience, I have distinguished three broad topics: (1) Groundwater travel time rule; (2) Model validation and performance assessment; and (3) Prof. Neuman's research. In addition, I am attaching the following documents: (1) a copy of Prof. Neuman's viewgraphs and of his draft essay; (2) a copy of an article distributed to me at the meeting ("The Yucca Mountain project: Another perspective", by Isaac J. Winograd, Environ. Sci. Technol., Vol. 24, No. 9, 1990).

SUMMARY OF PERTINENT POINTS:

1. Groundwater travel time rule

Prof. Neuman raised the issue of the importance of concentrated release (lethal to humans), as opposed to the total mass at some arbitrary compliance surface.

NRC management expressed the need for (new) guidance regarding the groundwater travel time (GWTT) rule, without changing the rule itself. I noted that the Center is working on this, and that some of the options considered by the Center would require additional definitions but not a change of the rule per se. I also expressed my (personal) view on the proper interpretation of GWTT: a first step would be to recognize that GWTT is necessarily a scale-dependent quantity, with respect to the scale of averaging involved in calculating (measuring or modeling) groundwater velocities; a second step would then be for researchers to provide guidance concerning the magnitude of the scale of averaging and how it should be taken into account to prove compliance. (Example of problems that will be involved in selecting the proper scale of averaging: the scale of the domain within compliance boundaries is much larger than fracture apertures).

Prof. Neuman emphasized the fact that research on dispersion is research on GWTT distribution, since the two are directly related (see below; see also attached copy of Prof. Neuman viewgraphs).

NRC management asked whether the GWTT travel time was too constraining in terms of the data collection effort that would normally be required to prove compliance. This question was apparently prompted by the conclusions of the National Academy of Science in their recent report on the DOE/NRC handling of the Yucca Mountain project. Another question was whether there was any "technical" problem in the fact that NRC and DOE were using the same test site (at Appache Leap I think). Prof. Neuman's answer to the latter question was essentially that there should not be a problem (on the contrary) as long as the NRC and DOE researches proceed independently.

2. Model Validation and Performance Assessment

Discussions on Model Validation (MODVAL) and Performance Assessment (PA) took a philosophical turn towards the end of the day. Several individuals participated extensively to the discussion. Each point of view was different, but some of the differences boiled down to emphasizing different aspects of the same problem. What follows is a brief, possibly biased account of some of the perceived differences of opinion regarding MODVAL.

For instance, Norm emphasized the difference, in his view fundamental, between model and theory. He concluded that less effort and/or precision is required for model validation (performance assessment), than for theory validation (research).

Shlomo emphasized the fact that model validation can never be completely achieved since validation procedures cannot take into account unsuspected/unknown processes. Therefore, the best that can be done is to further basic research in order to uncover the most we can about unknown phenomena. The public should be made aware of such (basic science) uncertainties, of the amount of effort spent in resolving them, and of what has been achieved in that regard.

Dick affirmed his belief that a lot can be accomplished in a simple way through simplified models and binding, conservative calculations. This was challenged on the grounds that we will never know whether our calculations are binding or not if the simplified model is too far off, however conservative we try to make it in terms of input data.

I focused on the logical incompatibility that exists between "validation" and "refutation". Assume for instance that A is a model (e.g. transport model) and B is a particular manifestation of it (e.g. the actual occurrence of breakthrough at a compliance boundary at time T). Then, given that A — B and B is true, can we affirm that A is true (validation)? Not according to standard logical inference. Rather, all we can say is: given that A — B, if B is found to be false, then A must be false (refutation). Tom indicated that most INTRAVAL tests to date have been presented in such a way as to avoid the appearance (if not the possibility) of model refutation. The psychological reasons of this seem obvious.

I also suggested a parallel argument with respect to hypothesis testing: traditionally, e.g. in the area of radar detection, the focus has been on Type I error (probability of a miss) rather than Type II error (probability of a false alarm). In model validation for geologic repository, however, if the null hypothesis is defined as "The model is valid", then the Type II error ("false alarm" — "adopt invalid model") seems more critical than the Type I error ("miss" — "reject valid model"). Someone who disagreed suggested that to reject a valid model may be as tragic as to adopt a wrong one if only one model is available.

I cannot do justice to the many other thoughts that were expressed on PA and MODVAL during the meeting. I'll just add that some practical aspects, e.g. probabilistic model validation procedures such as hypothesis testing and the like, were discussed in some detail, mostly in reference to INTRAVAL work.

3. **Prof. Neuman's Research**

Prof. Neuman spent most of the morning explaining some of his recent and current research work in hydrogeology (see attached copy of his viewgraphs). One of his purposes was apparently to make the case for his (and other) research using statistical continuum approaches for studying the flow and transport behavior of fractured rock formations. Another purpose of his talk was, clearly, to point out that research on contaminant dispersion is directly relevant to GWTT distributions and, hence, to NRC regulations.

Prof. Neuman started by presenting his previous work on the in-situ characterization and interpretation of saturated flow tests in the fractured granitic formation at the Oracle site near Tucson, Arizona. This work was funded by NRC. He then moved on to more recent or ongoing NRC-funded research. Briefly, here are a few points that I noted:

- Key question is: are fractured media essentially different from porous media? Illustration with slide show (fracture outcrops, etc).

- Fracture aperture data from Stripa site in Sweden (Geneviève Gentières): both wall and aperture plotted.

- No obvious correlation between (i) fracture density distribution at borehole, and (ii) packer test conductivity distribution at same borehole. Data from both the Oracle site (Arizona) and the Stripa site (Sweden) lead to this conclusion.

- Prof. Neretnieks mapped outflow along a drift at Stripa site, as part of INTRAVAL work. Concluded that fracture flow occurs as channel flow rather than sheet flow. Poor correlation between flow rate and fracture outcrop lengths along the drift. Better correlation between flow rate and number of fracture intersections, which carry most of the flow rate apparently.

- Development of proof that GWTT PDF is directly related to mean-square displacement, or equivalently to the diffusion-dispersion coefficient D. [Note: this seems perfectly obvious intuitively; in fact, this is true for non-probalistic as well as probabilistic interpretations of travel time "distribution" and "dispersion"; simple examples can easily be constructed, e.g. with just two tracer particles].

- Using a simple example with just one tracer particle, Prof. Neuman shows that the coefficient of variation (CV) of total cumulated mass released at compliance boundary is maximal at early times (i.e. before breakthrough of center of mass of the plume). [Note: I observed that the CV gives a relative, dimensionless measure of uncertainty; using Prof. Neuman's simple example, it can be seen that the maximum uncertainty in terms of the standard deviation (units of mass) is in fact attained much later, at the time of breakthrough of the center of mass of the plume].

- In transport modeling, calibration with additional measurements leads to decreased variances and dispersivities. The effect is to transfer information from the dispersive to advective terms. [Note: this type of transfer of information has been recognized and formalized in several ways; there is a broad consensus on this, although the most practical methods to integrate this into classical models are still being researched].

CONCLUSIONS:

This was an informative meeting on performance assessment and research for geosphere flow and transport, with a good balance between the managerial and technical/scientific points of views. Much of the debates that took place at this meeting were directly relevant to the Center activities in both the Performance Assessment and Geologic Setting areas.

PROBLEMS ENCOUNTERED:

None

PENDING ACTIONS:

None

RECOMMENDATIONS:

Attendance at such meetings plays an important role in publicizing NRC and CNWRA research efforts as well as obtaining up to date information on recent progress in key areas of research. It is recommended that such communication channels be kept open in the future, notably through research presentations by CNWRA staff at scientific conferences and workshops.

SIGNATURE: Rachid Ababou Dec. 11, 1990
Date

REFERENCES:

None

CONCURRENCE SIGNATURE AND DATE:

for JOHN L. RUSSELL DEC. 3, 1990
Date

LIST OF ATTACHED DOCUMENTS:

(1) Copy of Prof. Neuman's viewgraphs and of his draft essay on "Validation of Repository Assessment Models and the Role of Research".

(2) Copy of an article distributed to me at the meeting: "The Yucca Mountain project: Another perspective", by Isaac J. Winograd, Environ. Sci. Technol., Vol. 24, No. 9, 1990.

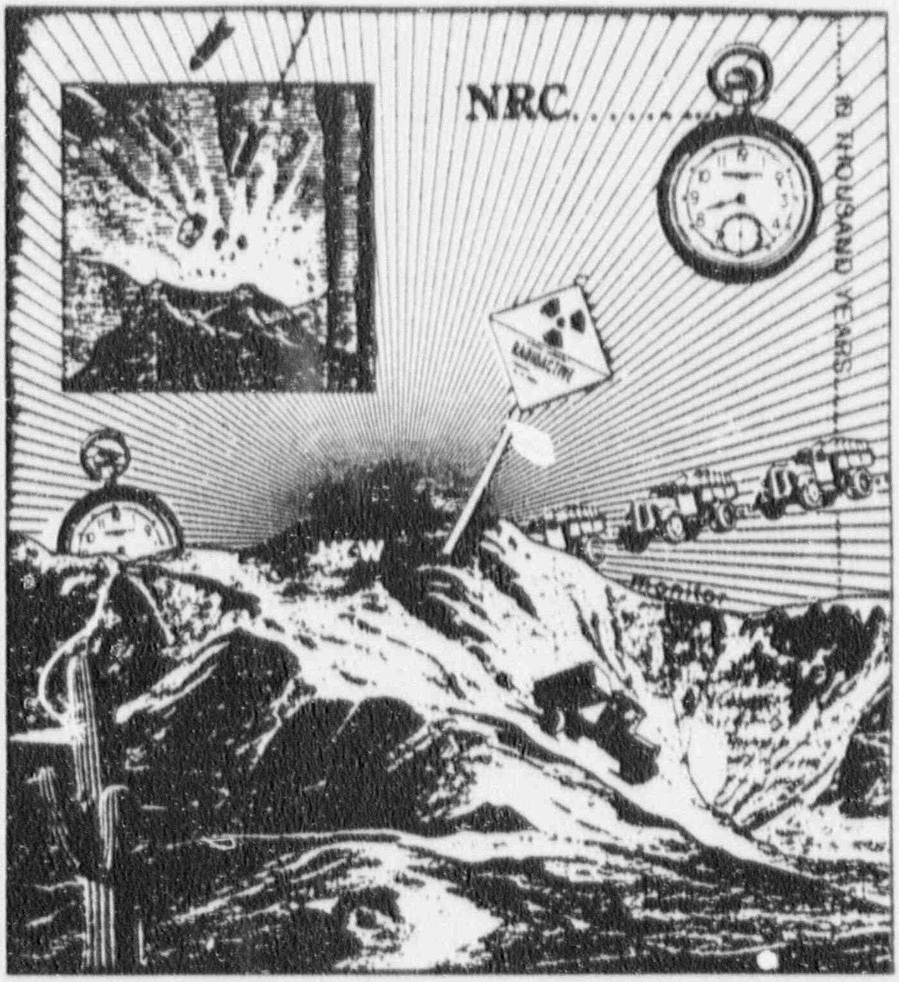
LIST OF ACRONYMS AND ABBREVIATIONS:

- Center: Center for Nuclear Waste Regulatory Analyses
- DOE: Department of Energy
- GWTT: Groundwater Travel Time
- INTRAVAL: International INTRAVAL Project (Validation of Geosphere Transport Models for Performance Assessment of Nuclear Waste Disposal)

R. Abdou

Info : P.A. + Mod. Va

The Yucca Mountain project: Another perspective



By Isaac J. Winograd

The recent commentary in your pages by Charles R. Malone *(1)* on the Yucca Mountain project deserves a response because the issues he raises go beyond Yucca Mountain to a host of present and future environmental conflicts. [Yucca Mountain in Nevada is the site chosen by the U.S. Department of Energy for exploration as a potential repository for high-level nuclear waste.] Malone is appropriately concerned about whether we can have "reasonable assurances that future geologic and hydrologic changes at the site will not result in transport of radionuclides to the accessible environment during the first 10,000 years following closure of the repository" (p. 1452). He views the "lack of validated models for predicting geologic and hydrologic processes over 10,000 years" as a major liability of the Yucca Mountain site. His bottom line is that "the limits of environmental science have been exceeded by the goals set for the nation's radioactive waste disposal program," and therefore he argues that "the debate over national policy for dealing with high-level nuclear wastes be reopened and that alternatives to the present course of action receive further consideration."

Malone's analysis of the Yucca Mountain endeavor is pertinent and thoughtful, but it is incomplete in several important respects. First, he categorically assumes that if a geologic environment is too complex to model exactly it is inherently unsuitable for waste emplacement. Second, he fails to mention that the alternatives to geologic disposal (at Yucca Mountain or elsewhere) are also fraught with major uncertainties. And third, he fails to inform readers that, unlike other geologic disposal sites considered thus far, disposal at Yucca Mountain is fully retrievable and could be reliably monitored. I will consider these matters in turn.

The assumption that precise 10,000-year "predictive" modeling is an essential requirement for determination of the "performance" of Yucca Mountain, or any other site, is an outgrowth of EPA and U.S. Nuclear Regulatory Commission (NRC) regulations *(2-4)*, which set discrete upper or lower limits for radionuclide release rates, groundwater travel times, and waste container lifetimes. As Malone correctly implies, and as I have pointed out elsewhere *(5)*, such models—though essential for guiding research, testing of worst-case scenarios, and eliminating marginal waste disposal sites—cannot readily be validated or, perhaps, even calibrated. I do not repeat the reasons I gave for this because Malone and I are in agreement on this matter. What Malone does not say is that EPA and the NRC recognize the need for nonquantifiable technical judgments in evaluating repository performance, though it is a matter of debate how such judgments can be used in the licensing process *(2-5)*. In any event, the folly of relying too heavily on mathematical modeling in geotechnical endeavors became apparent more than a decade ago, after the failure of the Teton Dam in 1976. As carefully noted by Ralph B. Peck *(6)*, it was an overreliance on numerical analysis—at the expense of judgment-based field work—that directly led to the failure of this dam. I am concerned that an overemphasis on models at Yucca Mountain may well result in the opposite situation: namely, the premature rejection of what may prove to be an otherwise acceptable, though not perfect, site for high-level radioactive waste (HLW). Selection or rejection of a dam or toxic waste disposal site must rest on technical judgment, not solely on the availability of "validated models."

What do I mean by technical judgment? Such judgment begins with the recognition that the problem of HLW disposal (or for that matter, perpetual surface storage of such wastes) is, as aptly phrased by Weinberg *(7)*, a transscientific problem—that is, a problem that involves events so rare that both their probabilities and consequences are beyond the ability of science and engineering to quantify with precision. Technical judgment also recognizes that mathematical models can be no better than the conceptual model guiding field observations; hence, it encourages the formulation of competing conceptual models. Technical judgment would favor selection of a disposal or storage site that provides multiple barriers to radionuclide transport—even if these barriers are only qualitatively established—over a site with a single, though quantitatively established, barrier to nuclide migration. In other words, a "defense in depth" approach would be heavily favored over placing all one's eggs in one basket, whatever its purported certitude. Briefly, technical judgment is multifaceted and does not rely on a single methodology, that is, modeling, but rather results from a blending of qualitative and quantitative approaches with weights experience deems appropriate.

Can technical judgment lead to erroneous decisions? Certainly. For this reason such judgment also requires an integration of multidecade monitoring into project design, as pursuasively argued by D'Appolonia *(8)*. Such validation and verification procedures allow for frank recognition that uncertainties remain. Fail-safe, or redundant containment, and retrievability, are similar logical extensions of the admission of uncertainties.

Malone correctly focused on the well-known limits of the environmental sciences but, unfortunately, failed to mention that the alternatives to geologic disposal or storage of HLW also are fraught with major uncertainties that also are not amenable to prediction by means of "validated models." The leading alternatives to geologic disposal of HLW on land that have been studied in the last two decades include: disposal in ice sheets; burial in deep-sea oozes; shooting of the wastes into space; and dry above-ground storage in concrete casks. The State of Nevada Agency for Nuclear Projects/Nuclear Waste Project Office recommends dry cask storage at reactor sites for up to 100 years, during which time, they argue, a superior disposal scheme might become available *(9)*. Alternatively, the wastes could be shipped to one of two national Monitored Retrievable Storage (MRS) facilities for indefinite holding. But even these two seemingly simple surface-based expedients are not free of risks. For example, are the probabilities and consequences of operator errors, of vandalism, of sabotage, or of an aircraft crashing into spent fuel storage areas adjacent to cities acceptable? Why was geologic disposal of HLW initially proposed over three decades ago? It was, of course, an attempt to preclude (or at least minimize) accidental, or mischievous, contact of humans and animals with HLW now and in the future.

Finally, Malone fails to inform his readers that, unlike other proposed geologic disposal sites—for example, in the deep sea, in basalt hundreds of feet below the water table, or in bedded salt—wastes disposed of at Yucca Mountain are readily retrievable, should unforeseen events make removal of the waste necessary or desirable. Indeed, as has been mentioned repeatedly in the literature *(10–13)*, one of the principal advantages of solid waste disposal in thick unsaturated zones in arid or semiarid terrain is ease of retrieval. HLW emplacement in the thick unsaturated zone at Yucca Mountain is, in reality, protracted storage in deep tunnels, rather than irretrievable disposal; it has, in fact, been viewed by Luther J. Carter *(14)* as a shallow subsurface MRS facility. (Study of the need for such a facility on the surface is required by the Nuclear Waste Policy Amendments Act of 1987.) Moreover, because the waste emplacement is in the fully accessible unsaturated zone, current estimates of groundwater recharge, repository temperatures, natural air convection, and so forth, can be checked repeatedly by *direct* monitoring for as many decades and perhaps centuries as is deemed necessary. Indeed, the unsaturated zone readily lends itself to the highly conservative geotechnical philosophy of "monitored decisions" proposed by D'Appolonia *(8)* for engineering decisions under uncertainty.

Technical judgment notwithstanding, let us be frank. There is unlikely to be a perfect site or disposal method for HLW or, for that matter, for each and every industrial toxic waste. We will have to select the best from an imperfect set of solutions. As of June 1990, Yucca Mountain appears to be a site deserving of further characterization; specifically, underground examination of the site is needed to test the initial findings arrived at by surface-based geologic mapping and test drilling.

