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U.S NUCLEAR REGULATORY COMMISSION
DIVISION OF WASTE MANAGEMENT

TRIP REPORT
NRC/CONTRACTOR MEETING
UNCERTAINTY IN HYDROGEOLOGIC EVALUATIONS
SILVER SPRING, MARYLAND
NOVEMBER 4-5, 1986

TECHNICAL ASSISTANCE IN HYDROGEOLOGY
PROJECT B - ANALYSIS
RS-NMS-85-009

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Technical Assistance in
Hydrogeology

NUCLEAR WASTE CONSULTANTS INC.

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Enclosure to
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November 19, 1986

009/N.5/.003
RS-NMS-85-009
Communication No. 111

U.S. Nuclear Regulatory Commission
Division of Waste Management
Geotechnical Branch
MS 623-SS
Washington, DC 20555

Attention: Mr. Jeff Pohle, Project Officer
Technical Assistance in Hydrogeology - Project B (RS-NMS-85-009)

Re: Trip Report - NRC/Contractor Meeting on Uncertainty in Hydrogeologic Evaluations of the Groundwater Travel Time Performance Objective

Dear Mr. Pohle:

This letter serves as the Nuclear Waste Consultants' (NWC) trip report for the NRC/Contractor meeting on Uncertainty in Hydrogeologic Evaluations of the Groundwater Travel Time Performance Objective, held at the Sheraton Potomac Hotel, Rockville, Maryland, November 4-5, 1986. Nuclear Waste Consultants' team was represented by Messrs. Adrian Brown and Mark Logsdon (NWC), Dr. David McWhorter (Water, Waste, and Land), and Dr. Daniel Stephens (Daniel B. Stephens and Associates), as requested by the NRC Project Officer. NWC considers that this meeting and the work that is anticipated to flow from it will be accountable under Task 5 of the current contract.

The purpose of the meeting was to develop a plan for the hydrogeology Technical Assistance contractors to prepare four topical reports related to different aspects of uncertainty relative to predicting groundwater travel time (GWTT). The four general areas are:

- o Sources of Uncertainty
- o Treating Uncertainty
- o Addressing Uncertainty in Testing
- o Addressing Uncertainty in Analyzing and Predicting GWTT.

The four topical reports are intended to support the NRC Staff's development of a final Generic Technical Position on Groundwater Travel Time. An annotated copy of the meeting agenda is attached (Attachment 1). Copies of the NWC Team's view-graphs and the Daniel B. Stephens and Associates' proposal to NWC concerning a numerical experiment (discussed at the meeting by Dr. Stephens) are presented as Attachment 2.

Following initial comments and direction from Mr. J. Pohle and Dr. T. Verma (NRC), the three principal contractor teams made presentations addressing the topics outlined on the agenda. All of the agenda items were covered in substantial detail during the two-day meeting, with ample time for questions and discussion from the floor, including from the large NRC Staff contingent. It is clear that there are differences in perspective and experience within and between the different contractor groups (as within and between the Staff and the contractors) that should go a long way towards assuring that the key technical concerns related to uncertainty are fully ventilated in the process of developing the topical reports.

At the conclusion of the contractor presentations and the team discussions, Mr. Pohle identified assignments and schedules for the topical reports. For each of the four topical reports, lead responsibility has been assigned to one of the two lead TA contractors, with the stipulation that the reports be developed as a team production between contractors. The topics, lead responsibilities, and tentative schedule for completion of the initial milestone (the development of detailed outlines) are as follows:

<u>TOPIC</u>	<u>LEAD CONTRACTOR</u>	<u>DATE FOR OUTLINE</u>
Sources of Uncertainty	Williams & Associates	11/24/86
Treating Uncertainty	NWC	2/13/87
Addressing Uncertainty in Testing	Williams & Associates	2/27/86
Addressing Uncertainty in Analyzing and Predicting GWTT	NWC	3/6/87

Mr. Pohle intends that all four topical reports will be completed by May 22, 1987, in order to fully support the Staff's GTP on GWTT, tentatively scheduled for finalization in mid-summer, 1987. Mr. Pohle indicated that he would provide formal documentation and written direction of these instructions in the very near future.

November 12, 1986

Staff of NWC and Williams and Associates have already met to discuss the implementation of the "Team Production" concept, and the two contractors anticipate working group sessions beginning this month on the Treating Uncertainty topic. NWC is confident that this new direction from the NRC Staff can be fully accommodated within the framework of the current contract and its deliverables.

If you have any questions about this trip report, please contact me immediately.

Respectfully submitted,
NUCLEAR WASTE CONSULTANTS, INC.

Mark J. Logsdon

Mark J. Logsdon, Project Manager

Att: Trip Report on Uncertainty Meeting, November 4-5, 1986

cc: US NRC - Director, NMSS (ATTN PSB)
DWM (ATTN Division Director)
Mary Little, Contract Administrator
WMGT (ATTN Branch Chief)

cc: M. Galloway, TTI
L. Davis, WWL
J. Minier, DBS

ATTACHMENT 1

Dave. 148

Mark Logsdon
NWC
11/4/86

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OCT 30 1986

AGENDA

UNCERTAINTY IN HYDROGEOLOGY RELATIVE TO PREDICTING GROUNDWATER TRAVEL TIME

WMGT/NMSS

November 4 and 5, 1986

Sheraton Potomac, Rockville, MD

1. Purpose: To plan and direct TA contractor efforts in preparing topical reports on uncertainty dealing with its sources, treatment, subsequent testing and analysis for uncertainty in making predictions of groundwater travel time. This activity supports preparation of a final generic technical position on groundwater travel time, a major milestone in the process of resolving the compliance demonstration issue on groundwater travel time.

2. Participants: NRC

✓ M. Groves
✓ J. Trapp
✓ J. Liggett (SPL)
✓ Mclartin } RES
✓ Cherry
✓ Kunkel }
✓

✓

J. Verma
J. Pohle
F. Ross
D. Codell
N. Coleman
M. Weber
A. Elzeftawy
M. Fliegel

Williams And Associates

R. Williams
K. Steinhorst
G. Winter
D. Ralston
S. Miller

NWC

A. Brown
M. Logsdon
D. Stevens
D. McWhorter
J. Yeh

3. Agenda Items:

Tuesday, Nov. 4

- A. 0900 - Introduction/Pohle
- B. 0930 - Direction in FY 87/Pohle - 5 year plan
- C. 1000 - Working interpretation of GWTT/Verma-Codell
- D. 1130 - Lunch
- E. 1300 - Sources Of Uncertainty/W&A
- F. 1330 - Sources Of Uncertainty/NWC
- G. 1400 - Sources Of Uncertainty/Sandia
- H. 1430 - Break
- I. 1500 - Treating Uncertainty/W&A

Discussion

I AMM

GWTT

- What Pathology?
- Classification
- Encapsulation
- Festest
- Uncertainty
 - Sources
 - Treatment
 - Testing
 - Analysis
- Alternative GWTT Bases
- Siting Criteria

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DATE : 86/10/27	:	:	:	:	:	:	:

11/5/86

- J. 1530 - Treating Uncertainty/NWC
- K. 1600 - Treating Uncertainty/Sandia
- L. 1630 - Open Discussion
- M. 1700 - Adjourn First Day

Wednesday, Nov. 5

- A. 0900 - Addressing Uncertainty In Testing/W&A
- B. 0930 - Addressing Uncertainty in Testing/NWC
- C. 1000 - Break
- D. 1030 - Addressing Uncertainty in Testing/Sandia
- E. 1100 - Discussion
- F. 1130 - Lunch
- G. 1300 - Addressing Uncertainty In Analyzing and Predicting GWTT/W&A
- H. 1330 - Addressing Uncertainty In Analyzing and Predicting GWTT/NWC
- I. 1400 - Addressing Uncertainty In Analyzing and Predicting GWTT/Sandia
- J. 1430 - Break
- K. 1500 - Discussion
- L. 1630 - Assignments/Schedules
- M. 1700 - Adjourn

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ATTACHMENT 2

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**ANALYSIS OF UNCERTAINTY IN PREDICTION OF
TRAVEL PATH AND TRAVEL TIME**

by

JIM YEH AND DANIEL B. STEPHENS & ASSOCIATES, INC.



DANIEL B. STEPHENS & ASSOCIATES, INC.
CONSULTANTS IN GROUND-WATER HYDROLOGY

REF ID: A
SEP 11 1986

• GROUND-WATER CONTAMINATION • UNSATURATED ZONE INVESTIGATIONS • WATER SUPPLY DEVELOPMENT •

September 9, 1986

Mr. Mark Logsdon
Nuclear Waste Consultants, Inc.
8341 S. Sangre de Cristo Road
#14
Littleton, CO 80127

Dear Mark:

Enclosed is a copy of a work plan which we believe may be useful to address uncertainty in travel time and radionuclide flux. The concepts were developed principally by Jim Yeh. As you know Jim has an excellent background in both numerical modeling and stochastic analysis. In fact, he teaches courses in stochastic methods and ground water hydraulics at Arizona, and he also has research in these areas supported by the NSF. I regard Jim as one of only a small group of hydrologists who has an excellent working-knowledge of uncertainty as it relates to hydrogeologic variability. If the proposal work is requested by you and the NRC, Jim would be the lead man on our team providing the theoretical guidance to our staff, whereas I would be responsible for the overall technical direction and provide the hydrogeological perspective.

I believe an NRC workshop on this subject would be an excellent idea. It would be critical to the success of such a workshop to bring in people who work directly in this field such as Lynn Gelhar, Al Gutjahr, Les Smith, Shlomo Neuman, Al Freeze, Chris Duffy, and Jim Yeh, etc.

Please give us your comments to this proposal when convenient.

Yours truly,

D.B. Stephens, cmc
Daniel B. Stephens, Ph.D.
President

DBS/cmc

Enclosure

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SUMMARY

The characteristics of ground-water travel time or radionuclide flux from a nuclear waste repository are mainly determined by the hydraulic properties of the geologic environment. The hydraulic properties exhibit considerable spatial variation. Because only limited amounts of field data are available, there is considerable uncertainty in any characterization of the hydraulic properties of the subsurface environment. This uncertainty is the factor that dictates a probabilistic approach to decision-making; if our knowledge of the hydraulic properties were perfect, deterministic simulations would be appropriate.

We propose to investigate the importance of using a stochastic approach to characterize the uncertainty in the prediction of ground-water travel time and radionuclide flux. Monte Carlo and conditional simulation techniques will be used to investigate the sensitivity of the uncertainties to the parameters characterizing the spatial variability. The result of the investigation will help us to address the data needs in the context of the NRC's regulatory responsibilities. For example, we will attempt to determine what parameters should be measured, what data density is needed to adequately characterize the uncertainties in ground-water travel time and radionuclide flux, where parameters should be measured and over what scale they should be

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determined to reduce the uncertainties. Comparisons between the deterministic and stochastic methods of analysis will be at the heart of our presentation of results.

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INTRODUCTION

The U.S. Nuclear Regulatory Commission (NRC) has established regulations pertaining to the underground disposal of high level radioactive waste, in the code of Federal Regulations, Title 10, Chapter 1, Part 60 (10 CFR 60). According to paragraph 122 of the regulations, the favorable waste disposal site will have a pre-waste-emplacement ground-water travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment that substantially exceeds 1000 years. Predicting impacts of the waste disposal on ground-water resources and its users is one of the crucial elements of the regulation. The reliability of the prediction of the impact to ground water is dependent in part upon the accuracy with which the geologic environment can be characterized. The NRC is also proposing to adopt regulations of the US Environmental Protection Agency (40CFR191) which establish thresholds for allowable cumulative releases of radionuclides to the accessible environment (an area within 5 km of the emplaced waste). In 10CFR 60.112 the NRC is proposing the following language: "The geologic setting shall be selected, so that for 10,000 years following permanent closure, cumulative releases of radionuclides to the accessible environment ...have a likelihood of less than one chance in 10 of exceeding the quantities calculated in

accordance with (paragraph) 60.115." The NRC and EPA regulations to protect ground water cited above require predictions of ground-water travel time and concentrations of radionuclides. It is clear from the regulations that an element of uncertainty is recognized to be inherent in the prediction.