I wish next to briefly state one of my own major concerns regarding the Yucca Mountain project. It is my strong impression—though admittedly that of an interested observer rather than participant—that past overemphasis on planning documents, quality assurance requirements, data management systems, and other administrative requirements has hindered an efficient geotechnical characterization of Yucca Mountain. When and if work there is resumed—following resolution of current litigation—I suggest a 4- to 6- year moratorium on, or at the least a significant reduction in, such paperwork to permit scientists and engineers to efficiently obtain data from underground workings, so as to reach an informed and mature judgment about this site. If the site still appears technically suitable after such intensive study, then pertinent quality assurance (see below) can be performed on key matters requiring replication. During the proposed 4- to 6-year moratorium on "paperwork" it would also be extremely helpful if the National Academy of Sciences would address, by one or more interdisciplinary committees, the following important questions, all of which go beyond Yucca Mountain to the endless environmental contestations now facing us and certain to multiply in the next several decades:

- What shall constitute "proof" in complex environmental issues—some perhaps transscientific—involving the earth, chemical, and biological sciences, and how shall it be arrived at?
- What constitutes adequate quality assurance in environmental endeavors involving these sciences?
- How can the public best be informed that neither science nor engineering can provide certitude in certain environmental matters such as HLW disposal?

The excellent paper by A.M. Weinberg *(7)* sets the stage for discussion of these critical questions and deserves careful study and discussion by all scientists, engineers, regulators, lawyers, politicians, and lay people involved in environmental disputations.

In summary, technical judgment—including awareness of vast archaeological and paleoecological records of delicate objects preserved for millenia in thick unsaturated zones in arid and semiarid terrain *(5, 15, 16)*—suggests that Yucca Mountain, though not problem free, is a site worthy at least of further study by means of underground workings. Let us not yet return to square one as Malone suggested. And, beyond Yucca Mountain, if our nation is going to insist on purported mathematically precise modeling of key factors entering into major environmental decisions, are we not dooming ourselves to environmental inaction in perpetuity? On the other hand, if we intend to act in some environmental matters, then it seems we have no choice but to apply technical judgment constrained by the integration of multidecadal monitoring into project design *(8)*.

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(3) "Disposal of High-Level Radioactive Wastes in Geologic Repositories"; U.S. Nuclear Regulatory Commission; U.S. Government Printing Office: Washington, DC, July 31, 1986; 10 CFR, Part 60.

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__Isaac J. Winograd__ is a research hydrologist with the U.S. Geological Survey in Reston, VA. His publications on the potential utility of thick unsaturated zones of arid regions for the isolation of solidified toxic wastes played an important role in the U.S. Department of Energy's decision to explore Yucca Mountain as a possible high-level radioactive waste repository.

Radhid Ababar.

PRESENTATION TO NRC

by S.P. Neuman

November 9, 1990

CONTENTS

1. Some questions regarding
    a. Relationship between NRC regulations and EPA standards
    b. Implications of NRC regulations with respect to site characterization and safety assessment
2. Some lessons about the characterization of fractured rock properties relevant to groundwater flow and transport in both saturated and unsaturated media (experimental, mainly 35 mm slides)
3. Relation between travel time and dispersion in random groundwater velocity fields (theory)
4. Implications of scale effect (theory validation)
5. Validation of safety assessment models and the role of research
    a. Introduction
    b. The role of positive evidence in validation
    c. Near-field versus far-field model validation and the concept of robustness
    d. Performance assessment of engineered versus natural repository system components
    e. Role of geosphere flow and transport research in validation
6. Open discussion

EPA Standards According to
WORKING DRAFT 2 OF 40 CFR Part 191, 1-31-90

191.13 Containment Requirements: (a) Disposal systems for spent nuclear fuel or high-level or transuranic radioactive wastes shall be designed to provide a *reasonable expectation*, based upon *performance assessments*, that the *cumulative releases* of radionuclides to the accessible environment *for 10,000 years* after disposal from *all significant processes and events* that may affect the disposal system shall: (1) have a likelohood of less than one chance in 10 of exceeding the quantities *calculated according to Table 1* (Appendix B) [Release Limit per 1,000 MTHM or other unit of waste] ; and (2) have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities *calculated according to Table 1* (Appendix B).

"Performance assessment" means an *analysis* that: (1) *identifies the processes and events* that might affect the disposal system; (2) *examines the effects of these processes and events on the performance* of the disposal system; and (3) *estimates the cumulative releases of radionuclides considering the associated uncertainties*, caused by all significant processes and events. These estimates shall be incorporated into **AN OVERALL PROBABILITY DISTRIBUTION OF CUMULATIVE RELEASE** to the extent practicable.

EPA is also considering options for **INDIVIDUAL AND GROUND-WATER PROTECTION REQUIREMENTS** such as

191.5 ... to provide a reasonable expectation that *for X [1,000 or 10,000] years* after disposal, undisturbed performance of the disposal system shall not cause the *annual commited effective dose equivalent* due to all potential pathways from the disposal system *to any member of the public* in the accessible environment *to exceed Y [25 or 10] millirems*. These pathways shall include the *assumption that individuals consume 2 liters per day* of drinking water *from any high-yield aquifer outside of the controlled area.*

191.16 (a) ... to provide a reasonable expectation that, *for X years* after disposal, undisturbed performance of the disposal system shall *not cause: (1) any increase in the levels of radioactivity in any portion of a special source of ground water etc.*

"Committed effective dose equivalent" means the total dose equivalent received over a lifetime by an individual following an intake of radionuclides into the body, multiplied by appropriate weighting factors ...

10 CFR Ch.1, 1-1-90 Edition

60.113(a)(2) ... The geologic repository shall be located so that prewaste-emplacement *groundwater travel time* along the *fastest path* of likely radionuclide travel from the disturbed zone to the accessible environment shall be *at least 1,000 years* or such other travel time as may be approved or specified by the Commission.

60.122(b)*Favorable conditions*(7) Pre-waste-emplacement *groundwater travel time* along the *fastest path* of likely radionuclide travel from the disturbed zone to the accessible environment that *substantially exceeds 1,000 years.*

How does this travel time relate to measurable site characteristics and to EPA Standards?

60.102(e)(2) ... The engineered barrier system works to control the release of radioactive material to the geologic setting and *the geologic setting works to control the release ... to the accessible environment. Isolation* means inhibiting the transport of radioactive material so that *amounts and concentrations* of the materials *entering the accessible environment will be kept within prescribed limits.*

How precisely do these amounts and concentrations relate to travel time, measurable characteristics of the geology, and EPA standards?

60.21(c) The Safety Analysis Report shall include: ... (1)(ii)(C) An evaluation of ... performance ... *giving the rates and quantities of releases* of radionuclides to the accessible environment *as a function of time*;

In what relation to EPA standards? This evidently requires reliance on models of time-dependent transport. The latter must further be validated:

60.21(c)(1)(ii) The assessment shall contain: (F) An explanation of measures used to *support the models used to perform the assessments* required in paragraphs (A) through (D). *Analyses and models* that *will be used to predict future conditions and changes* in the geologic setting *shall be supported by using an appropriate combination of such methods as field tests, in situ tests, laboratory tests which are representative of field conditions, and natural analog studies*. 60.101(a)(2) ... For ... long-term objectives and criteria, what is required is reasonable assurance making allowance for ... uncertainties involved, that the outcome will be in conformance with those objectives and criteria. *Demonstration of compliance* with such objectives and criteria *will involve* the use of *data from accelerated tests and predictive models* that are *supported by* such measures as *field and laboratory tests, monitoring data and natural analog studies*.

What must be measured in the field and/or laboratory, how and on what scale(s) in space-time, to allow the QUANTITATIVE ESTIMATION of travel time along the fastest path, amounts and concentrations entering the accessible environment, and rates and quantities of releases to the accessible environment as a function of time, as well as the associated estimation uncertainty, once release rates from the engineered repository have been specified?

In what precise way is such quantitative estimation aided by "detailed information" *of the kind required in* 60.21(c)(1)(i), *particularly* (A) The orientation, distribution, aperture, in-filling and origin of fractures, discontinuities, and heterogeneities; (B) The presence and characteristics of other potential pathways such as solution features, breccia pipes, or other potentially permeable features? *How, in what quantity, and on what scale(s) need such information be collected?*

What "hydrogeologic properties and conditions" [60.21(c)(1)(i)(D)] *must be determined, how, in what quantity, and on what space-time scale(s) to make such quantitative estimation possible?*

To what extent, if any, can models and analyses which attempt to make such quantitative estimates be validated? What is the meaning and importance of this term? What validation strategy, if any, should the NRC adopt?

APERTURE CONFIGURATION
OF A NATURAL FRACTURE IN WELDED TUFF

by

Brian Charles Vickers

A Thesis Submitted to the Faculty of the
DEPARTMENT OF HYDROLOGY AND WATER RESOURCES
In Partial Fulfillment of the Requirements
For the Degree of
MASTER OF SCIENCE
In the Graduate College
THE UNIVERSITY OF ARIZONA

1990

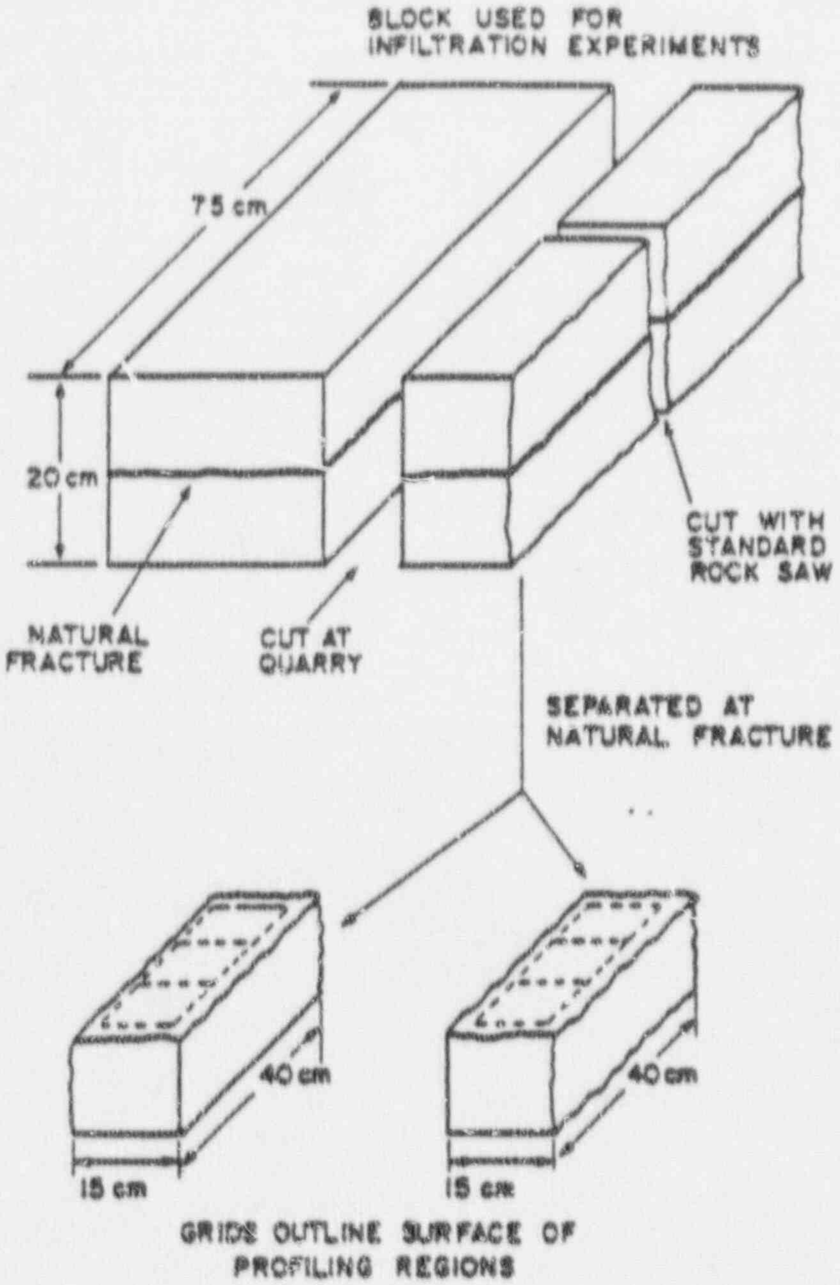


Figure 3.2 Exposure of Fracture Surfaces

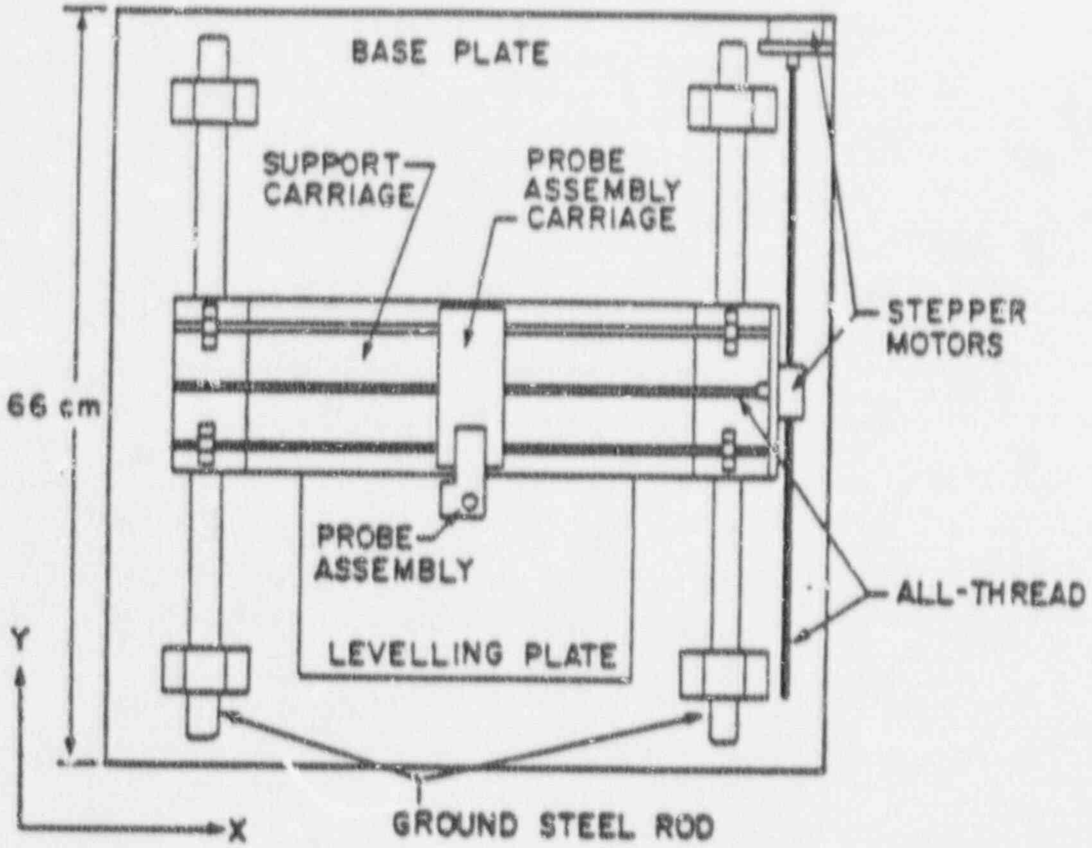


Figure 3.1 Schematic of Profilometer
(Modified from Farrington 1983)

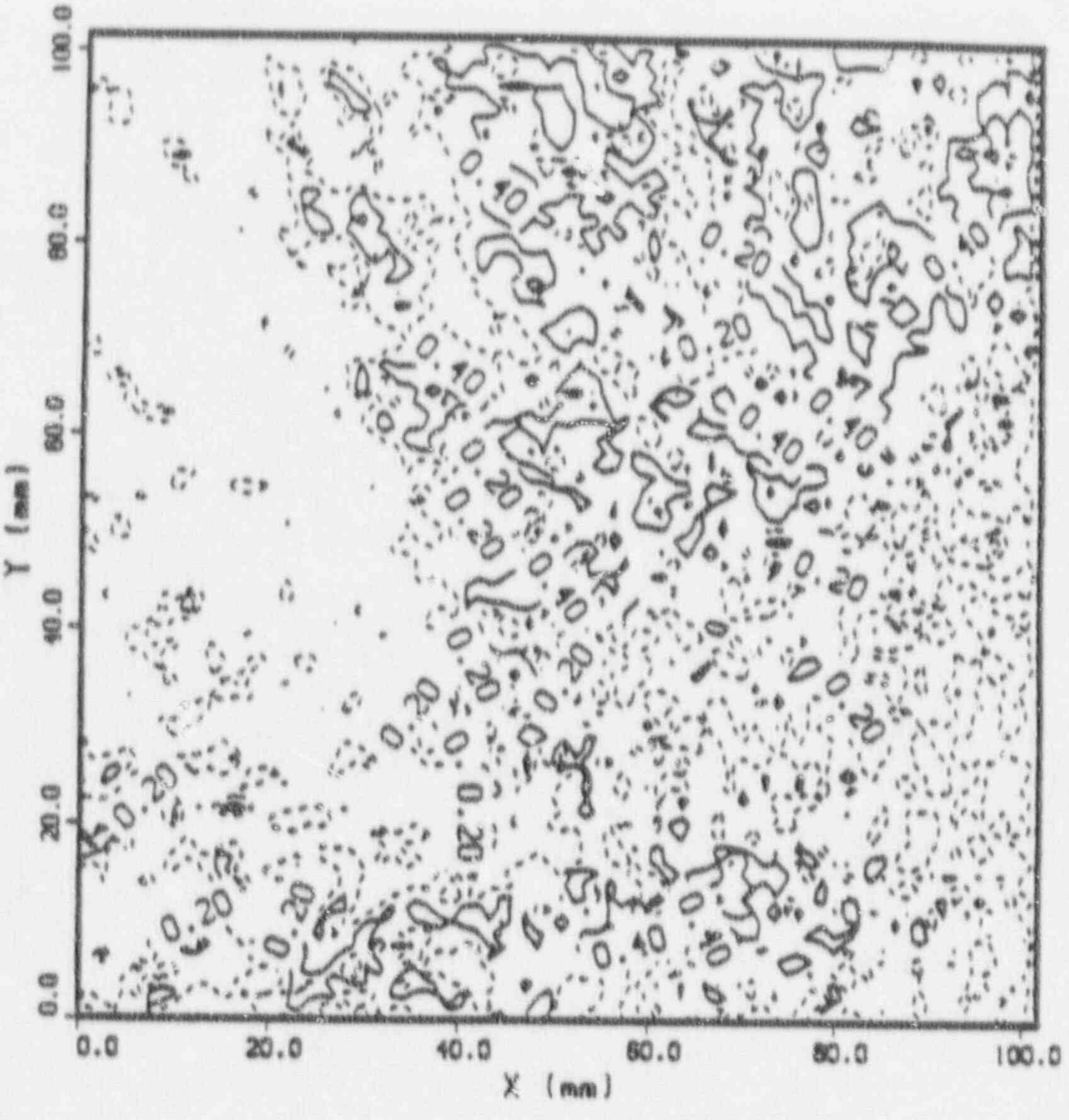


Figure 4.10 Contour of Apertures (Section 1)
(Contour interval = 0.2 mm)

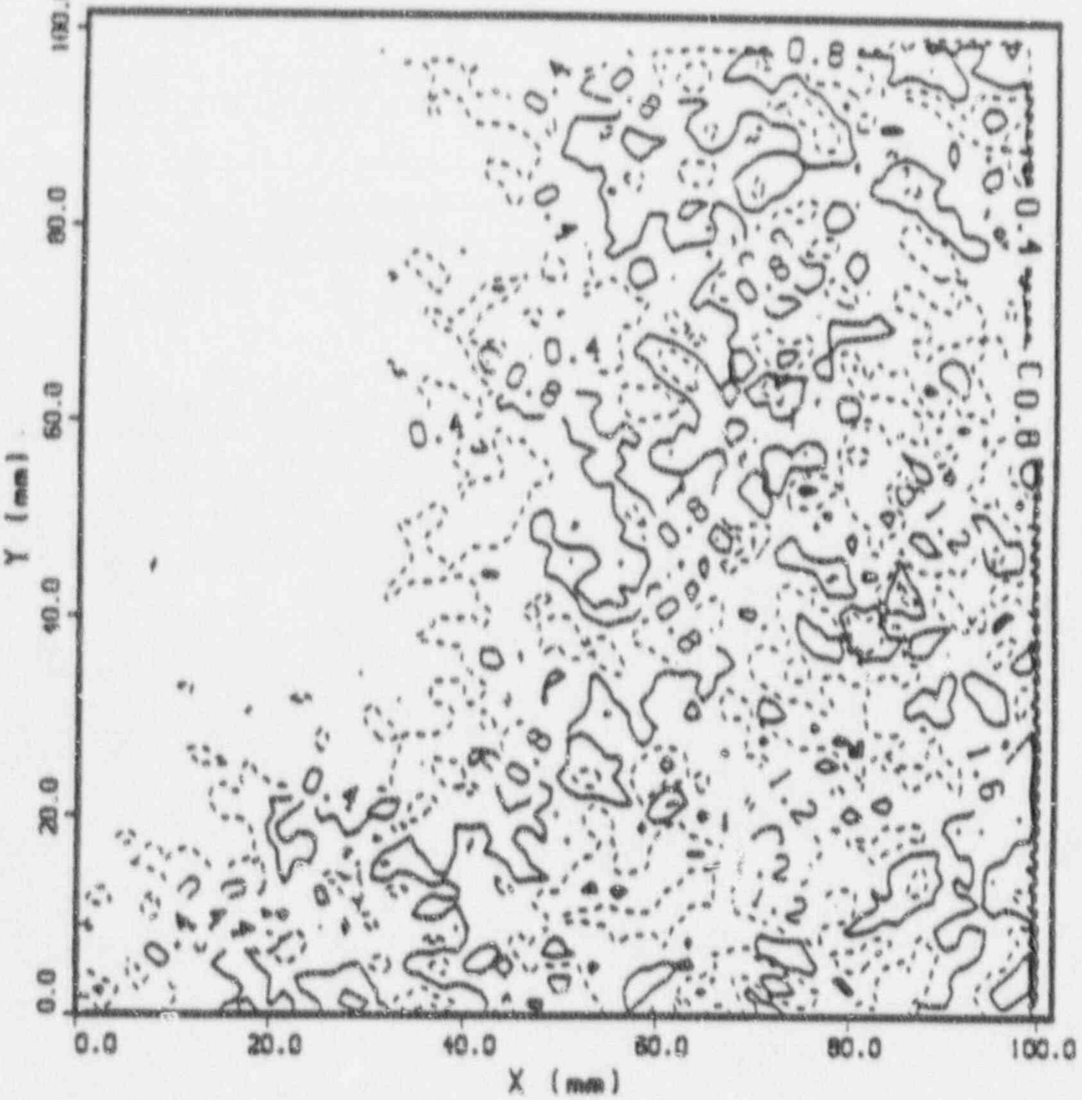


Figure 4.11 Contour of Apertures (Section 2)
(Contour interval = 0.4 mm)

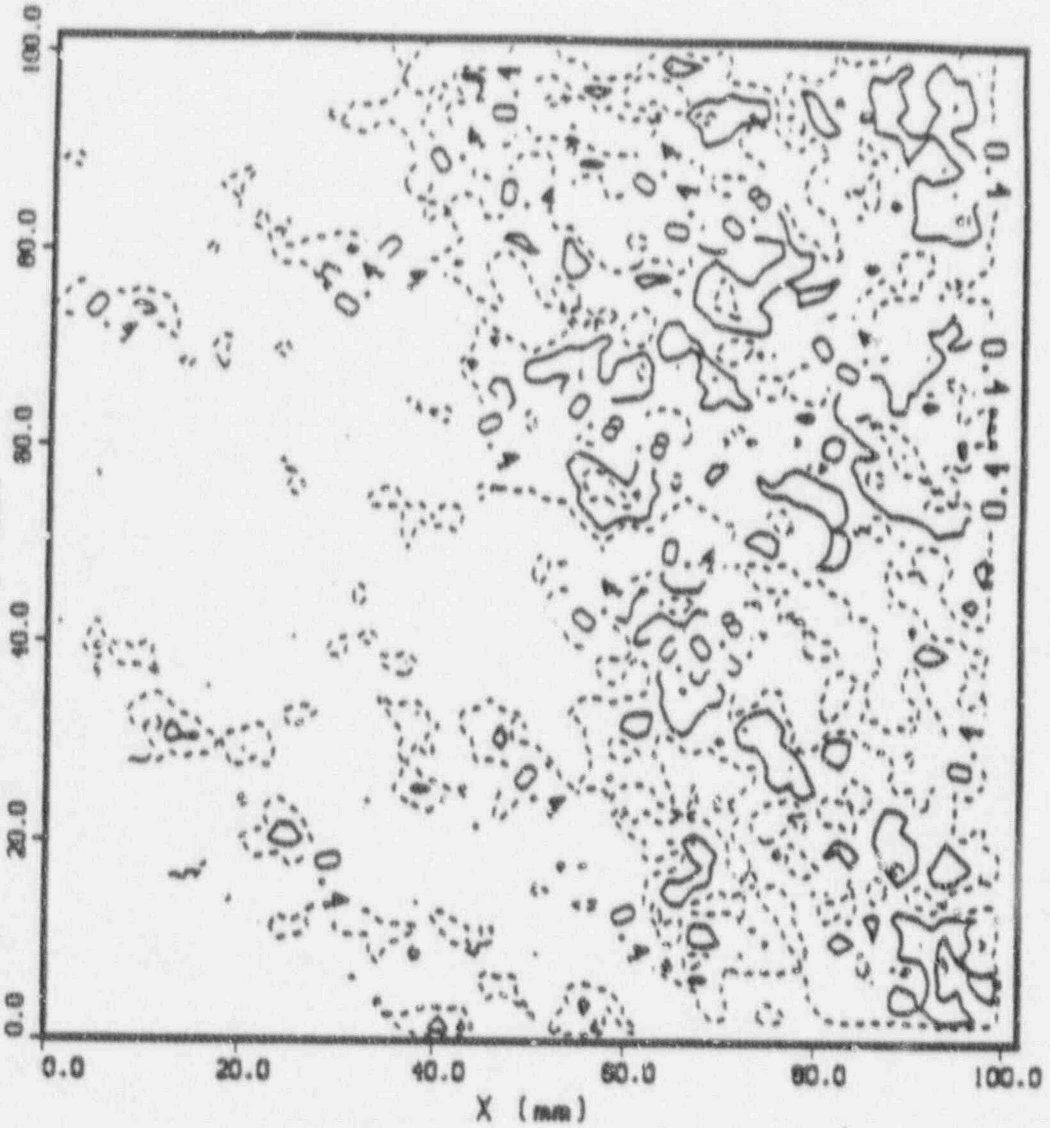


Figure 4.12 Contour of Apertures (Section 3)

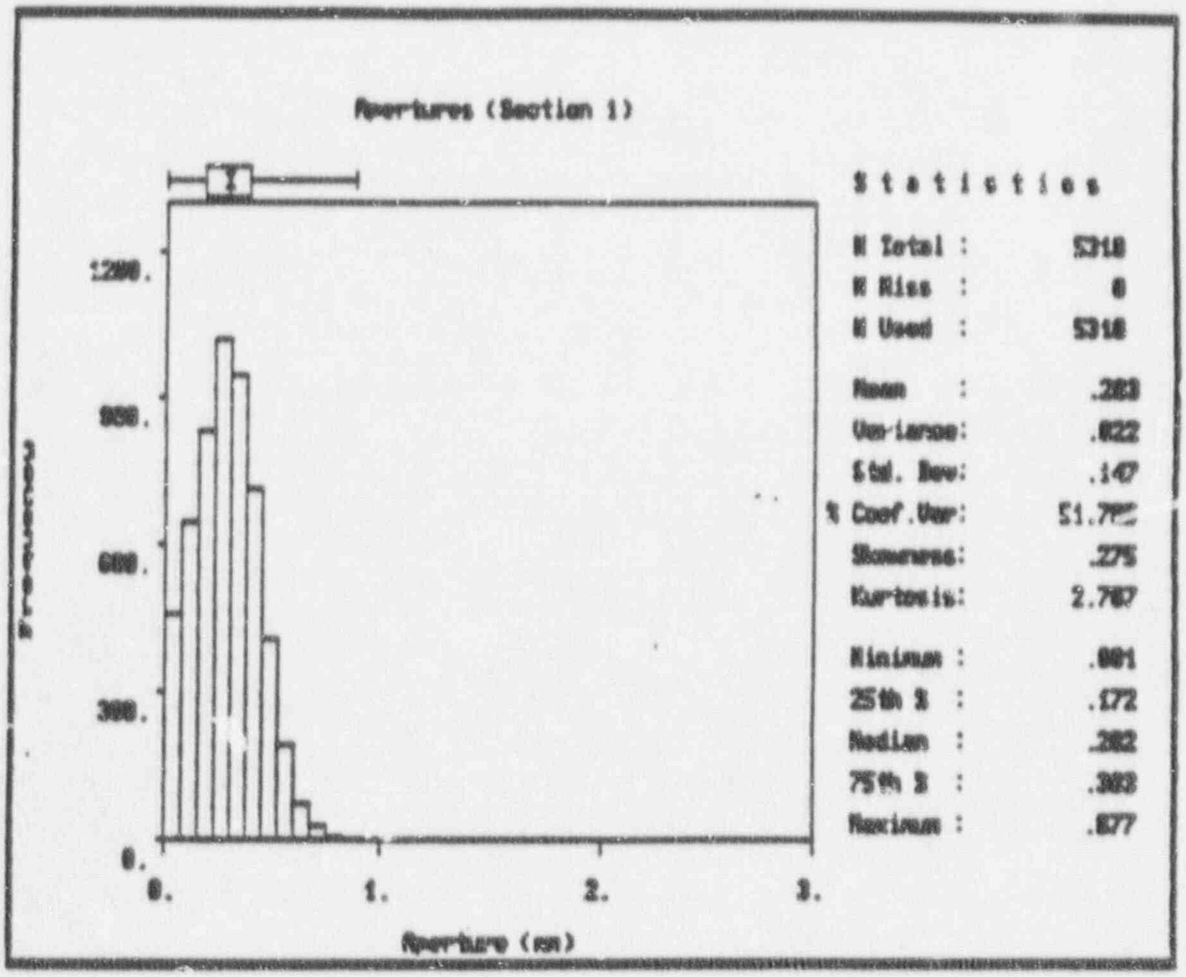
(Contour interval = 0.4 mm)

Table 5.5

Estimation of Drift and Model Parameters (Pure Nugget Model)

		Drift Parameters (1)			
Data Set	GLSR Iter (2)	bo	b1	b2	Nugget
1AP (3)	*(4)				0.018
	0	0.0782	0.00251	0.00120	0.017
	1	0.0782	0.00251	0.00120	0.017
2AP	*				0.076
	0	0.225	0.0154	-0.00651	0.059
	1	0.225	0.0154	-0.00651	0.059
3AP	*				0.080
	0	0.0869	0.00541	0.00161	0.068
	1	0.0869	0.00541	0.00161	0.068

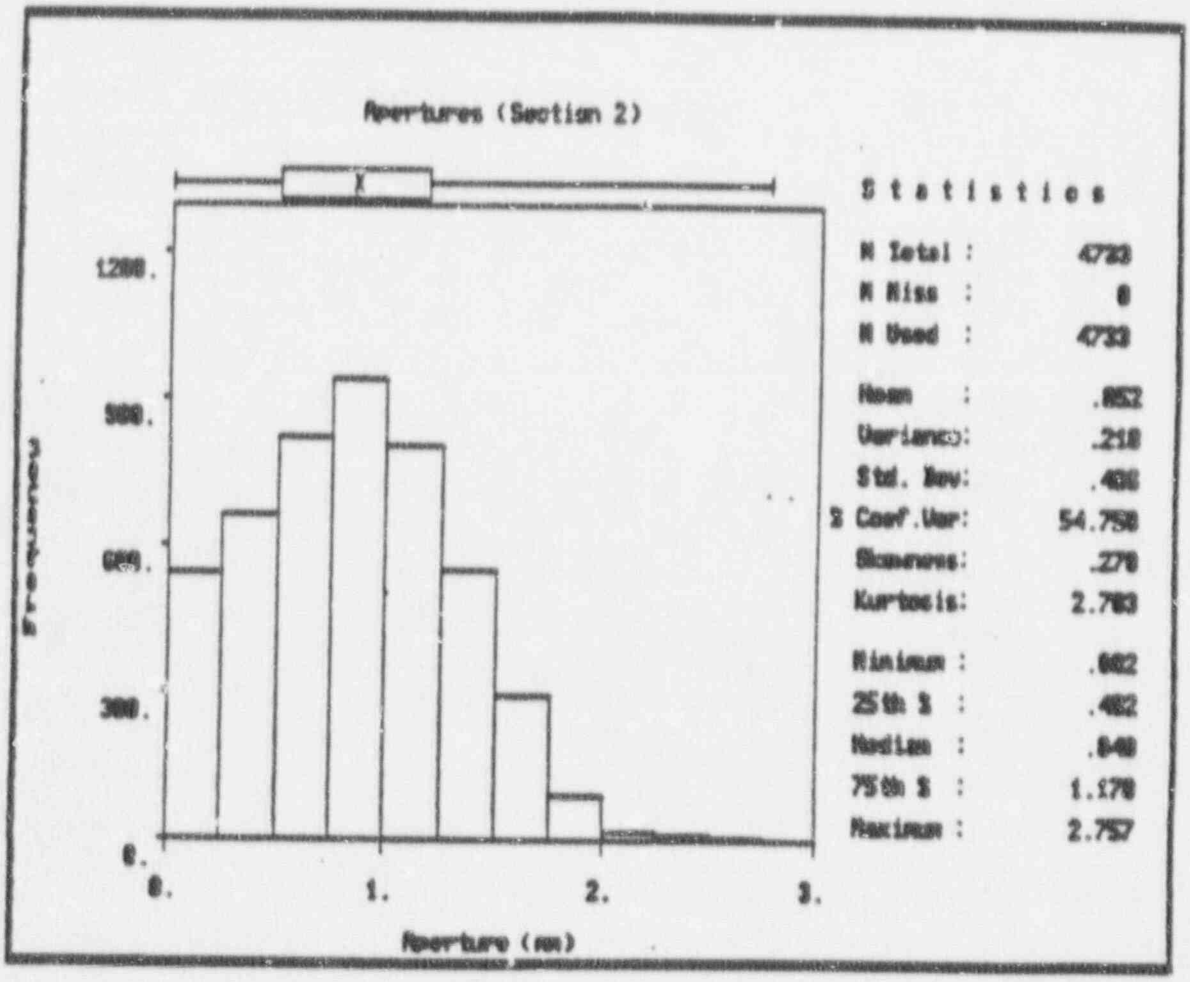
1. Coefficients of polynomial Y
2. Generalized Least-Squares Regression Iteration
3. Apertures calculated for section 1
4. Model fit by eye



Statistics

N Total :	5318
N Miss :	0
N Used :	5318
Mean :	.283
Variance:	.022
Std. Dev:	.147
% Coef.Var:	51.7[illegible]
Skewness:	.275
Kurtosis:	2.707
Minimum :	.001
25th % :	.172
Median :	.282
75th % :	.383
Maximum :	.877

Figure 5.7 Histogram of Apertures (Section 1)



Statistics	
N Total :	4733
N Miss :	0
N Used :	4733
Mean :	.852
Variance:	.218
Std. Dev:	.466
% Coef.Var:	54.758
Skewness:	.270
Kurtosis:	2.703
Minimum :	.002
25th % :	.482
Median :	.840
75th % :	1.170
Maximum :	2.757

Figure 5.8 Histogram of Apertures (Section 2)