There are many sources of uncertainty in these predictions. These sources are: inappropriate conceptual representation of true responses of aquifers, errors in computation due to roundoff associated with digital computation and due to numerical approximation of the governing partial differential equations for ground-water flow and transport, uncertainty due to data collection and estimation, and the uncertainty in characterizing the hydrologic properties of the field site. The uncertainty associated with models and computational aspects have been adequately addressed in the literature and ground-water textbooks. The uncertainty due to error in collection and calculation of hydrologic properties in general usually can be controlled and reduced to a minimum. The remainder is the uncertainty in characterizing the hydrogeologic properties in the field site. This uncertainty arises from the fact that only a limited amount of field measurements are available and the fact that the hydrogeologic proper-

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ties of the formations vary spatially. Therefore, we, hydrogeologists, are facing many questions such as how much confidence do we have in our predictions? How much data is necessary to make the predictions with the required degree of confidence? How does the location of the data collection points, the spacing between points, and the scale of test used to make the measurement affect the uncertainty in the predictions? Answers to these questions relate not only to the regulations, but also to the design of a field data collection program - the site characterization plan. Answers to these questions are difficult and have only begun to receive attention from researchers in about the past decade. These researchers have recognized that geologic environments are highly heterogeneous, and some describe the spatial variability using stochastic methods. Most hydrologists tend to utilize deterministic approaches to calculate groundwater travel time and transport. However, with a deterministic approach the hydrogeologic parameters are assumed to be perfectly known everywhere, and therefore, there is no uncertainty which can be determined. Unfortunately, hydrogeologic parameters cannot be determined everywhere in the system, thus there is uncertainty in the hydrogeologic characteristics of the system. An approach to quantify uncertainty in ground-water travel time or solute transport due to parameter variability has not been clearly

established. There have been no sufficiently well-documented field-scale experiments completed to date which allow us to verify any specific approach.

Spatial variability of hydrologic properties in aquifers has long been recognized. Due to difficulties in characterizing the variability in terms of deterministic functions, statistics are commonly used. Generally, the hydraulic conductivity values exhibit a log-normal distribution and the standard deviation of hydraulic conductivities can be very large (Freeze, 1975). For example, Byers and Stephens (1983) found a large degree of variation in hydraulic conductivity in a small fluvial sand area that would generally be assumed homogeneous. However, the variation in hydraulic conductivity values is not entirely random in space. The values tend to correlate over a large distance (Bakr, 1976; Smith, 1980; Russo and Bresler, 1981; and Vieira et al, 1982 and others). In other words, the hydraulic conductivity values tend to be similar at adjacent sampling locations and the similarity decreases as the sampling distance increases. The distance beyond which the hydraulic conductivity values are no longer correlated is called the correlation scale. This spatial correlation structure is directly related to the size of stratifications or laminations of sediments (Byers and Stephens, 1983).

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Classical deterministic analyses of flow and solute transport through heterogeneous aquifers either employ an equivalent homogeneous porous medium concept or discretize the aquifers into zones or layers of different hydraulic conductivity values based on a limited amount of field data. Each zone or layer is usually assumed to be homogeneous. The results of the analysis are subject to uncertainty, because of a limited number of tests to adequately represent the domain, and because it is not certain whether the scale of the field measurement is consistent with the size of the discretized zones used in the model.

Consider an area of 5 km radius which is defined as the distance to the accessible environment in the EPA standard and NRC regulation. It may be necessary to collect thousands or millions of samples of hydrologic properties at a small scale within the geologic formations in order to accurately predict the ground-water travel time throughout this radius with a very high degree of confidence, if a deterministic approach is used to model flow in a spatially varying hydrogeologic setting. Obviously, such a detailed characterization of the site is of little practical interest. Alternatively, one may argue that tests of hydraulic properties over a scale of kilometers may integrate the heterogeneities so that the single composite value (mean or effective hydraulic conductivity) is that which

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should be used in the deterministic model. However, field tests (for instance, tracer tests) at this scale are impractical.

On the other hand, some hydrogeologists recognize the fact that due to the small scale of most of our measurements spatial variability of hydrologic properties exists, but is subject to uncertainty. To deal with the uncertainty in hydrologic property values, they treat the properties as stochastic processes characterized by their joint probability density functions. (Note that the spatial variability, itself, is deterministic if we can measure the hydrologic properties at every part of the aquifer.) To ensure mass conservation and other physical principles, they utilize deterministic partial differential equations for flow and transport to predict the behavior of the aquifer. For example, let us examine the travel path of a particle released from the waste site in a heterogeneous aquifer to the accessible environment. We might have hydraulic conductivity and porosity measurements at some locations within the aquifer but for making predictions of travel path we have to "guess" the values of these properties at locations where no samples were taken. Thus, the aquifer that we are dealing with is no longer a deterministic one. If the parameters are not measured everywhere, we may want to make numerous predictions based on various possible combinations of parameters. The path of the

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particle calculated from the governing equations in each trial certainly is different. Therefore, the predicted particle travel time through this heterogeneous aquifer is no longer a single value but a random variable characterized by its probability density function. Thus, the likelihood that the particle reaches the accessible environment within a certain time-frame is addressed.

Certainly, the travel time distribution depends on the joint probability functions of the hydrologic properties. Generally, the joint probability density function of a stochastic process can be characterized by the mean, variance, and correlation function. However, in order to employ the stochastic approach, one has to assume that these statistical parameters can be accurately estimated from a subset of the entire aquifer under consideration. It should be pointed out that if an accurate estimate of these statistical parameters requires as many data as in an accurate deterministic approach, then there is no need to use any stochastic approach.

This report is a pre-proposal for consideration by the NRC. In it we outline numerical experiments which we believe will be useful for a) evaluating the importance of characterizing heterogeneity in hydrogeologic parameters, and b) guiding data collection efforts to minimize uncertainty in predicting ground-water travel time and cumulative radionuclide releases to

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the accessible environment.