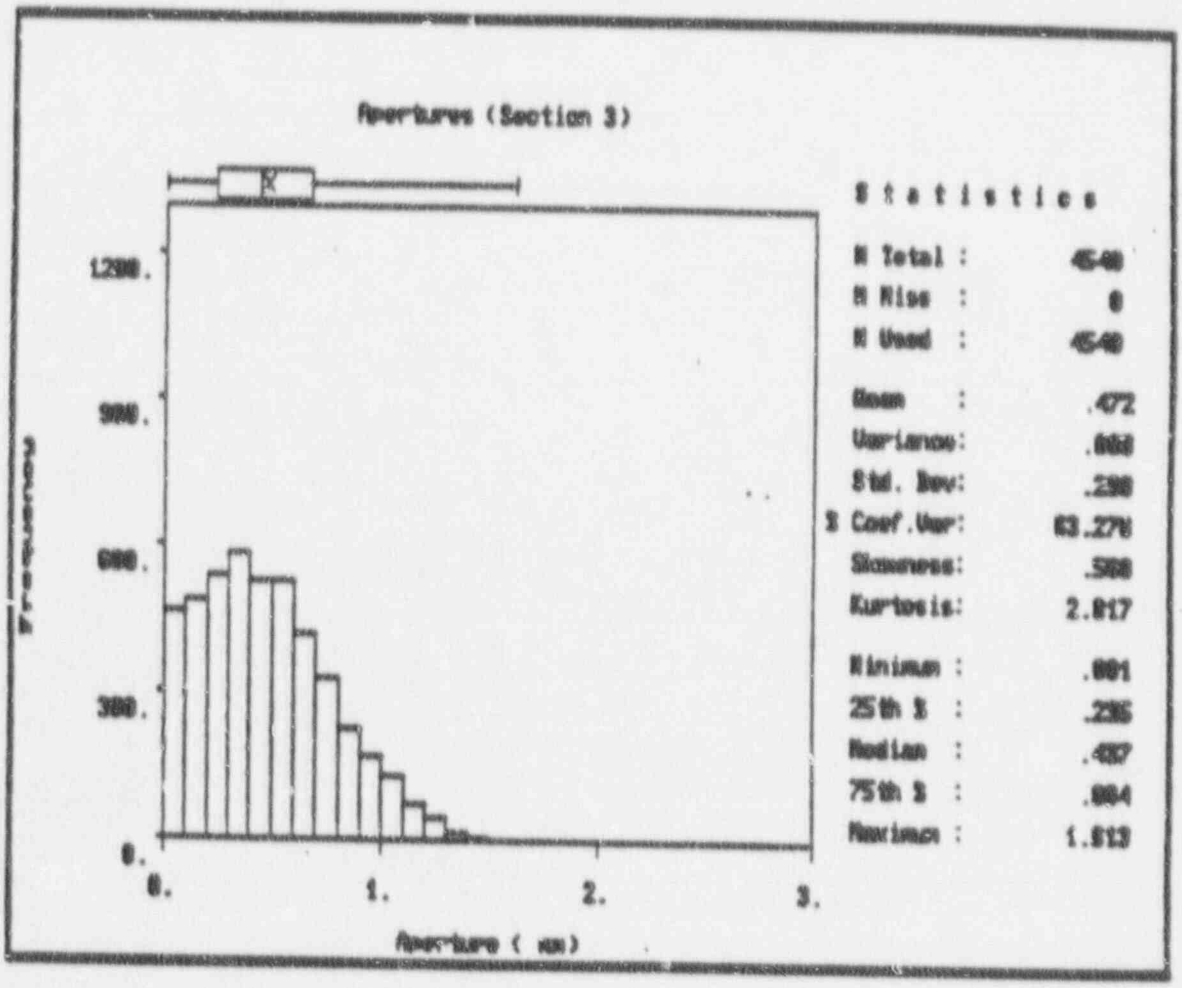
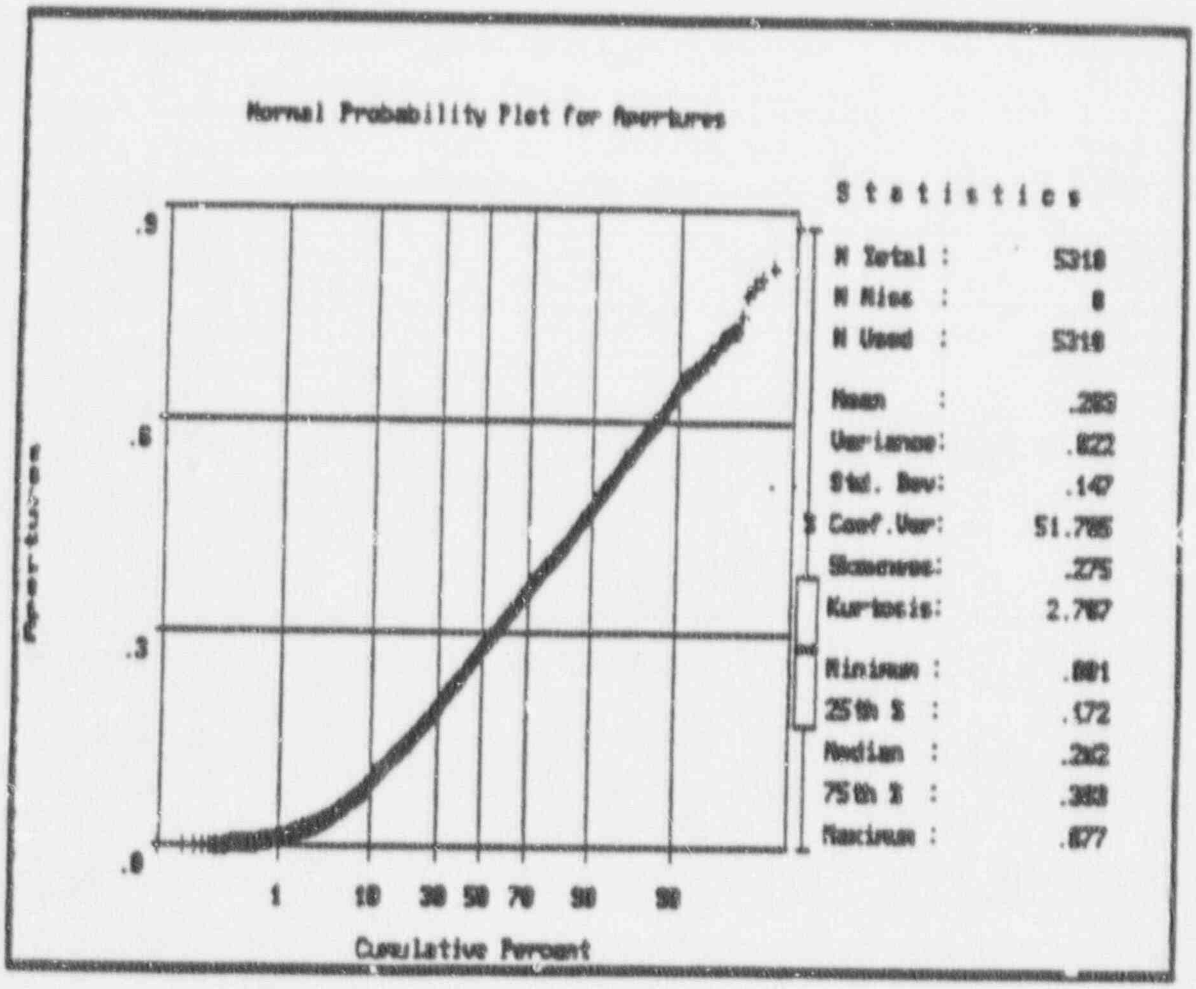


Figure 5.9 Histogram of Apertures (Section 3)



```
S t a t i s t i c s
N Total :       5310
N Miss  :          0
N Used  :       5310
Mean    :       .283
Variance:       .022
Std. Dev:       .147
% Coef.Var:   51.785
Skewness:       .275
Kurtosis:      2.787
Minimum :       .001
25th %  :       .172
Median  :       .282
75th %  :       .383
Maximum :       .877
```

Figure 5.11 Normal Probability Plot (1AP)

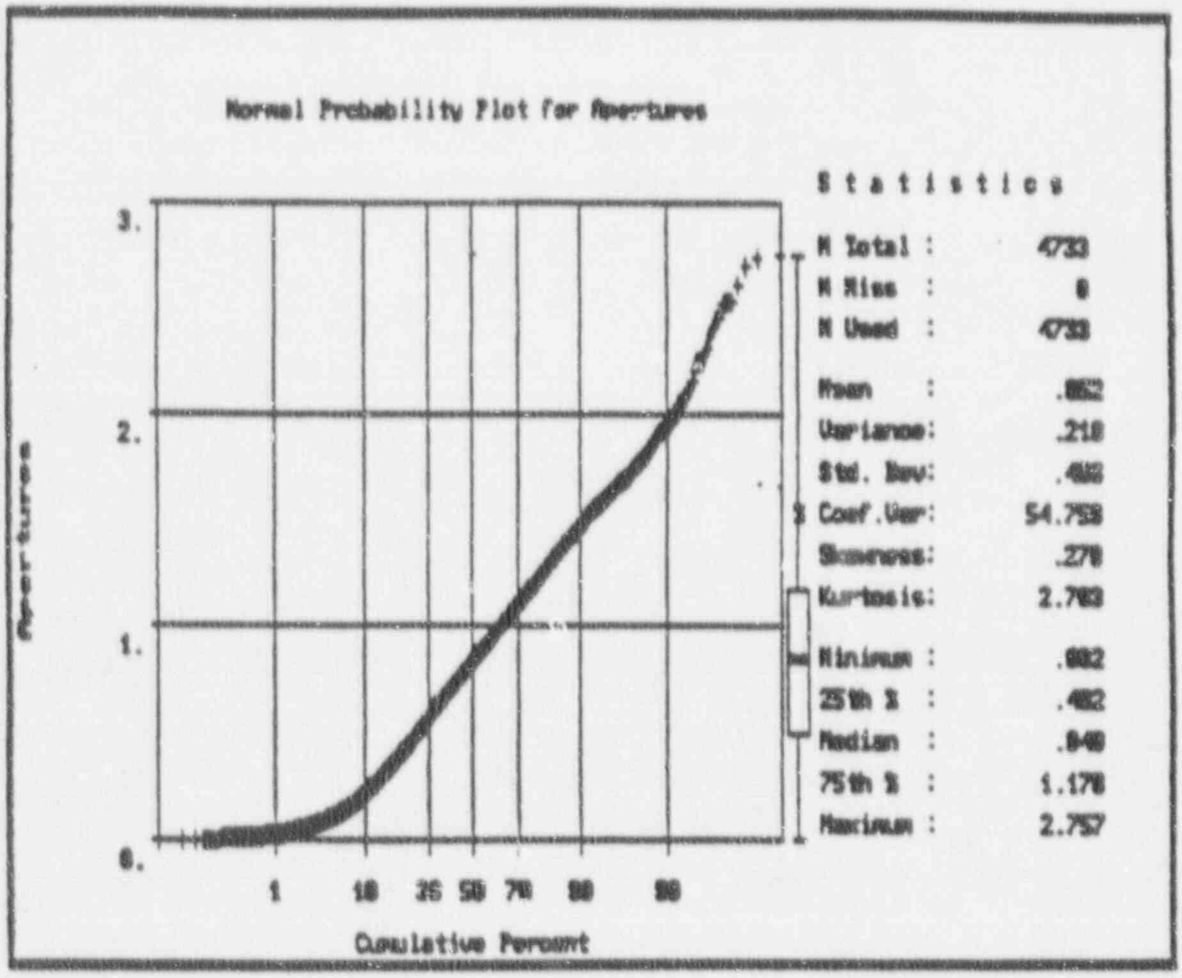


Figure 5.12 Normal Probability Plot (2AP)

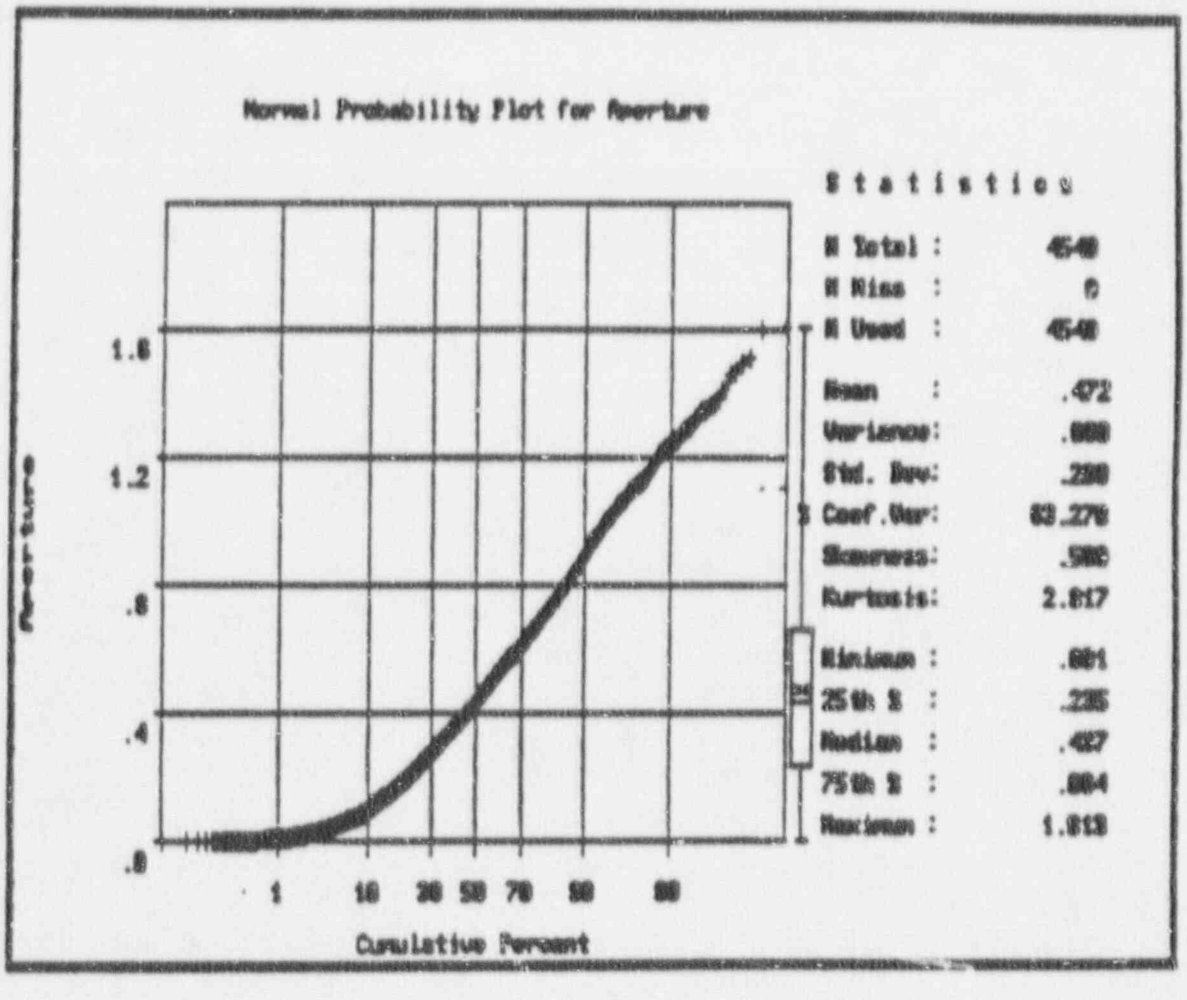


Figure 5.13 Normal Probability Plot (3AP)

Table 5.2

K-S Goodness of Fit Test

Data Set	K-S Z (1)	2-Tailed Probability	Reject Ho (2) (α=0.05)
1AP	2.008	0.001	Yes
2AP	2.344	0.000	Yes
3AP	3.881	0.000	Yes
1SK	6.283	0.000	Yes