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SUMMARY OF LITERATURE

Various stochastic approaches have been used to analyze ground-water flow and contaminant movement in heterogeneous and saturated porous media. Types of stochastic methods used include the spectral method (Gelhar, 1976; Bakr et al., 1978; Gutjahr et al., 1978; Mizell et al., 1982; Gelhar and Axness, 1983), Monte Carlo simulation techniques (Freeze, 1975; Smith, 1978; Smith and Schwartz, 1980, 1981a, and 1981b) and those used by Dasan (1982), Simmons (1982), Tang et al., (1982), and Matheron and de Marsily (1980), and finally the conditional simulation (Delhomme ,1979). Most of the above methods of analysis have been discussed in part of a report to the NRC by Gutjahr (1986). In the following paragraphs, we will review some of these analyses which are less abstract and pertinent to the analysis of uncertainty in the prediction of ground-water travel times and radionuclide flux.

The most relevant research related to radionuclide transport uncertainties at salt sites proposed for high level waste repositories appears to be that of Smith and Schwartz (1980; 1981 a,b). They conducted computer experiments to investigate the uncertainty in prediction of mass transport in ground-water flow due to the lack of complete knowledge of spatial distribution of hydrologic properties. Hundreds of realizations of two-dimensional auto-

correlated hydraulic conductivity fields were generated. A particle tracking model was used to simulate the movement of a large number of tracer particles in each synthetic hydraulic conductivity field. They pointed out that the mass transport phenomenon is strongly controlled by the spatial structure of sediments, and that the uncertainty in model prediction can be significant.

More specifically, they found that :

(1) as the variance in hydraulic conductivity increases, the time of first arrival of tracer particles decreases (Figure 1a). Because the preferred paths through the flow domain have relatively higher conductivities for the larger value of the variance of hydraulic conductivity, the leading particles can move more quickly through the system.

(2) as the heterogeneity increases, the standard deviation in the exit time distributions also increases (Figure 1b). This increase reflects a greater uncertainty in the prediction of solute transport through these media.

(3) a greater variability in the exit times is observed as the correlation scale increases, as shown in Figure 2. This indicates the importance of considering the correlation scale in the analysis of uncertainty in the ground-water travel time and path analysis.

The importance of correlation length on ground-water travel

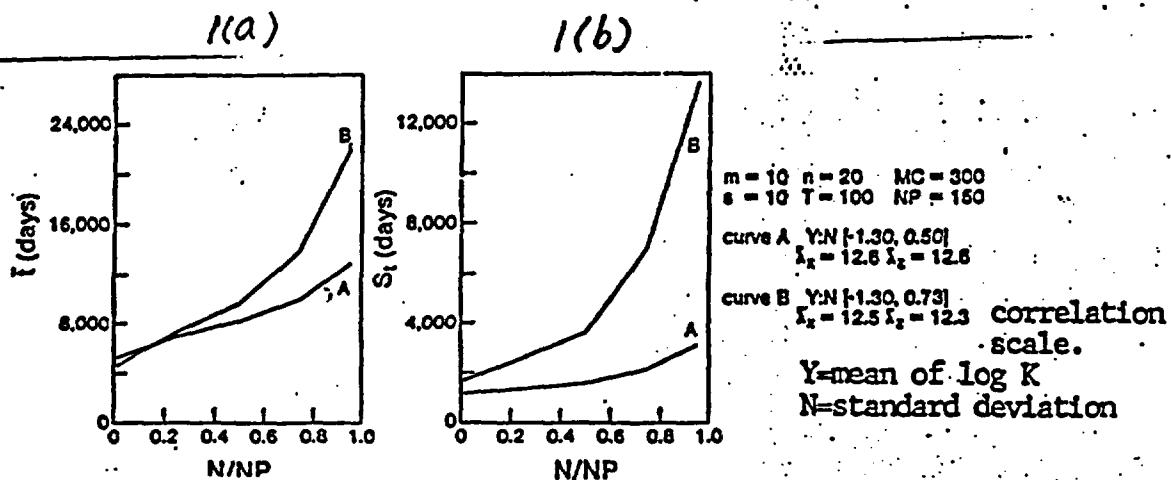


Fig. 1. Influence of the standard deviation σ in the logarithm of hydraulic conductivity on the mean time t and the standard deviation S_t for the breakthrough curve.

N/NP = relative concentration.

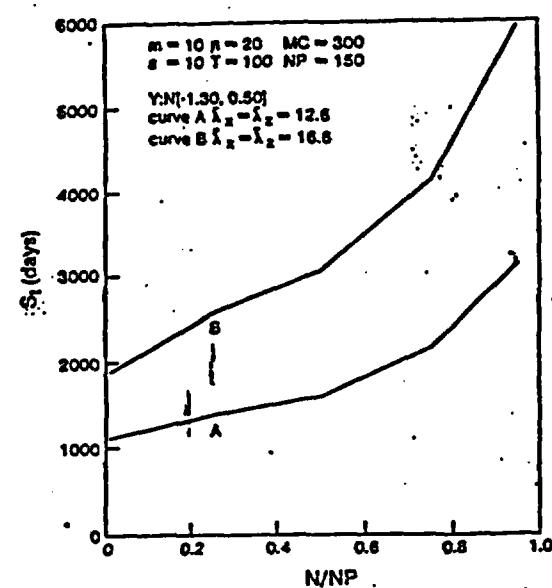


Fig. 2. Influence of larger integral scales in hydraulic conductivity on the standard deviation in the exit times for the breakthrough curve. (Smith and Schwartz, 1980)

Eliminate
 $m =$ $n =$ $MC =$
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time was also demonstrated by Clifton et al (1985), who found that the mean travel times are greater in the medium with the larger correlation scale (Figure 3).

These conclusions demonstrate the importance of considering the spatial structures of the hydraulic conductivity in the stochastic analysis of uncertainties in prediction of solute transport and ground-water travel time and path. To further address the significance of uncertainty in the data base derived from site characterization plans with respect to 10 CFR 60 and 40 CFR 191, we are proposing the scope of work which is described as below.