1. Kolmogorov-Smirnov Z value.
2. The null hypothesis is that the data are from a normal distribution.

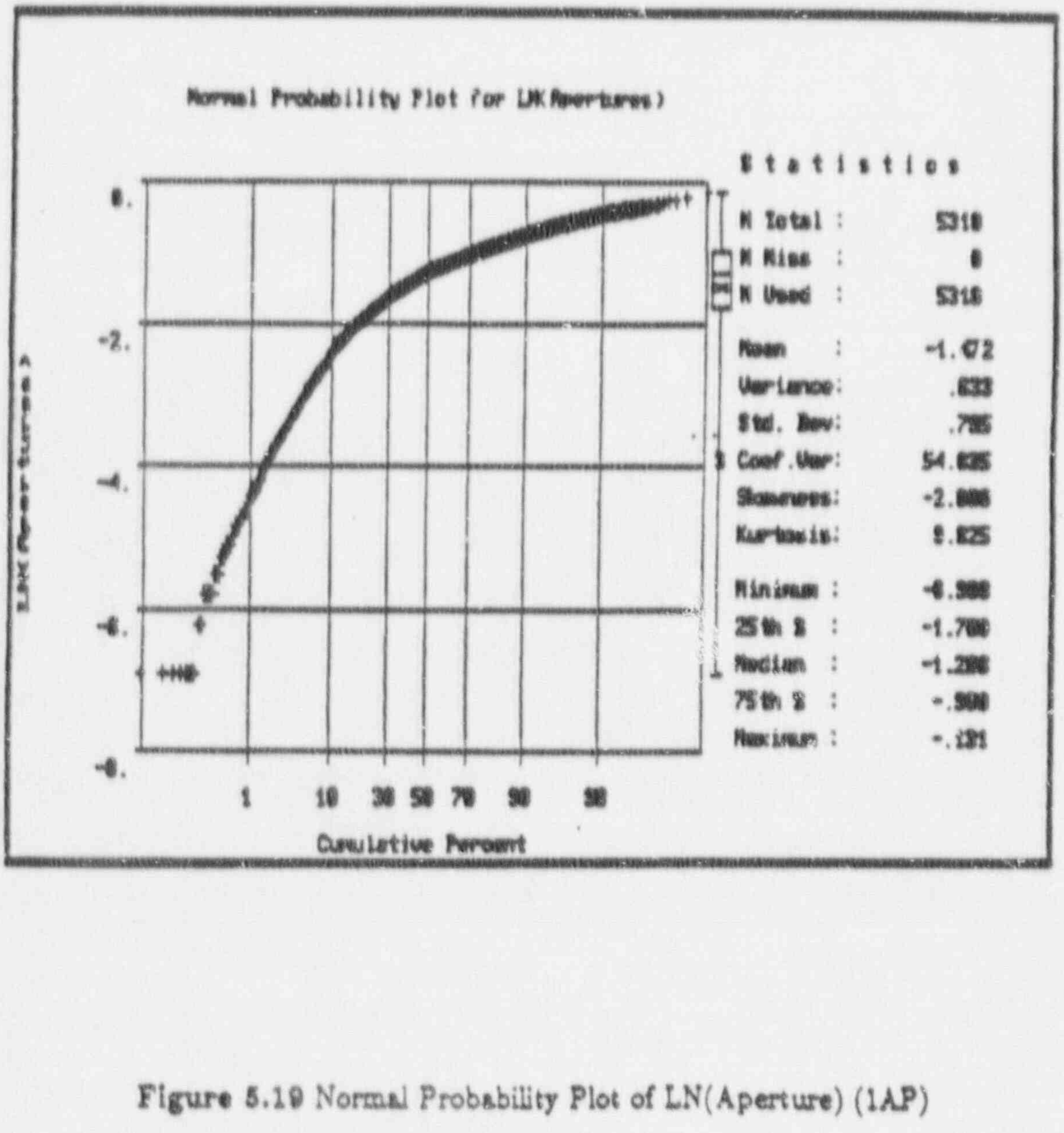
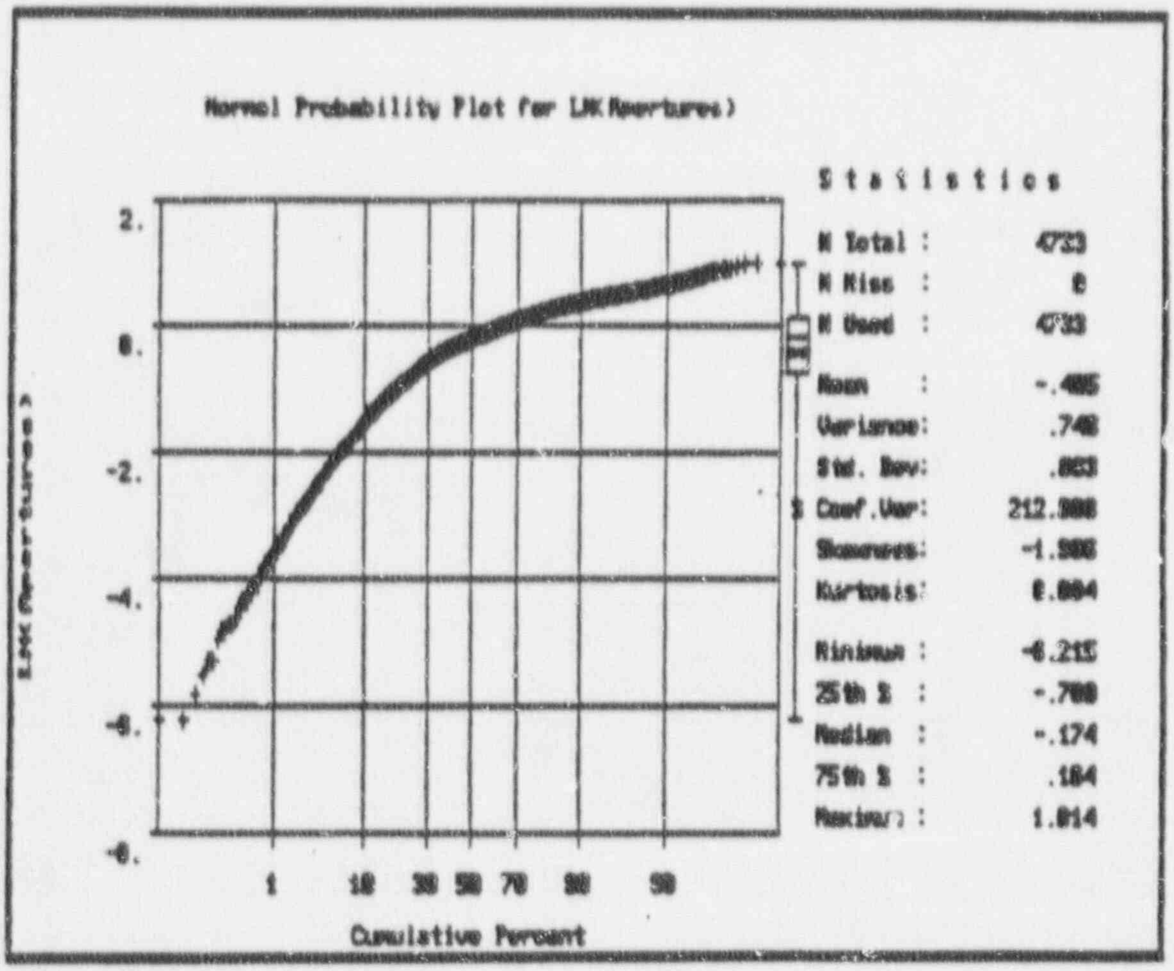


Figure 5.19 Normal Probability Plot of LN(Aperture) (1AP)



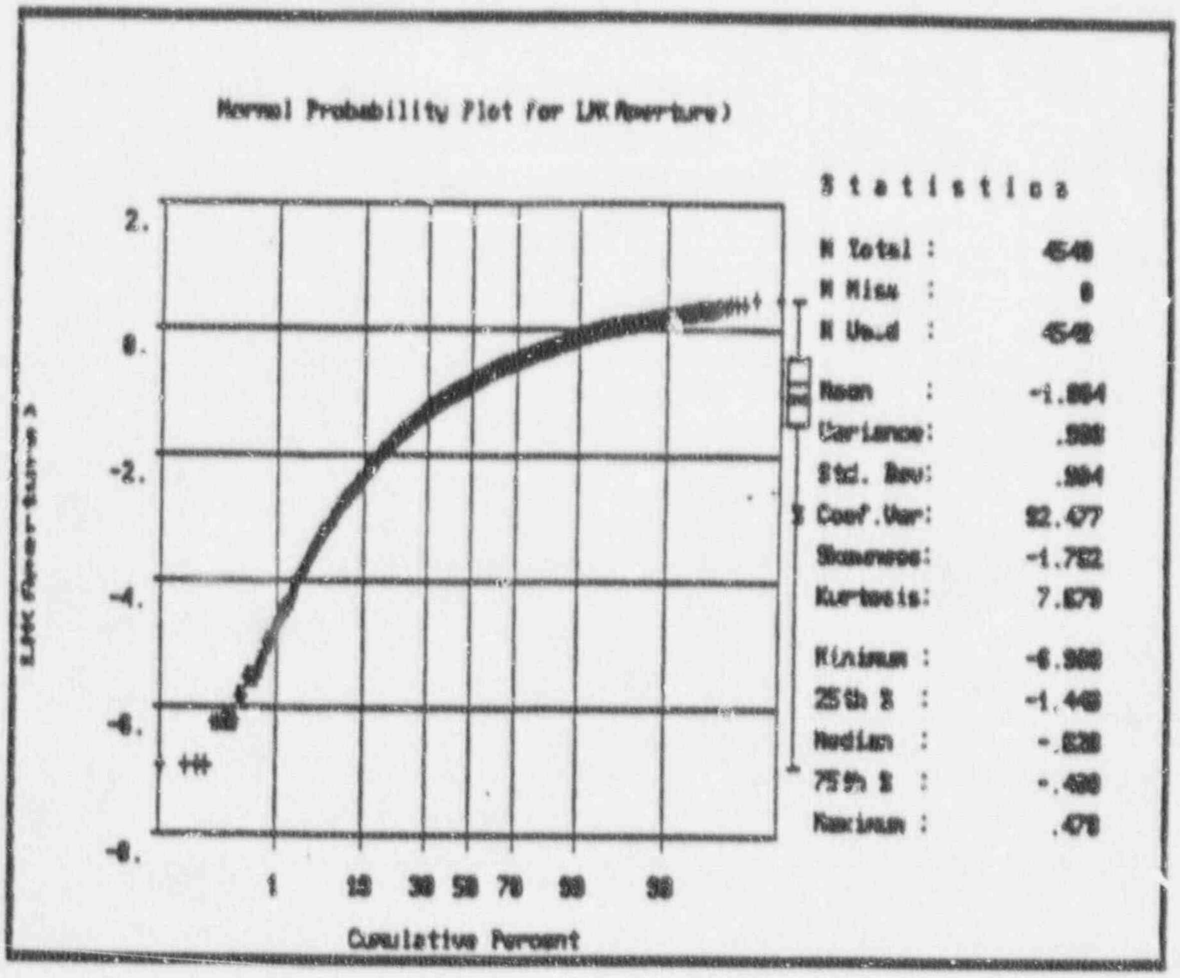
```
Statistics

N Total :      4733
N Miss  :         0
N Used  :      4733

Mean    :     -.405
Variance:      .748
Std. Dev:      .865
Coef.Var:   212.988
Skewness:    -1.900
Kurtosis:     0.004

Minimum :    -6.215
25th %  :     -.700
Median  :     -.174
75th %  :      .184
Maximum :     1.014
```

Figure 5.20 Normal Probability Plot of LN(Aperture) (2AP)



Statistics

N Total :	4540
N Miss :	0
N Used :	4540
Mean :	-1.084
Variance:	.988
Std. Dev:	.994
Coef.Var:	92.477
Skewness:	-1.782
Kurtosis:	7.870
Minimum :	-6.908
25th % :	-1.440
Median :	-.828
75th % :	-.400
Maximum :	.470

Figure 5.21 Normal Probability Plot of LN(Aperture) (3AP)

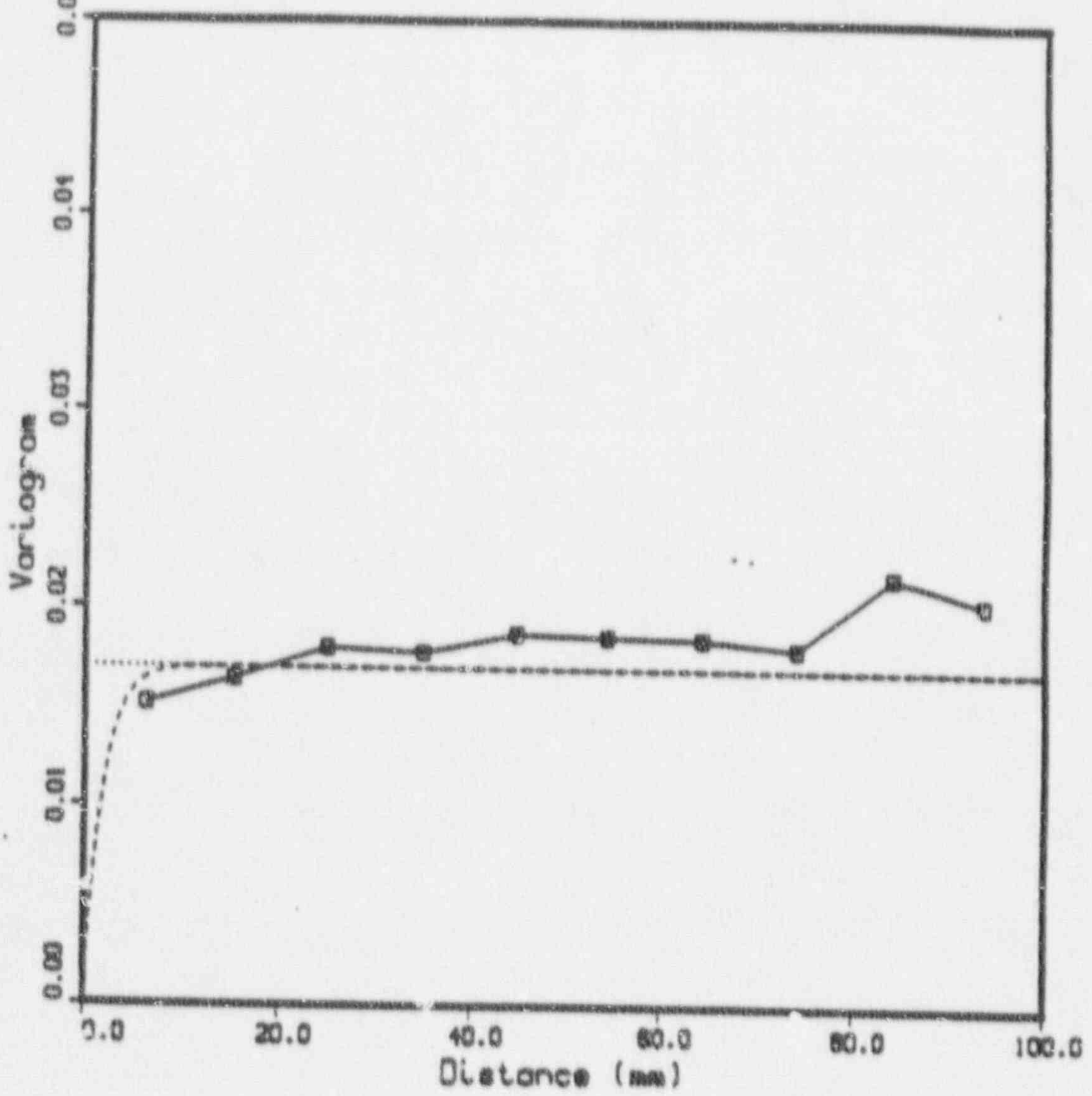


Figure 5.23 Estimated Models for Residuals Variogram (1AP)

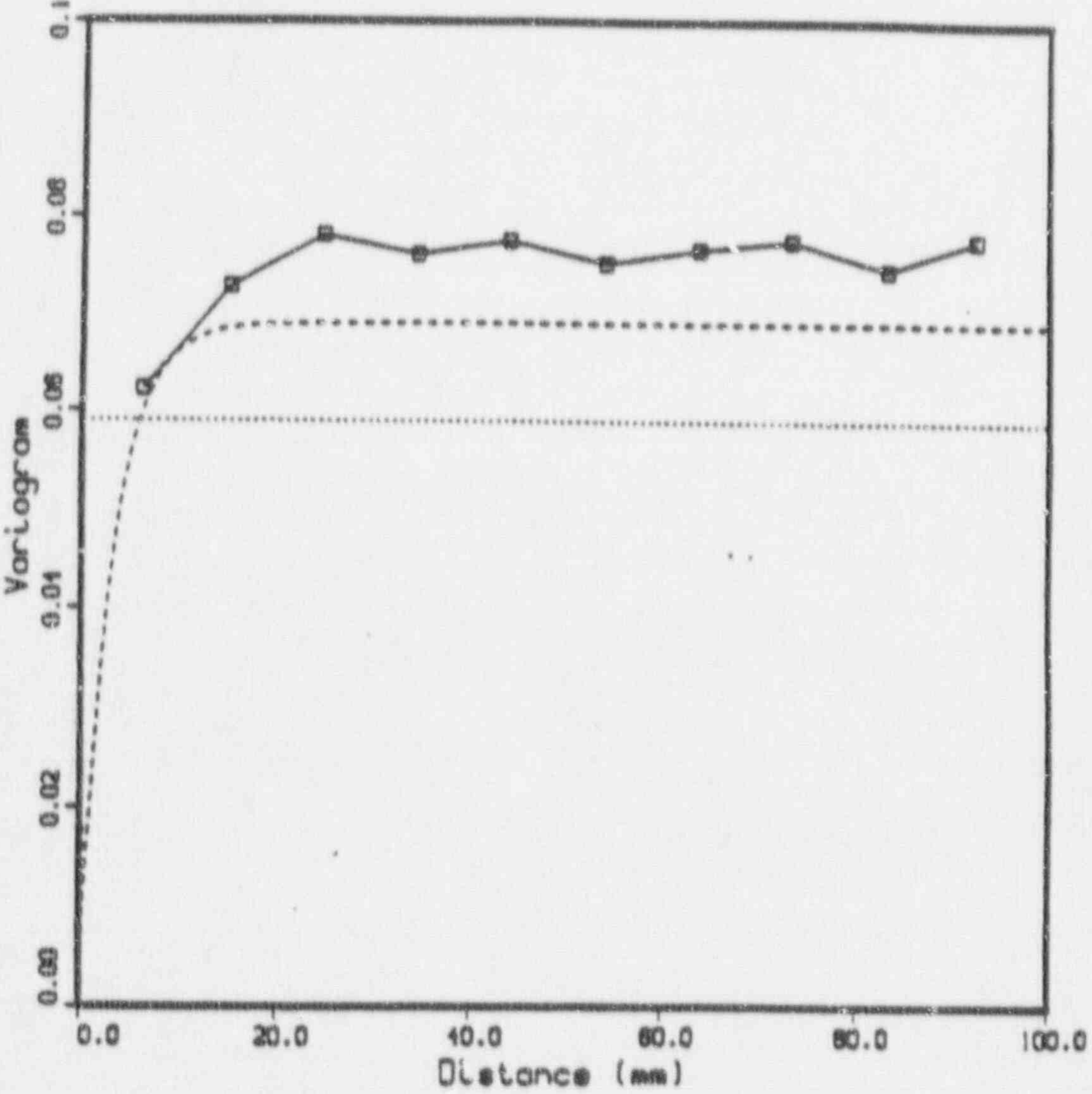


Figure 5.24 Estimated Models for Residuals Variogram (2AP)