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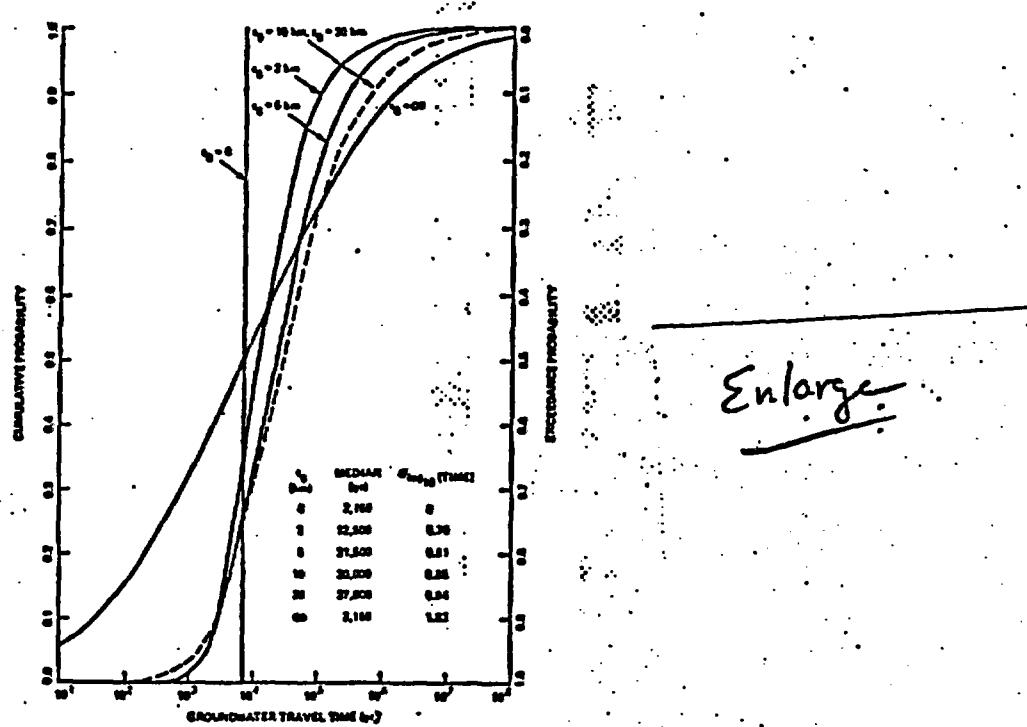


Figure 3. Distribution of Groundwater Traveltimes for Models with Different Log-Transmissivity Correlation Ranges, s_0 . (Clifton et al., 1985)
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A three phased investigation is proposed. The first is a survey and analysis of available scientific literature, the second phase includes an analysis of the importance of the spacing and scale of measurement of hydraulic properties using a deterministic approach, and the third phase pertains to the use of stochastic models in addressing uncertainty in flow and transport.

Phase 1. Literature Review, Compilation of Concepts, and Glossary

The first phase of the work plan will be a detailed review of literature on uncertainties in solute transport or ground-water travel time and path which are attributed to hydrogeologic parameters. We will critically review all the relevant scientific articles related to the analysis of uncertainties in prediction of ground-water travel time and path or in mass transport, and we will examine the significance of the findings to the NRC's waste management program. We will furnish a phase I report that clearly explains and illustrates the stochastic concept and the methods for stochastic analysis so that subsequent discussions are based upon common understanding. A glossary of the terminology in the stochastic analysis will be provided so that managers and seologists,

hydrologists and others who are not familiar with stochastic jargon may have a convenient reference tool when reviewing papers dealing with uncertainty and stochastic analysis.

Phase 2. Deterministic Simulation to Compare Travel Time in Uniform and Spatially Varying Media

The purpose of this phase is to assess the ability of using deterministic simulations to address the uncertainties in predicting groundwater travel time at a hypothetical repository site. In this phase of the task we first will assemble a hypothetical two-dimensional heterogeneous aquifer with a known variance in hydraulic conductivity values and correlation functions. For convenience, this hypothetical aquifer, rectangular in shape, will be our analog of a real-world site, in lieu of working with compiled data from a well-characterized ground-water basin. We anticipate that the rectangular flow domain will be very finely discretized at regular intervals, and it will have pairs of constant head and impermeable boundaries on opposite sides (Figure 4). The prescribed hydraulic parameters in each grid block or element could be considered analogous to measured, and therefore known, values obtained from in situ tests which sample over a space equal to the size of the grid block. (We are not addressing uncertainty due to measurement error here.) With

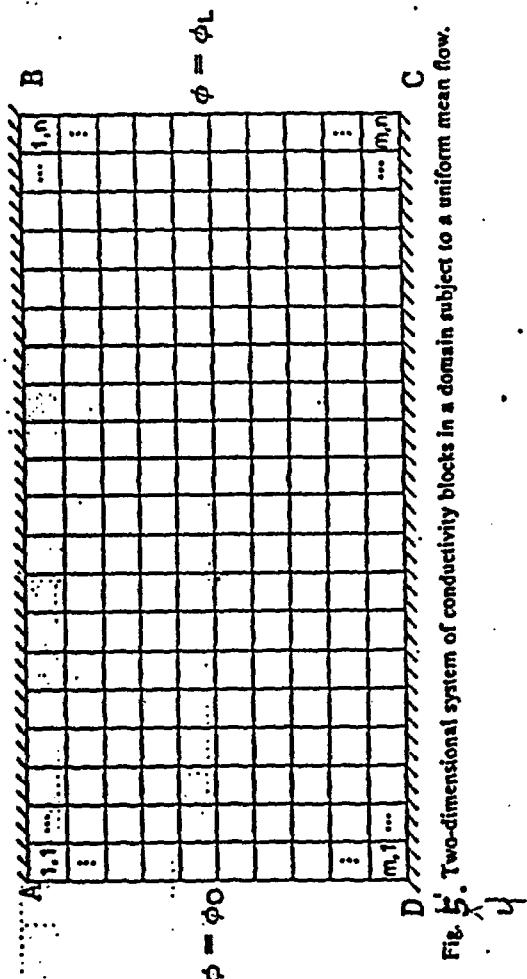


FIG 4

this hypothetical porous media, we will determine the travel times and paths of tracer particles released from the inflow constant head boundary using a numerical model of flow which conserves mass. The deterministic result will represent the ground-water travel time in an aquifer where the exact spatial distribution of the hydrologic properties is known. It will serve as a standard for numerous subsequent deterministic and stochastic analyses.

During site characterization it is unlikely that tests for hydraulic properties will be conducted at regularly spaced locations at a relative density which approaches that just described to represent the real-world analog. In fact, within the accessible environment, the test locations will probably be very sparse and somewhat random, but more densely spaced near the repository. To evaluate how many sample sites are needed to predict the travel time distribution from the real-world analog, we will select a small subset of data points from the finely discretized domain. These values of hydraulic properties will be contoured in much the same manner one might contour sparsely spaced field data. At the locations, or grid blocks, for which there are no "measured" data, parameters will be assigned by interpolation based on the contouring. These data will be used in the ground-water flow model to estimate ground-water travel time and path. Numerous repetitions of the experiment

will be conducted using different numbers of samples and locations where field data might be obtained during site characterization of the hypothetical aquifer. The results of this analysis, when compared to results from the assumed-real data base, will allow us to assess the feasibility of using only a few measured data to reproduce the ground-water travel time determined for the real-world analog. We will also investigate the number of samples required to reproduce the result obtained with the assumed complete data set. We believe this analysis will be relevant to the field sampling design in the site characterization plans for the repository site.

Another important aspect of uncertainty associated with evaluating data needs for flow and transport predictive models, pertains to the importance of the scale of parameter measurement. From a practical viewpoint alone, one may easily argue that a few large-scale tests are a better alternative to a very large number of local scale tests to characterize a repository. However, is there a significant difference in results of ground-water travel time distributions using the different data bases? Starting from the very finely discretized domain representative of our real-world analog, we will run simulations in which we will sequentially increase the size of the finite difference or finite element blocks in the flow model so that the hydraulic

conductivity value in each block represents an average value of several smaller blocks used in the previous analysis. The final case will be one in which all the heterogeneities are integrated into a single value using some effective mean of all the data from the finely discretized real-world analog. The ground-water travel time calculated using these average values will, then, be compared to the results from the hypothetical aquifer.

Phase 3. Stochastic Analysis of Flow and Transport and Implications for Site Characterization Plans

The objective of Phase 3 is to investigate the relevance of using a stochastic approach to address uncertainties in predicting ground-water travel time and solute transport. From the results of this analysis, we will be able to determine the data needs for assessing the uncertainties. The results of the analysis may also allow us to provide information useful to establish guidelines for the data collection program, such as where to sample, and how many samples are required to more fully characterize the flow system parameters and to reduce uncertainties.

We are proposing:

- (1) to investigate the degree of uncertainty in predictions of flow and transport through a hypothetical two-dimensional aquifer due to a lack of complete knowledge of the spatial variability of

hydraulic properties; (2) to determine the reduction of the uncertainty in predictions that can be achieved by some additional knowledge of hydraulic property values at various sampling points; (3) to investigate the effects of errors in estimating statistical parameters characterizing the spatial variation and correlation structure of hydrologic properties; and (4) to apply to one of the candidate repository sites, to the extent possible, the conditional simulation procedures (Appendix 1) and assess the degree of uncertainty in the predictions and the data needs.

In the first step of the stochastic analysis we will generate random fields of hydraulic conductivity and porosity using non-conditional simulation techniques (spectral or turning-bands methods). To do this, we will use the same statistical properties (mean, variance, correlation length) which were employed to construct the hypothetical, real-world analog of the aquifer described previously under the section pertaining to deterministic modeling. This step will in effect produce many realizations of possible aquifer properties based solely on the statistical characteristics which are known a priori. None of the parameter fields generated by this method is likely to be identical to the real-world analog at all locations. However, they should have the same mean, variance, and correlation function. Parameters

then will be assigned at nodes or grid blocks of a finely discretized two-dimensional flow domain identical to the one described previously for deterministic modeling (Figure 4). For each realization of the parameters we will predict ground-water travel time and solute transport and compile the results in the form of a cumulative probability. These results would be expected to produce considerable dispersion and uncertainty, because there are no locations in the aquifer under consideration where data are actually known and held constant. This case represents expected uncertainty in results using mean hydraulic conductivity and porosity.

Then we will assess the importance of including field measurements. To obtain 'field measurements' we will select locations from our finely discretized real-world aquifer analog and assume that at these locations there is no uncertainty in hydraulic properties. The conditional simulation procedure will be invoked to produce many realizations of hydraulic properties, preserving the measured values at their respective locations. We will vary the number of 'measurements' as well their locations to assess the importance of test site location, such as it may relate to site characterization activities. For each realization we will again predict ground-water travel time and solute transport and compile cumulative probability

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density functions for arrival time and concentration. This step will be repeated by adding more locations from the real-world aquifer analog where parameters are assumed to be known from 'field measurements'. By comparing the various cases, we expect that the dispersion in the probability density function should decrease as the uncertainty in knowledge of hydraulic properties decreases. As the number of known data points increases, the cumulative probability density function from the stochastic result should approach a step function which is representative of the deterministic analysis of flow and transport in the real-world aquifer analog.

In the procedures described in preceding paragraphs, the true statistical properties over the aquifer were assumed to be known and were kept the same in all cases. (Recall that we arbitrarily designated them in order to construct the real-world aquifer analog.) However, the true statistical properties within the entire accessible environment would not likely be obtained from only a few testing or sampling locations. The statistics derived from these locations would only represent those of the sample set; when the sample set is sufficiently large it may be representative of the population. Therefore, there are likely to be errors in predictions of ground-water travel path and travel time or solute transport because statistics from the sparse data base are different

from those of the population. (These statistics are used to obtain estimates of hydraulic properties at locations for which there are no data.) To examine the significance of this source of uncertainty, we will return to the several sets of 'field measurements' selected for the analysis just described. Recall that each data set contains more values than the previous one. The mean and covariance structure will be determined for each data set. Conditional simulations then can be carried out with the estimated covariance functions to generate several realizations of random parameter fields with which several ground-water travel time distributions can be obtained from the numerical simulators. Mean and variance of ground-water travel times and concentration thus can be evaluated. The effect of uncertainty in parameter estimation will be determined through the comparison of the ground-water travel time and solute distributions obtained from the previous analysis.