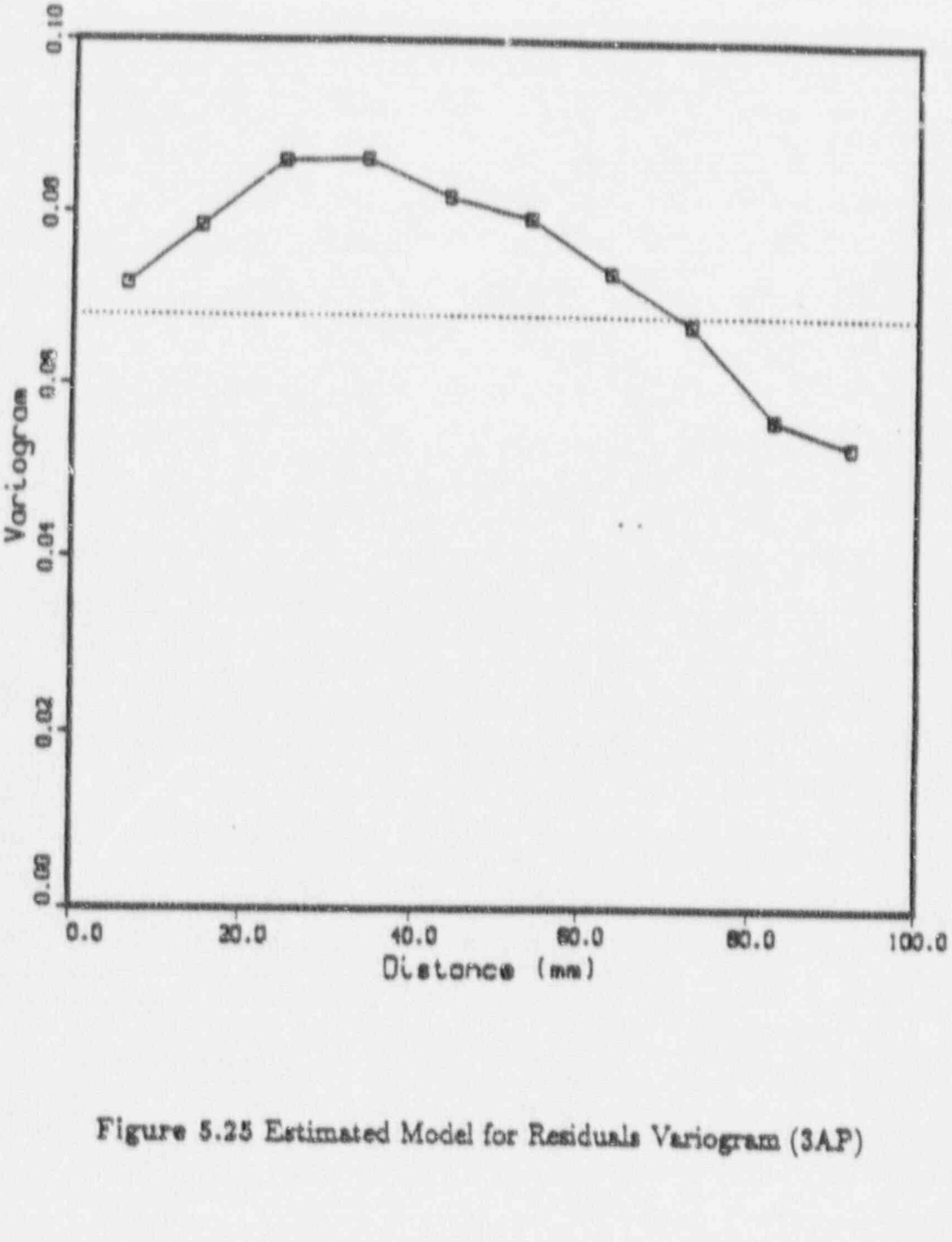


Figure 5.25 Estimated Model for Residuals Variogram (3AP)

Table 5.4

Estimation of Drift and Model Parameters
(Exponential Model with Nugget)

Data Set	GLSR Iter (2)	Drift Parameters (1)			Model Parameters		
		bo	b1	b2	Nugget	Sill	a (6) (mm)
1AP (3)	*(4)				0.010	0.008	25
	0	0.0782	0.00251	0.00120	0.000009	0.0169	1.84
	1	0.0864	0.00251	0.00110	0.000005	0.0170	1.84
	2	0.0864	0.00251	0.00110	0.000002	0.0170	1.84
2AP	*				0.040	0.035	20
	0	0.225	0.0154	-0.00651	0.00126	0.0677	3.10
	1	0.190	0.0158	-0.00619	0.00133	0.0677	3.10
	2	0.190	0.0158	-0.00619	0.00135	0.0677	3.10
3AP (5)	*				0.055	0.027	20

1. Coefficients of polynomial Y
2. Generalized Least-Squares Regression Iteration
3. Apertures calculated for section 1
4. Model fit by eye
5. Program did not converge after 20 iterations
6. Integral Scale

RELATIONSHIP BETWEEN TRAVEL TIME AND DISPERSION IN RANDOM GROUNDWATER VELOCITY FIELDS

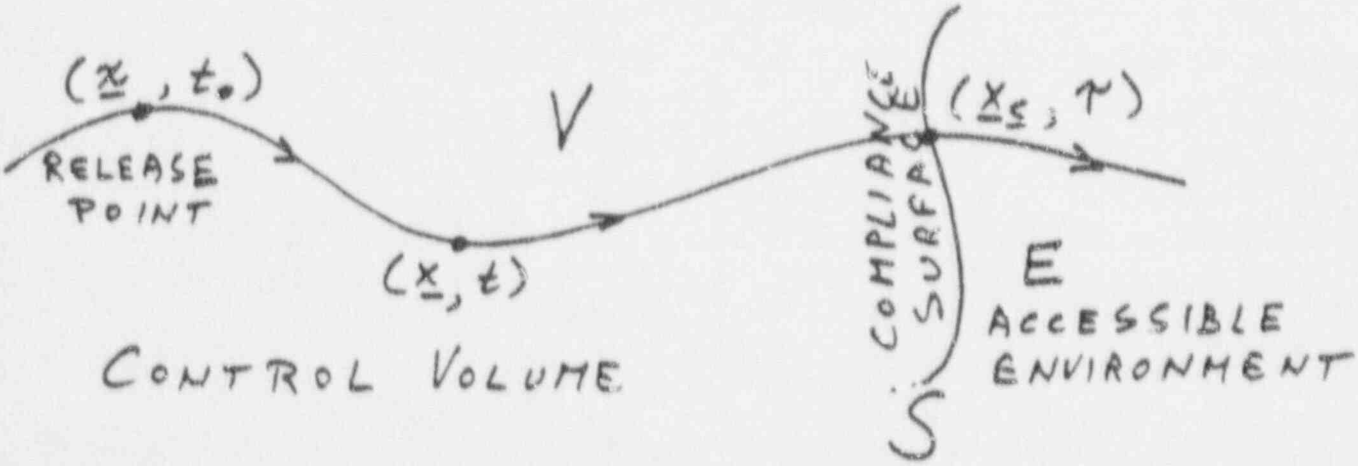
Consider the random Eulerian velocity field

$$u(x,t) = U(x,t) + u'(x,t) \tag{1}$$

such that

$$<u(x,t)> = \text{Ensemble mean velocity} = U(x,t) \tag{2}$$

$$<u'(x,t)> = \text{Ensemble mean velocity fluctuation} = 0. \tag{3}$$



Let S be a *Control or Compliance Surface* enclosing the *Repository Control Volume* V from the *Accessible Environment* E. Following G.I. Taylor's [1921] *theory of continuous motions*, consider an indivisible solute "particle" of mass M_0 released from the repository to the host rock at point χ and time t_0, then traveling along a random trajectory to cross S into E at point x_S following a *Travel or Residence Time* τ. We assume for simplicity, and without a loss of generality, that

1. All streamlines emanating from repository intercept S;
2. Randomness stems from spatial variability of advective velocity field and associated estimation errors.

Following Dagan [1987, 1989] we write

Total particle displacement

= Advective displacement + Brownian Displacement

$$X_t = X + X_B \tag{4}$$

where the Brownian component accounts for classical (local) Fickian dispersion. The *displacement covariance* of each component is

$$\Omega = \langle (X - \langle X \rangle)(X - \langle X \rangle)^T \rangle \qquad \text{for advection} \tag{5}$$

$$\Omega_B = 2dt \qquad d = \text{local dispersion tensor.} \tag{6}$$

Assuming for simplicity a constant water content θ, the *ensemble mean concentration* due to this particle is

$$\langle c(x, t; \chi, t_0) \rangle = \langle \frac{M_0}{\theta} \delta(x - X_t) \rangle = \frac{M_0}{\theta} f(x; t, \chi, t_0) \tag{7}$$

where

$$f(X_t; t, \chi, t_0) = \text{pdf of } X_t\text{, evaluated at } X_t = x. \tag{8}$$

Define the *effective dispersion tensor*

$$D(t-t_0) = \frac{1}{2} \frac{d\Omega(t-t_0)_t}{dt} = d + \frac{1}{2} \frac{d\Omega(t-t_0)}{dt} \tag{9}$$

which *depends on travel (residence) time.* Then if the displacements are Gaussian, or otherwise to a leading-order of approximation, f as well as <c> can be shown to satisfy the *pseudo-Fickian advection-dispersion equation*

$$\frac{\partial \langle c \rangle}{\partial t} + U \cdot \nabla \langle c \rangle = \nabla \cdot D(t-t_0) \nabla \langle c \rangle. \tag{10}$$

The nature of $D(t-t_0)$ has been investigated based on a linear approximation by Dagan [1984, 1987, 1989], and based on a higher-order quasilinear approach by Neuman and Zhang [1989] and Zhang and Neuman [1989].

Following Dagan [1989], we define

$G(\tau;S,\chi,t_0)$ = the *cumulative probability that a particle released from the repository location* χ *at time* t_0 *crosses the compliance surface* S *into the accessible environment E during any time* $t_0 < t \leq \tau$. Then

$$G(\tau;S,\chi,t_0) = 1 - \int_V f(\mathbf{x};\tau,\chi,t_0)\,d\mathbf{x}. \qquad (11)$$

By virtue of (7), this can be written as

$$G(\tau;S,\chi,t_0) = 1 - \frac{\theta}{M_0}\int_V \langle c(\mathbf{x};\tau,\chi,t_0)\rangle\,d\mathbf{x} = \frac{\langle M_S(\tau;\chi,t_0)\rangle}{M_0} \qquad (12)$$

$\langle M_S(\tau;\chi,t_0)\rangle$ = mean (!) mass having reached the accessible
environment E during $t_0 < t \leq \tau$.

Since the 2nd moment Ω of f depends on D by virtue of (9), or equivalently <c> depends on D by virtue of (10), we have established a clear and unequivocal relationship between the cumulative probability G of the (random) travel time τ, as well as the mean cumulative release to the accessible environment, $\langle M_S(\tau;\chi,t_0)\rangle$, and the effective dispersion tensor D!

(V)

<c> is only an *estimate of the real concentration* c, and $\langle M_S\rangle$ is only an *estimate of the real cumulative release* M_S. By virtue of (12), our ability to estimate M_S depends on our ability to estimate the integral of c over V. We will see later [Neuman, 1990a, b] that the *estimation error, or uncertainty* in c and/or M_S, are closely related to the magnitude of D, which in turn depends on the *uncertainty associated with site-characterization of the advective velocity field*. The more poorly is this field characterized, the larger are D and the resulting uncertainties in c and/or M_S.

Let $g(\tau;S,\chi,t_0)$ = *pdf of a particle released from the repository location* χ *at time* t_0 *crossing the compliance surface S into the accessible environment E during* $\tau \leq t \leq \tau + d\tau$. Then from (11)

$$g(\tau;S,\chi,t_0) = -\int_V \frac{\partial f}{\partial \tau}\, d\mathbf{x} \tag{13}$$

or equivalently from (12)

$$g(\tau;S,\chi,t_0) = -\frac{\theta}{M_0}\int_V \frac{\partial \langle c(\mathbf{x},\tau;\chi,t_0)\rangle}{\partial \tau}\, d\mathbf{x} = \frac{1}{M_0}\,\frac{\partial M_S}{\partial \tau} = \frac{\langle J_S \rangle}{M_0} \tag{14}$$

$\langle J_S(\tau;\chi,t_0)\rangle$ = mean (!) mass flow rate into the accessible environment E at time τ.

Like $\langle M_S \rangle$, the mean mass flow rate $\langle J_S \rangle$ depends on f and/or $\langle c \rangle$ and hence on D.

The mean mass flow rate into E at time τ, due to the release of mass $dM_0(\chi) = \theta c_0(\chi) d\chi$ at time t_0 from each point χ within a repository volume V_0, is

$$\langle J_S(\tau;V_0,t_0)\rangle = \int_{V_0} \theta c_0(\chi)\, g(\tau;S,\chi,t_0)\, d\chi. \tag{15}$$

For a continuous release at the mass rate $Q(\chi,t_0) = \partial M(\chi,t_0)/\partial t_0$ the mean mass flow rate into E is

$$\langle J_S(\tau;V_0)\rangle = \int_0^{\tau}\int_{V_0} Q(\chi,t_0)\, g(\tau;S,\chi,t_0)\, d\chi\, dt_0. \tag{16}$$

NOW, ABOUT UNCERTAINTY:...

Returning to the single particle of mass M_0, assume that G is known and $d = 0$ (negligible local dispersion). Then the pdf of M_S is bimodal, with probability G that $M_S = M_0$ (particle is in E) and probability (1 - G) that $M_S = 0$ (particle is in V):

IN THIS CASE, EASY: $f(M_S)$ is BIMODAL

$$f(M_S) = (1 - G)\delta(M_S) + G\delta(M_S - M_0). \tag{17}$$

From (12), the mean of M_S is

$$\langle M_S \rangle = M_0 G. \tag{18}$$

✓

The variance is

$$\begin{aligned}\mathrm{Var}(M_S) &= \langle (M_S - \langle M_S \rangle)^2 \rangle = \langle (M_S - M_0 G)^2 \rangle \\ &= \int_{-\infty}^{\infty} (M_S - M_0 G)^2 f(M_S)\, dM_S \\ &= (M_0 G)^2 (1 - G) + (M_0 - M_0 G)^2 G = M_0^2 G(1 - G)\end{aligned} \tag{19}$$

✓!!! ≠ Concl

If you look at the variance of Ms, it's max. for G = 1/2 !

and the coefficient of variation

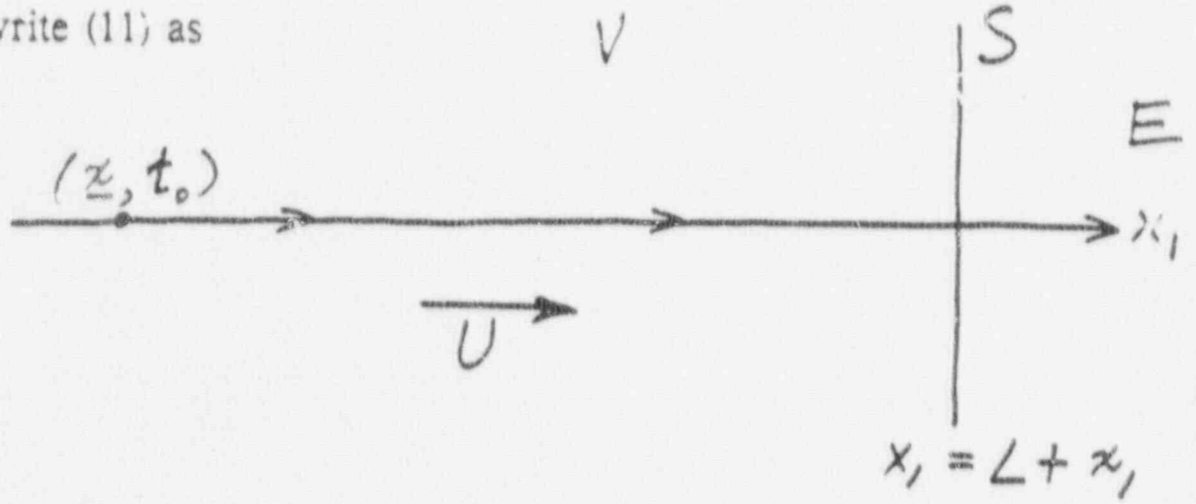
$$CV(M_S) = \frac{\sqrt{\mathrm{Var}(M_S)}}{\langle M_S \rangle} = \sqrt{\frac{1 - G}{G}}. \tag{20}$$

It follows that at early time, when $\langle M_S \rangle$ and G are small, $CV(M_S)$ is very large and thus the uncertainty about the particle's release to the accessible environment is very large. This uncertainty is compounded by the uncertainty about G itself: As implied by (11) - (12), to evaluate G one must be able to evaluate the integral of f or <c> over the control volume V. As was already made clear, this cannot be accomplished without a knowledge of D.

BUT.

✓

Uniform Mean Flow in Semi-infinite Stationary Medium: If one takes the mean flow to take place uniformly (for simplicity, or lack of data to justify doing otherwise) in a semi-infinite medium toward a planar compliance surface S, located a distance L from the repository release point χ, and the displacement process X_t to be stationary, one can rewrite (11) as



$$G(\tau - t_0; L - \chi_1) = 1 - \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{L} f(x_1-\chi_1, x_2-\chi_2, x_3-\chi_3; \tau - t_0)\, dx_1\, dx_2\, dx_3$$

$$= 1 - \int_{-\infty}^{L} f_1(x_1-\chi_1; \tau - t_0)\, dx_1 \qquad (21)$$

$f_1(x_1-\chi_1;\tau-t_0)$ = 1-D marginal pdf of particle displacement

= probability that particle released at χ_1 at t_0

is within the strip x_1 and $x_1 + dx_1$ at time $\tau - t_0$.

If X_t is Gaussian, or otherwise to leading order of approximation, f_1 satisfies the *pseudo-Fickian advection-dispersion equation*

$$\frac{\partial f_1}{\partial t} + U\frac{\partial f_1}{\partial x_1} = D_L(t-t_0)\frac{\partial^2 f_1}{\partial x_1^2} \qquad (22)$$

so that computation of the travel time cpf G depends only on longitudinal dispersion, not on transverse dispersion.