The last part of the third phase is to extend the geostatistical method to the proposed repository site of the Deaf Smith County site. In this case a cross-sectional model similar to that employed by the Texas Bureau of Economic Geology will be used. The cross-sectional model will include the Ogallala Formation, Dockum Group, Permian Evaporite Strata, and Deep-Basin Brine Aquifer. Each formation will be assigned a mean

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and variance of hydraulic conductivity. Conditional simulations will then be employed to analyze the uncertainties in ground-water travel time and concentration distributions. We will investigate the sensitivity of the uncertainties in groundwater travel time and concentration to the statistical parameters (such as correlation scales, variances, means, and distributions) of each formation. The results of the analysis will provide us with the information about the importance of these parameters and thus, direct our attention to the data needed to fully characterize the uncertainties and to reduce the uncertainties. For example, more densely spaced hydraulic conductivity measurements in the Permian Evaporite Strata and Deep-Basin Brine Aquifer near the vicinity of the proposed repository may reduce the uncertainties in travel time and radionuclide flux predictions. Therefore, the results of this analysis may assist the NRC in establishing a sampling guideline for the DOE site characterization program.

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BUDGETARY CONSIDERATIONS

The entire scope of work described herein is beyond the scope of the current contract. However, Phase 1 and possibly significant parts of Phase 2 could be completed under the current contract between Nuclear Waste Consultants and the NRC. We estimate professional time to complete the three phases of the work plan would be roughly 1, 3 and 12 man-months, respectively. Technical support, technical review and administration time would be in addition to this effort.

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APPENDIX 1

GENERAL CONCEPT OF CONDITIONAL SIMULATIONS

If the in situ hydraulic properties of the formation were perfectly known, the groundwater travel time and path could be determined by applying various deterministic mathematic models. Unfortunately, perfect knowledge of in situ hydraulic properties is not available. The information available at the planning stage for a repository site is usually very fragmentary and limited to the properties of a few samples. The estimations deduced from this information, for example through Kriging (a method of estimation of random fields), are far too imprecise for the accurate determination of the groundwater travel time and path using a deterministic approach.

Conditional simulation provides a solution to this problem. Each conditional simulation is considered to be a plausible version of the unknown hydraulic properties of the heterogeneous aquifer. The complete theory of conditional simulation is given by Matheron (1973) and Journel' and Huijbregts (1978). Briefly, the procedures to be used to conduct the conditional simulation in this proposed study are first to generate nonconditional simulations (i.e., the synthesis of different realizations of the random field of saturated hydraulic conductivities, having the actual covariance function that has been inferred from the

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data). The first step can be obtained by various methods, such as those, for instance, based on spectral analysis (Jenken and Watts, 1968) or the so-called turning bands method (Journel, 1974; and Montoglio and Wilson, 1982). One realization from this analysis may be presumed to be representative of the variability of the real system. In the second step we condition the simulations obtained in the first step based on measured data (i.e., making the interpolation consistent with the known values of parameters.) For the second step, one has to employ Kriging. Kriging, is an interpolation scheme which preserves the known parameter values at the sample points. In addition, it preserves the spatial covariance of the phenomenon. From the actual sample values, $Z(x)$, Kriging yields an estimate Z^* at any point x . For example, in Figure 5a, if we measured the parameter Z at the five locations Kriging would produce intermediate values which closely approximate the known values. If x is not a sample point, the true value $Z(x)$ is not available, and the Kriging error $Z(x)-Z^*(x)$ remains unknown. But $Z(x)=Z^*(x)+[Z(x)-Z^*(x)]$. Kriging (e.g., interpolating permeability values) can be performed using as input data the values (e.g., permeability predictions) from a given nonconditional simulation at the actual sample locations. The sample value obtained from the given nonconditional simulation $S(x)$ can be decomposed as the sum of the Kriging estimate $S^*(x)$ and the Kriging error,

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i.e., $S(x) = S^*(x) + [S(x) - S^*(x)]$ (Figure 5b). Since this is derived from the nonconditional simulation, all terms are known. By substituting $S(x) - S^*(x)$ for $Z(x) - Z^*(x)$, the conditional simulation $Z_s(x)$ is defined as