Uncertainty of Concentration c [Neuman, 1990b]: Express the actual concentration c as

$$c(\mathbf{x},t) = <c(\mathbf{x},t)> + c'(\mathbf{x},t) \quad (23)$$

$<c(\mathbf{x},t)>$ = unbiased *estimate* of $c(\mathbf{x},t)$

$c'(\mathbf{x},t)$ = zero-mean *estimation error.*

Then, for $t_0 = 0$ and a space-time stationary velocity field $\mathbf{u}(\mathbf{x},t)$ with

$<\mathbf{u}(\mathbf{x},t)> = \mathbf{U}$ = uniform and constant in time,

the *covariance of the estimation error* between two points $\mathbf{y}$ and $\mathbf{x}$ is

$$<c'(\mathbf{y},t)c'(\mathbf{x},t)> = \nabla^T <c(\mathbf{y},t)> \Omega(t) \nabla<c(\mathbf{x},t)> \quad (24)$$

$$\frac{d\Omega(t)}{dt} = 2D(t) \quad (25)$$

$$D(t) = \int_0^t \Lambda(\lambda)\, d\lambda \quad (26)$$

$\Lambda(t)$ = Lagrangian covariance (mean over random particle trajectories) of velocity fluctuations $\mathbf{u}'(\mathbf{x},t)$ about their constant mean $\mathbf{U}$.

If, instead of assuming stationarity, we set

$<\mathbf{u}(\mathbf{x},t)> = \mathbf{U}(\mathbf{x},t)$ = unbiased *estimate* of $\mathbf{u}(\mathbf{x},t)$

(not necessarily uniform or constant in time)

$\mathbf{u}'(\mathbf{x},t)$ = zero-mean *estimation error*

(now generally nonstationary)

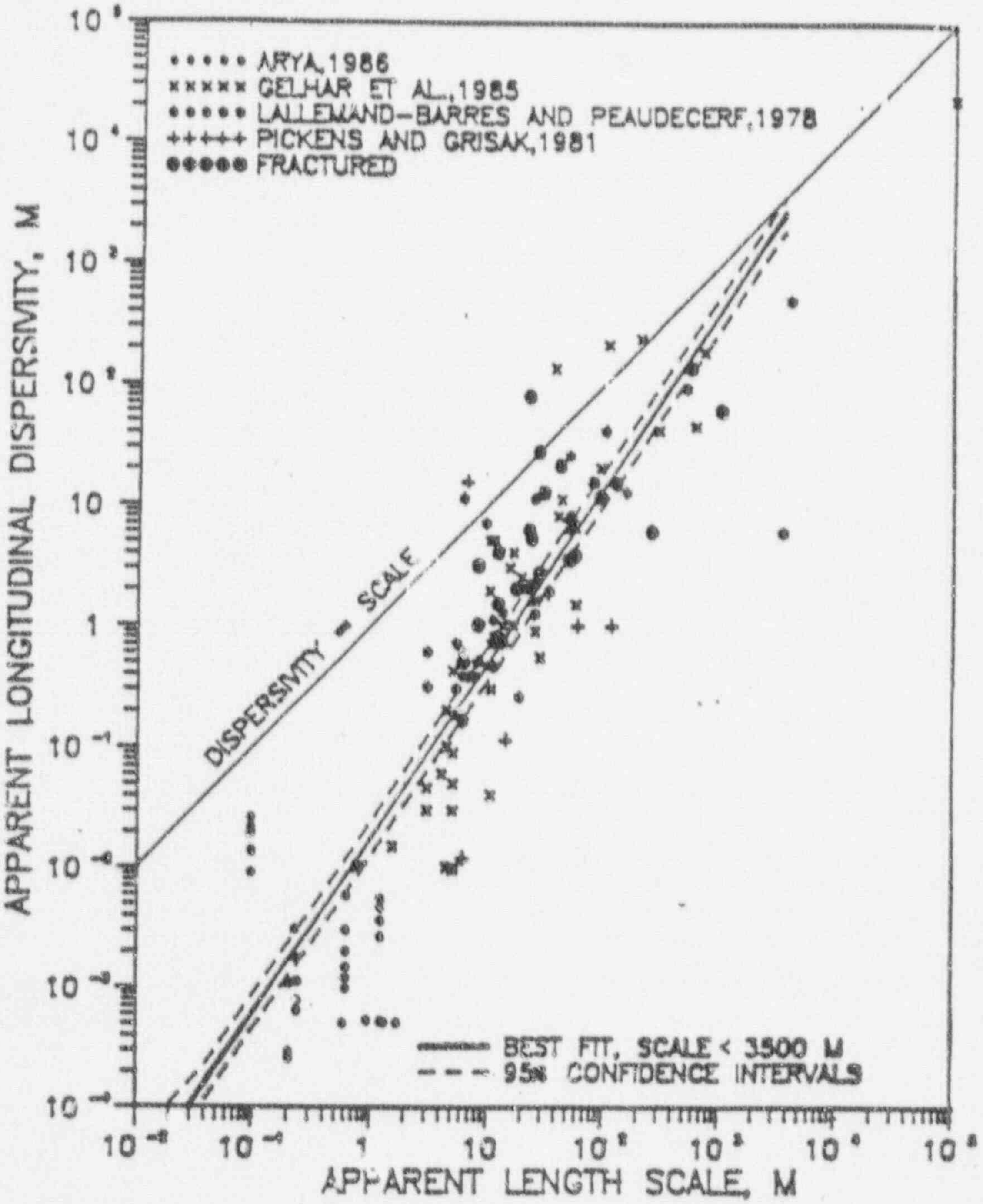
then $<c>$ satisfies a more complex equation of the form

$$\frac{\partial<c(\mathbf{x},t)>}{\partial t} + \mathbf{U}(\mathbf{x},t)\cdot\nabla<c(\mathbf{x},t)> = -\nabla\cdot\mathbf{J}_D(\mathbf{x},t) \quad (27)$$

$$\mathbf{J}_D(\mathbf{x},t) = \text{dispersive flux dependent on } \Lambda(\mathbf{x},t). \quad (28)$$

The better is the estimate of $\mathbf{U}(\mathbf{x},t)$, the smaller is the covariance $\Lambda(\mathbf{x},t)$ of the errors $\mathbf{u}'(\mathbf{x},t)$ and the dispersive flux $\mathbf{J}_D(\mathbf{x},t)$! *Information is thus transferred from the dispersive to the advective term!*

✓ Well known



••••• ARYA,1986
××××× GELHAR ET AL.,1985
••••• LALLEMAND-BARRES AND PEAUDECERF,1978
+++++ PICKENS AND GRISAK,1981
●●●●● FRACTURED
DISPERSIVITY = SCALE
BEST FIT, SCALE < 3500 M
95% CONFIDENCE INTERVALS
APPARENT LONGITUDINAL DISPERSIVITY, M
APPARENT LENGTH SCALE, M
10⁵
10⁴
10³
10²
10
1
10⁻¹
10⁻²
10⁻³
10⁻²
10⁻¹
1
10
10²
10³
10⁴
10⁵

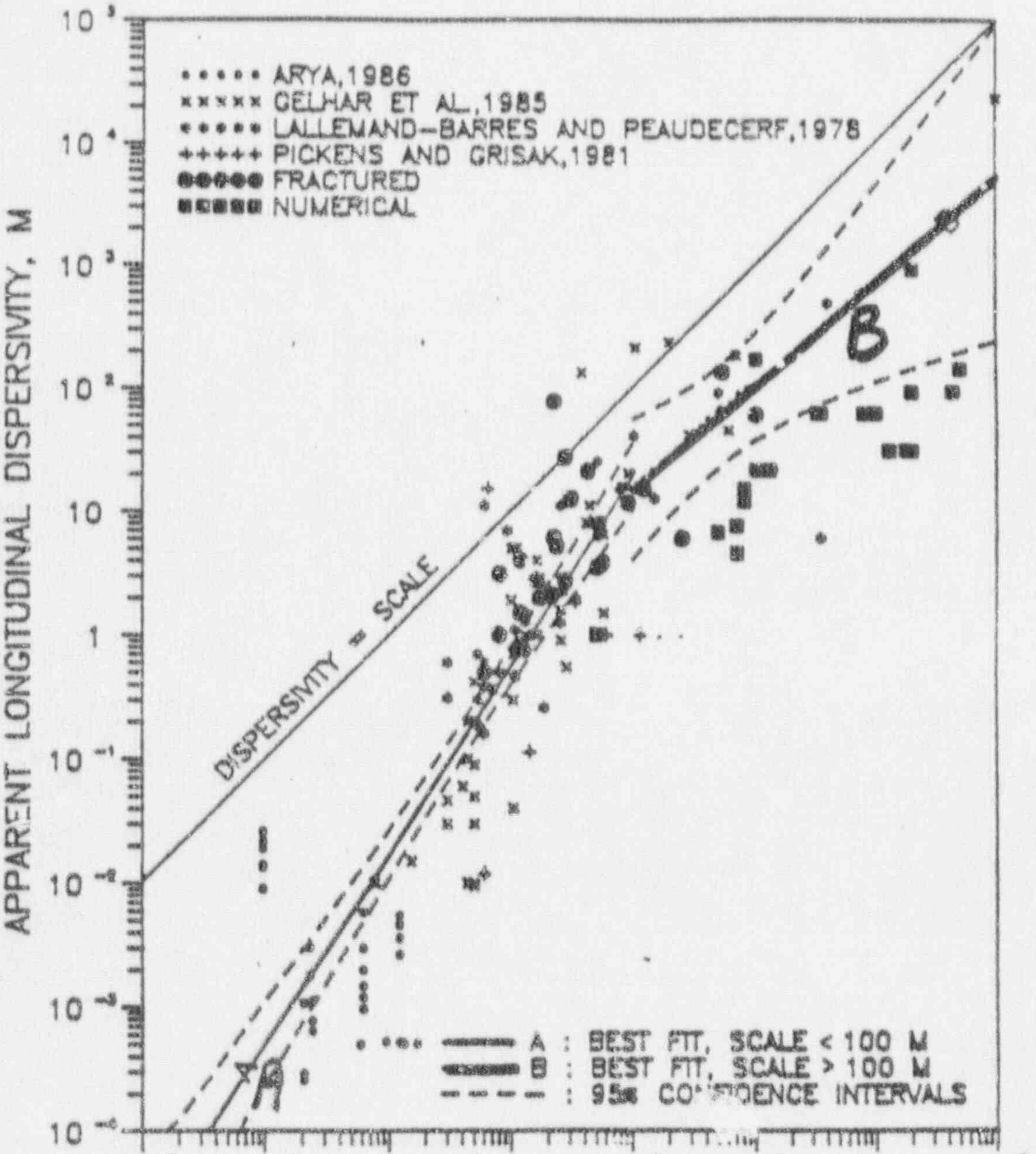
FIG. 1

IMLICATIONS OF SCALE EFFECT

The observed increase of apparent longitudinal dispersivity with observation or experimental scale in saturated media implies (Neuman, 1990a):

1. Heterogeneous geologic media are not statistically homogeneous with respect to saturated log hydraulic conductivity (there are no unique mean, variance, correlation scales) except, at best, locally. Heterogeneities may appear on a multiplicity of scales and their effect must be superimposed. Hence site characterization on one scale does not carry over to other scales; a thorough understanding of geologic conditions in the near field of a repository is not sufficient to predict flow and transport in the far field; *characterization is required on all scales of the control volume*. Where this is not practical, the alternative is to rely on *scaling rules* such as that of Neuman (1990a). No such scaling rules presently exist for unsaturated media; much *theoretical work*, supported by *multiscale experiments and observations* are required to derive them.

2. Saturated flow and transport properties of fractured media scale, on the average, like those of porous media. Hence the *validity* of many *distinctions* commonly drawn between these two types of media may be *in question*.


ARYA,1986
GELHAR ET AL.,1985
LALLEMAND-BARRES AND PEAUDECERF,1978
PICKENS AND GRISAK,1981
FRACTURED
NUMERICAL
DISPERSIVITY = SCALE
A
B
A : BEST FIT, SCALE < 100 M
B : BEST FIT, SCALE > 100 M
95% CONFIDENCE INTERVALS
APPARENT LONGITUDINAL DISPERSIVITY, M
10^5
10^4
10^3
10^2
10
1
10^-1
10^-2
10^-3
10^-4
APPARENT LENGTH SCALE, M
10^-2
10^-1
1
10
10^2
10^3
10^4
10^5

3. Neuman's (1990a) scaling rule is derived from apparent dispersivities calculated without information about flow or transport properties of specific heterogeneities (*fractures, channels, other pathways*), taking the advective velocity to be that of a *uniform medium*. Apparent dispersivities from calibrated numerical models increase more slowly with scale; in such models medium properties vary slowly (usually remaining constant within zones containing numerous finite difference cells) and advective velocities show corresponding large-scale fluctuations which would not show in a uniform medium. Knowledge of these large-scale property and velocity variations means that now only smaller-scale fluctuations remain uncertain, allowing the dispersivity which represents them to decrease. This demonstrates that *information has been transferred from the dispersive to the advective term* of the transport equation; the less well a site is characterized, the more crude is the description of advective velocities (and travel times) and therefore the dispersivity must increases to reflect this lack of information.

The data thus *validate the theoretical prediction* that *advection and dispersion are two sides of the same coin* and treating them as two distinct phenomena is inappropriate; dispersion is not a local medium parameter but a *non-local parameter* which depends on residence time and reflects all that is unknown about the advective field; transport models which treat dispersivity as a constant independent of information content *underestimate the uncertainty in contaminant fluxes, concentrations, and travel times.*

- CALIBRATION HELPS DEFINE SPACE-TIME VARIATIONS IN $\langle v \rangle$:

UNCALIBRATED
(UNCONDITIONAL) MODEL

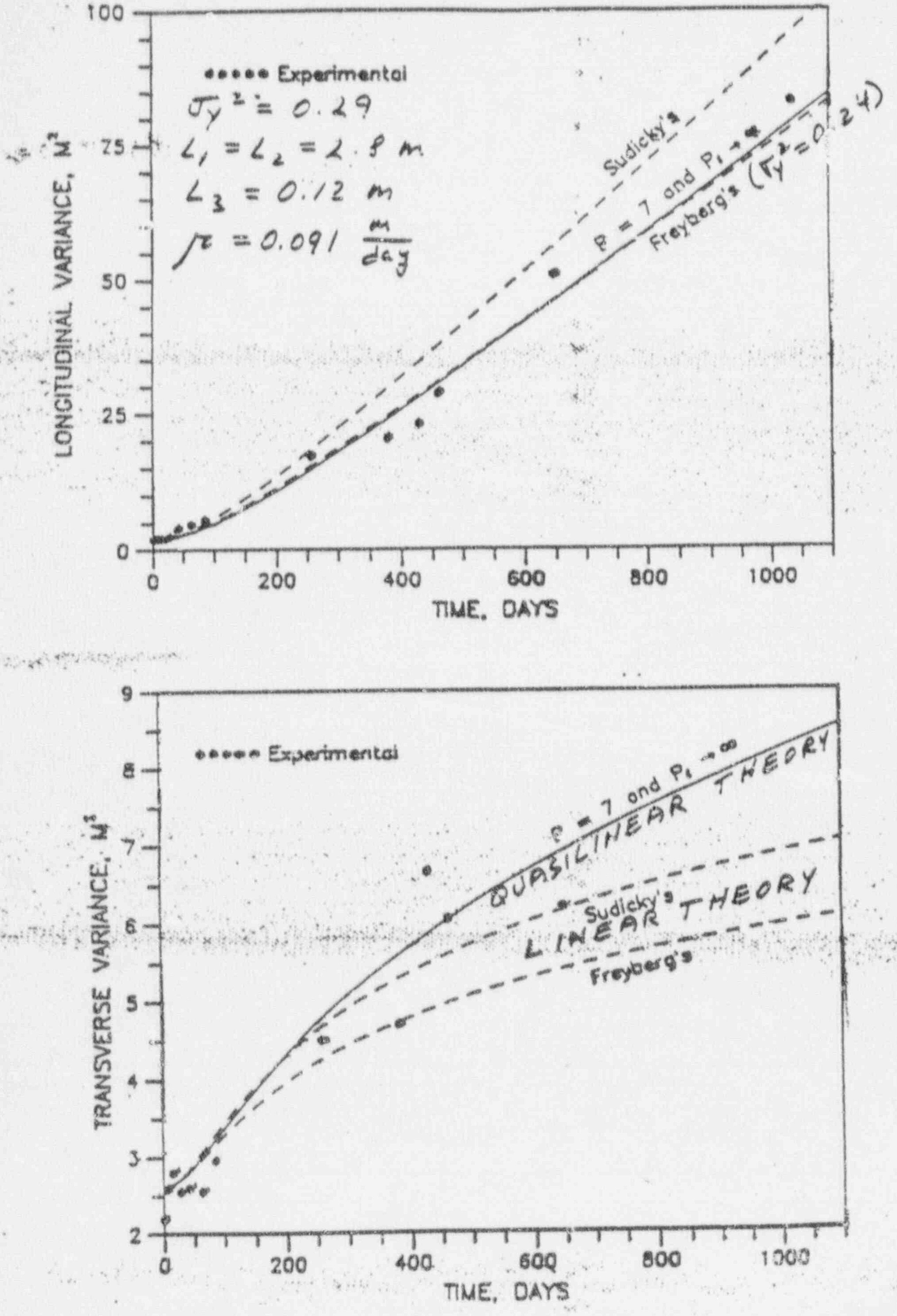
CALIBRATED
(CONDITIONED) MODEL

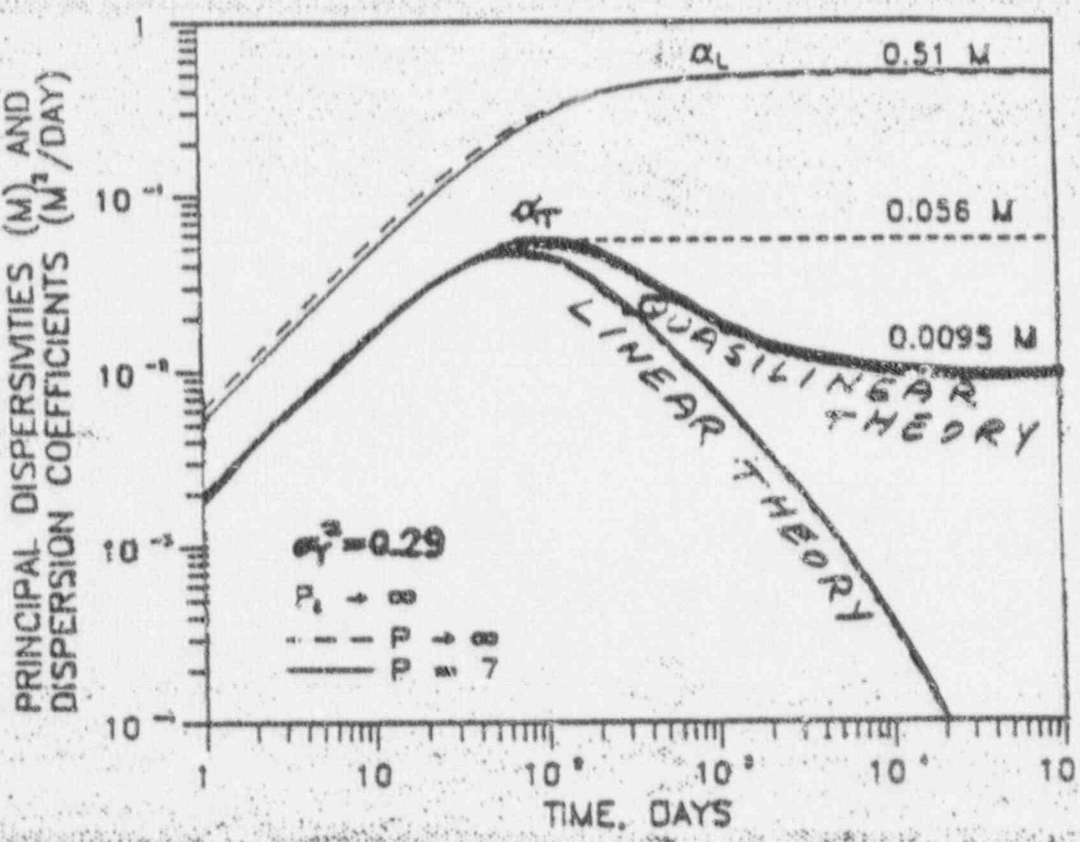
v' VARIANCE LARGE	v' VARIANCE SMALLER
v' CORRELATION SCALE LARGE	v' CORRELATION SCALE SMALLER
v' HOMOGENEOUS	v' NONHOMOGENEOUS
$\underline{\underline{D}}(t)$ RELATIVELY LARGE ACCOUNTS FOR 100% OF v VARIATION	$\underline{\underline{D}}(x,t)$ SMALLER ACCOUNTS ONLY FOR PART OF v VARIATION, THE REST BY $\langle v \rangle$

CALIBRATION IS SEEN TO AFFECT THE MAGNITUDE AND NATURE OF $\underline{\underline{D}}$, TRANSFERRING INFORMATION FROM DISPERSIVE TO ADVECTIVE TERM. (O.K. – well known)

INFORMATION CONTENT AFFECTS MODEL STRUCTURE AND PARAMETERS.

BORDEN EXPERIMENT





LONGITUDINAL SPREAD NON-FICKIAN TILL
1,000 DAYS (2.8 YEARS).

TRANSVERSE SPREAD NON-FICKIAN TILL OVER
10,000 DAYS (28 YEARS).

VALIDATION OF REPOSITORY SAFETY ASSESSMENT MODELS AND THE ROLE OF RESEARCH

For a repository to be licensed without facing a successful political and legal challenge it must meet with public acceptance and the concurrence of experts. Without a concensus among leading experts in all relevant fields about the safety of a repository there is little chance for public confidence which is a prerequisite for acceptance.

It is incorrect to assume that if a hydrogeologic environment is too complex to model with confidence it is inherently unsuitable for waste disposal. It is equally incorrect to deny the crucial role of quantitative models in repository safety assessment. Hence there is a need to insure that such models are *valid* tools for this purpose.

Should experts and the public sense a lack of firm scientific and experimental support for safety assessment calculations by the DOE or NRC, they may decide to act as intervenors and (Davis and Goodrich, 1990) "use validation as an issue in litigation against either the DOE (before a license application for construction of a repositor or the NRC (after a license is granted)."

Indeed, "the issue of validation was the basis for the decision in a court case involving the State of Ohio and the EPA (23 ERC 2091 [6th Cir. 1986]) ... the court ruled that the EPA had acted arbitrarily in using the CRSTER code ... for establishing limitations on sulfur dioxide emissions from two electric utility plants. The Court decided that the EPA had failed to establish the accuracy or trustworthiness of the model as compared with the actual discharge from the plants. In other words, the EPA did not perform a site-specific validation of the model."

The Arizona Daily Star, October 27, 1990, p. 5B: "A Phoenix-area citizens group said yesterday that it found major flaws in proposed permits for Ensco Inc.'s hazardous-waste incinerators near Mobile ... Hausen said the state estimated the cancer risk with a set of computer models based on unvalidated assumptions. "It's an inexact science ... there are a lot of unknowns ... even an EPA researcher says it will take 20 years of field data to validate, or refute, the models - that's too risky for us."

As (J.-P. Olivier, OECD/NEA, GEOVAL-90) "there are at least two decades ... ahead of us before the first high-level waste repositories become operational," the DOE and NRC should act immediately and vigorously to pursue both short-term and long-range scientific research goals in support of model validation.

The Ohio-EPA court case implies that in addition to supporting safety assessments by firm scientific theory and evidence in a generic sense (through *generic validation*), one must further prove that these scientifically sound models in fact apply to the site in question (through *site-specific validation*). Generic validation is a prerequisite for site-specific validation but the latter depends further on the information content of data describing the particular site in question.

DOE October 1989 Draft Validation Methodology for PA Models identifies the three key elements of such validation as "1) a record of model development; 2) a description of the laboratory and field investigations and the resulting data supporting the development of the model; and 3) technical reviews." Their validation "methodology is essentially an attempt to document the scientific method." The draft says little about how "the scientific method" is to be pursued in the context of validation. While proper documentation is important, it in itself does not constitute validation.

The Role of Positive Evidence in Validation

Model validation is equivalent to the testing of a scientific theory by requiring ample positive evidence that the model or theory are correct and "work," *i.e.*, that they have met with repeated successes in explaining and reproducing pertinent observations and experimental data.

Kuhn (1970) points out that Popper (1959) "denies the existence of any verification procedure at all. Instead, he emphasizes the importance of falsification, i.e., of the test that, because its outcome is negative, necessitates the rejection of an established theory." This negativist attitude does not appear conducive to the creation of a concensus among relevant experts that a proposed geologic repository is safe, as would appear necessary for public acceptance.

Kuhn counters Popper by noting that "If any and every failure to fit [theory and data] were ground for theory rejection, all theories ought to be rejected at all times. On the other hand, if only severe failure to fit justifies theory rejection, then the Popperians will require some criterion of 'improbabilty' or of 'degree of falsification.' In developing one they will almost certainly encounter the same ... difficulties that ha[ve] haunted the advocates of various probabilistic verification theories ... probabilistic theories disguise the verification situation as much as they illuminate it."

Kuhn (1970) does not deny the need for falsification through the exposure of "anomalies" that cannot be explained with existing theories or models, nor does he reject the role of probabilistic methods in validation. Instead, he requires a combination of negative evidence that the existing theory or model fail to explain and/or reproduce an observed anomaly, and positive evidence that a new theory or model can do so *better*, leading to the adoption of the new theory or model by the majority of scientists as valid.

In Kuhn's opinion, "it makes little sense to suggest that verification is establishing the agreement of fact with theory. All historically significant theories have agreed with the facts, but only more or less." However, "it makes a great deal of sense to ask which of two actual and competing theories fits the facts *better*."

One way to answer the latter question is by means of model identification criteria based on likelihood concepts such as those used by Carrera and Neuman (1986) to select between alternative heterogeneity patterns in a given aquifer flow model, by Samper and Neuman (1989) to select between alternative spatial covariance structures of hydrochemical and isotope data from the Madrid Basin in Spain, and by Carrera and coworkers to formally test the justification for including matrix diffusion and other phenomena in models of transport to reproduce laboratory data from Harwell in England under INTRAVAL Case 1.

Kuhn (1970): "Few philosophers of science still seek absolute criteria for the verification of scientific theories. Noting that no theory can ever be exposed to all possible relevant tests, they ask not whether a theory has been verified but rather about its probability in the light of the evidence that actually exists."

The broader is the available data base used to support a theory or model, the more are experts willing to accept this theory or model as being valid. However, no matter how broad this base may be, there always is a possibility that new observations or experiments may become available which the existing theory or model can neither reproduce nor explain. Such observations or experiments constitute surprises to those whose frame of mind is set by the currently accepted theory or model; the latter theories and models clearly cannot predict surprises and, therefore, must not be used for extrapolation outside their established domain of validation. A scientific concensus is thus necessary but not sufficient for validation.

When the body of such new observations and experiments becomes weighty enough to cast doubt on the validity of the existing theory or model, attempts are made to modify or replace them by a new theory or model which possess a broader range of validity. This is presently happening to fundamental theoretical and modeling concepts related to fluid flow and contaminant transport in complex geologic media.

There are numerous attempts to replace the established theoretical framework of hydrogeology in strongly heterogeneous media with a new one. There is an urgent need to confirm or deny (through "confirmatory research") many of the key new concepts (*discrete fracture models, stochastic continuum models, channel models, effective flow and transport parameters, pseudofunctions for unsaturated flow, scaling ideas*) by conducting large-scale, long-term field experiments of the kind presently carried out or planned by some participants of INTRAVAL.

Some existing theories and models which make up components of current PA models are expected by leading groundwater scientists to fail when applied outside their experimentally established range of validity. This should make the DOE and NRC extremely cautious whith PA models which rely on extrapolation into untested medium, process, parameter, space, or time domains for which there is no *experimental frame of reference*. Such models have a high chance of being rejected as unreliable by at least some relevant experts, which in turn may shake public confidence in the safety assessment process to a sufficient degree so that public acceptance is compromised.

Near-Field versus Far-Field Model Validation and the Concept of Robustness

McCombie *et al.* (1990) consider the NAGRA model of the [saturated] near-field to be relatively *robust* in providing "confidence that the results are either correct ... or ... overpredict detriment" so that "any errors either will have little effect on performance or will be on the conservative side ... A robust model would be a simulation of well-understood processes in which the required databases are well defined."

"Critical ... is that the overall repository performance (as measured by a global parameter like release or dose) is relatively insensitive to, or is demonstrably[!] conservative in the case of, variations in the conceptual model framework or individual parameters within established ranges. This second condition means that performance assessment predictions with large uncertainties can be acceptable provided that the band of results lie well below defined targets. A robust model with no excessive demands on validation results from a combination of a simple system [not simple model!] with large reserves of performance and a conservative approach to choice of models and data."

The repository can be "design[ed] for robustness by lowering waste loadings or increasing storage times before disposal."

McCombie *et al.* conclude that "With limited requirements on the host rock" one should "be able to sufficiently validate an appropriate near-field release model" in saturated environments.

Far-field transport models are "less robust" and "defining even the initial characteristics and boundary conditions ... for a far-field model is inherently more difficult and uncertain than in the near-field case." Such models are highly sensitive "to parameter/conceptual model variations [which] minimises the safety reserves involved and hence its robustness. Validation is inherently more difficult ... A specific problem is the distance scales considered ... The near field covers a volume small enough to be well characterized in the actual system or in appropriate analogues. The far field is so extensive that it is more difficult to achieve sufficient data 'density'."

Niederer (1990) agrees that "There is very little experience with processes ... in the deep underground ... not sufficient to create ... concensus on the relevant models." Validation "is particularly important for ... models of geospheric migration because scientific experience with the deep underground is scarce."

Eisenberg (1990) adds that "the time periods for the application of repository performance assessment models are so long ... that direct comparison of system performance with model prediction cannot be accomplished; therefore, the inductive approach to model validation is inapplicable ... the site geology, geochemistry, hydrology, rock mechanics, etc. are aspects of a highly complex, heterogeneous natural system ... the behavior of the system can only be observed inferentially and only at a finite number of measuring points in space and time. These limitations apply to both the boundary observables and to the much more difficult-to-obtain interior structure and behavior. The inability to confirm the interior structure of the system or to confirm the processes relating such structures to each other and to system performance, severely limits the degree to which validation can be carried out ... The state-of-the-art of scientific theory for various aspects of performance assessment modeling are not advanced enough to assure a basis of a priori knowledge sufficient to produce valid models by deductive reasoning."

This underlines (McCombie *et al.*, 1990) "the importance of the use of realistic models" based on sound scientific principles and warns that oversimplified PA models based on deductive reasoning may lack validity.

Performance Assessment of Engineered Versus Natural Repository System Components

PA is a useful concept when applied to the design of man-made systems such as nuclear reactors and engineered portions of a repository. The inclusion of a non-engineered geologic environment in the definition of a repository system for the purpose of PA has no precedence in engineering practice and poses the single most difficult challenge for safety assessement.

The geologic environment is part of nature which man can *integrate* into an engineered system but one which man cannot *design*; it is neither man-made nor does it *perform* to man's specifications. Hence PA as commonly applied in engineering practice does not strictly apply to it. Such application has allowed modelers to adopt the misleading notion that mathematical and systems analytical concepts which have been tested (with partial success) in the context of engineering PA (say in the area of nuclear reactors) are transferable to the analysis of environmental response. Such transferability has not been demonstrated and there is little hope that it will be in the future.

Groundwater flow and transport models have never been validated against observed or experimental behavior of the natural system over time spans longer than a few years (maximum decades) and spatial scales larger than a few hundred meters (maximum a kilometer or two, both in highly permeable unfractured aquifers and subject to considerable debate). Models of groundwater flow and transport in unsaturated porous soils have never been validated on time scales exceeding a few weeks (at best months) or spatial scales exceeding a few tens of centimeters (at best meters). Models of groundwater flow and transport in unsaturated fractured tuffs have never been validated at all.

Some current DOE and NRC research effort is directed toward developing such models and validating them on extremely modest temporal and spatial scales. There is virtually nothing to indicate that the best available models can be relied on to simulate groundwater flow and transport on spatial and temporal scales relevant to repository PA within a specified margin of error (or at a given level of statistical confidence).

Hydrogeologic models relevant to Yucca Mountain will probably never be validated on any but relatively modest spatial and temporal scales. Can anything be done so experts and the public become convinced that geologic disposal of spent fuel and high level radioactive wastes is safe?

Role of Geosphere Flow and Transport Research in Validation

Relying too heavily on engineered barriers at the expense of the host rock in safety assessment may defeat the very purpose, or *raison d'être*, of a deep geologic repository. The geology must bear a good share of responsibility (given considerable credit) for waste isolation otherwise the concept of deep geological disposal may lack both rational and economic justification.

What strategy then must the DOE and NRC adopt to help resolve the difficulty in validating (*i.e.*, rendering credible) the geosphere components of safety assessment models? I agree with Niederer (1990), Olivier (1990), and Eisenberg (1990) that "the main reliance of validation should be on *scientific substance* and logical rigor," in this order. Though it is neither possible nor necessary (McCombie *et al.*, 1990) "to aim for 'absolute truth' or for perfect accuracy ... the best possible understanding of system behavior and a realistic modelling of important processes involved should ... always be aimed at."

The only way that scientific substance can be improved is through a well-funded, vigorous and rigorous research program which gradually expands the domain of present knowledge in areas critical to model validation, primarily geosphere flow and transport where scientific concensus seems most lacking.

The primary focus of DOE and NRC research should be on experimental and theoretical issues related to safety assessment on which expert concensus is presently lacking. Such studies may confirm or deny the validity of current performance assesment models or some of their key components, hence they fall well within the purview of NRC "confirmatory research." However, many outstanding issues are so fundamental that no resolution can realistically be expected without a much greater allotment of talent, time and money than is presently the case in the U.S. Without pursuing a more vigorous effort to resolve these issues, there is little hope for a concensus among hydrogeologists and groundwater scientists that current models of flow and transport in fractured tuffs, not to speak particularly of Yucca Mountain, are reliable. Without such a concensus, there is little hope for public confidence and therefore a greatly reduced prospect for defensible licensing.

A major prerequisite for public acceptance of government decisions about a high-level repository is that the agencies can back them with demonstrably excellent science and technology; a mature public may support such decisions even in the face of unresolvable uncertainties, duly acknowledged. The same public may be justified in rejecting such decisions if they are based on less than what the best science and technology of the day could potentially deliver given adequate government support and encouragement.

The notion that DOE and NRC research on geosphere flow and transport should be driven by needs perceived on the basis of performance assessment models is highly problematic. It is true that certain performance measures, when calculated on the basis of existing PA models, may appear robust by being insensitive to some processes or parameters built into these models. This, however, should not be sufficient ground for the dismissal of such processes and parameters as unimportant or undeserving of serious research.

First, performance measures may change in the future due to a re-evaluation of, or challenges to, current rules (groundwater travel-time is a highly ambiguous performance measure which is being justly criticized as lacking in scientific rationale).

Second, unless the processes and parameters in question are well understood and the corresponding components of the PA model have been properly validated, one cannot be sure that the implied robustness or lack of sensitivity is not merely the result of a misconception on the part of the modeler. One such common misconception is that cumulative release to the accessible environment is insensitive to radionuclide dispersion in the host rock and hence the process of dispersion need not be seriously researched.

Instead of subordinating research on geosphere flow and transport to licensing needs perceived on the basis of PA models, the case of model validation (and hence licensing) would be better served if such research was to progress toward long-term scientific goals in a relatively independent manner.

Geosphere flow and transport do not qualify as engineering problems for which tangible "solutions" can be expected within a predetermined time frame to satisfy licensing User Needs; rather, they are geoscience problems which one can study but not solve. Possible (but not inevitable) byproducts of such a study may include improved laboratory and field methods, analytical tools, and computational models.

The new DOE plan to delay repository operations to the year 2010 provides an opportunity for the DOE and NRC to seriously pursue such long-term research goals, and a good prospect for this research to be translated into tangible products within a similar time frame. Regardless of whether or not such tangible products are in fact obtained, the important thing to agree upon is that the primary goal of geosphere model validation must be the resolution, through long-term research, of fundamental issues which hamper concensus among scientists about the nature and quantification of geosphere flow and transport phenomena.