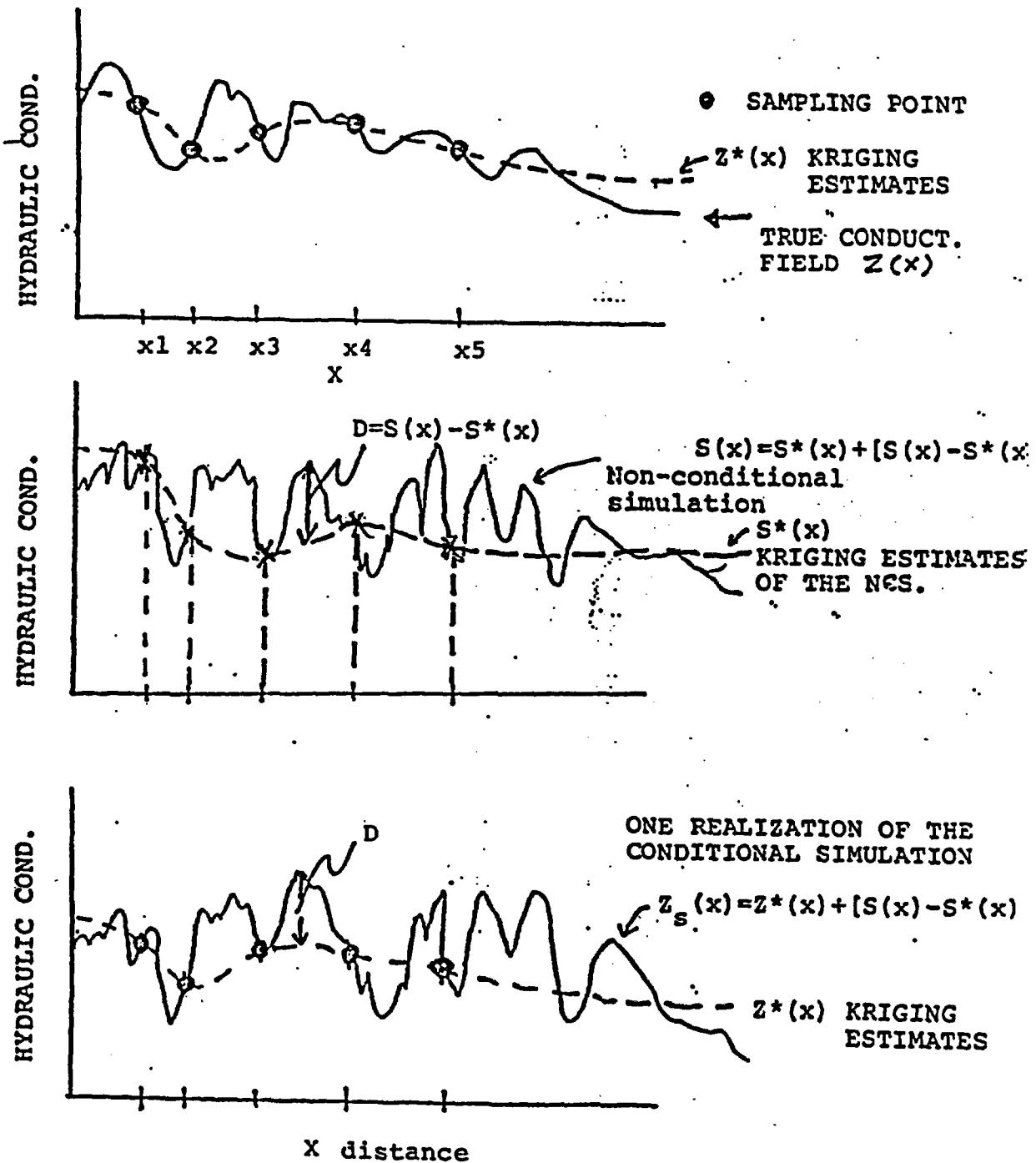
$$Z_s(x) = Z^*(x) + [S(x) - S^*(x)]$$

Therefore, $Z_s(x)$ is consistent at the sample points with the sample values; $Z_s(x)$ and $Z(x)$ have the same covariance functions; and the average of many conditional simulations at a given point x is the Kriging estimate, and their variance the Kriging variance (Figure 5c).

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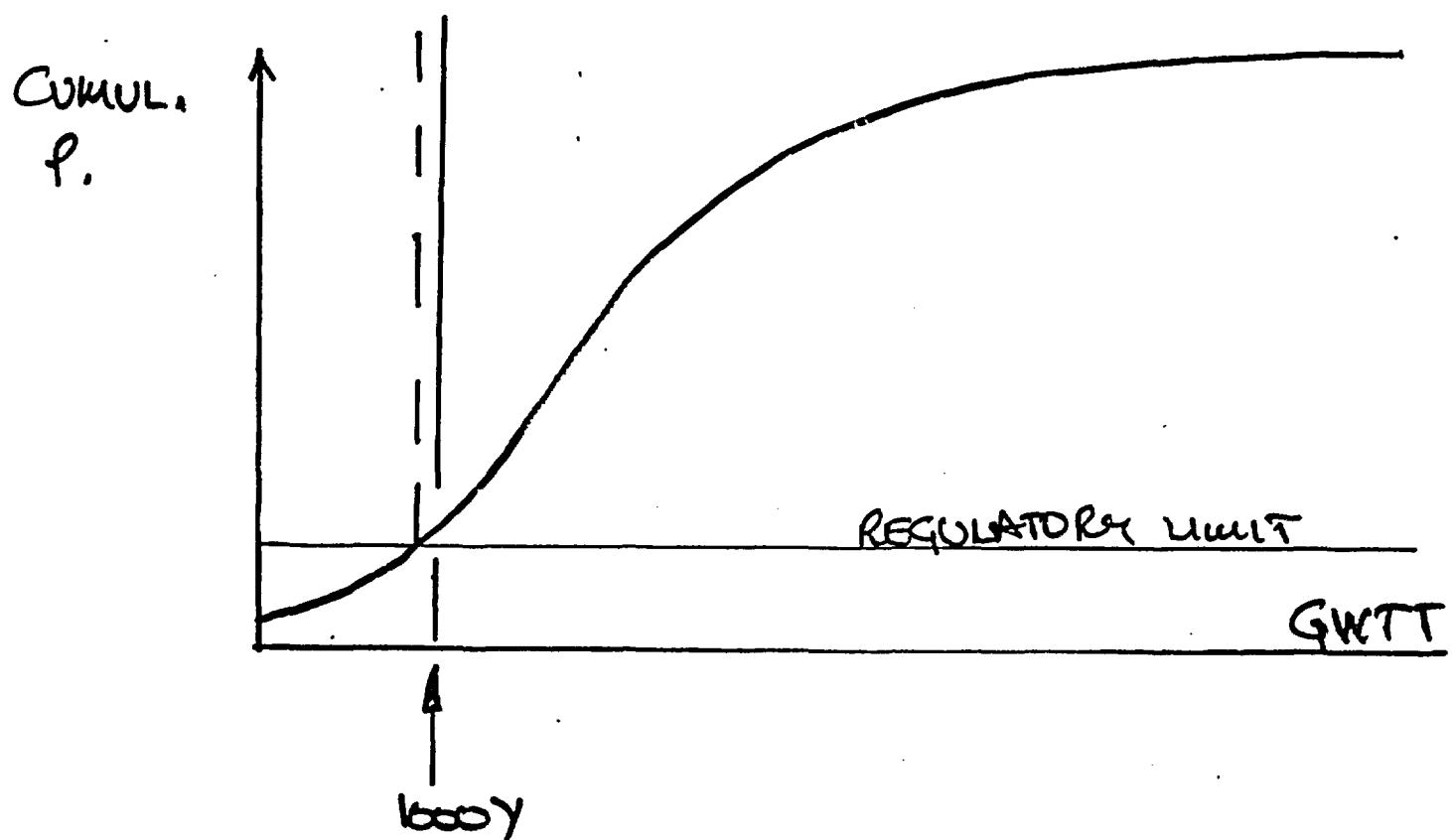
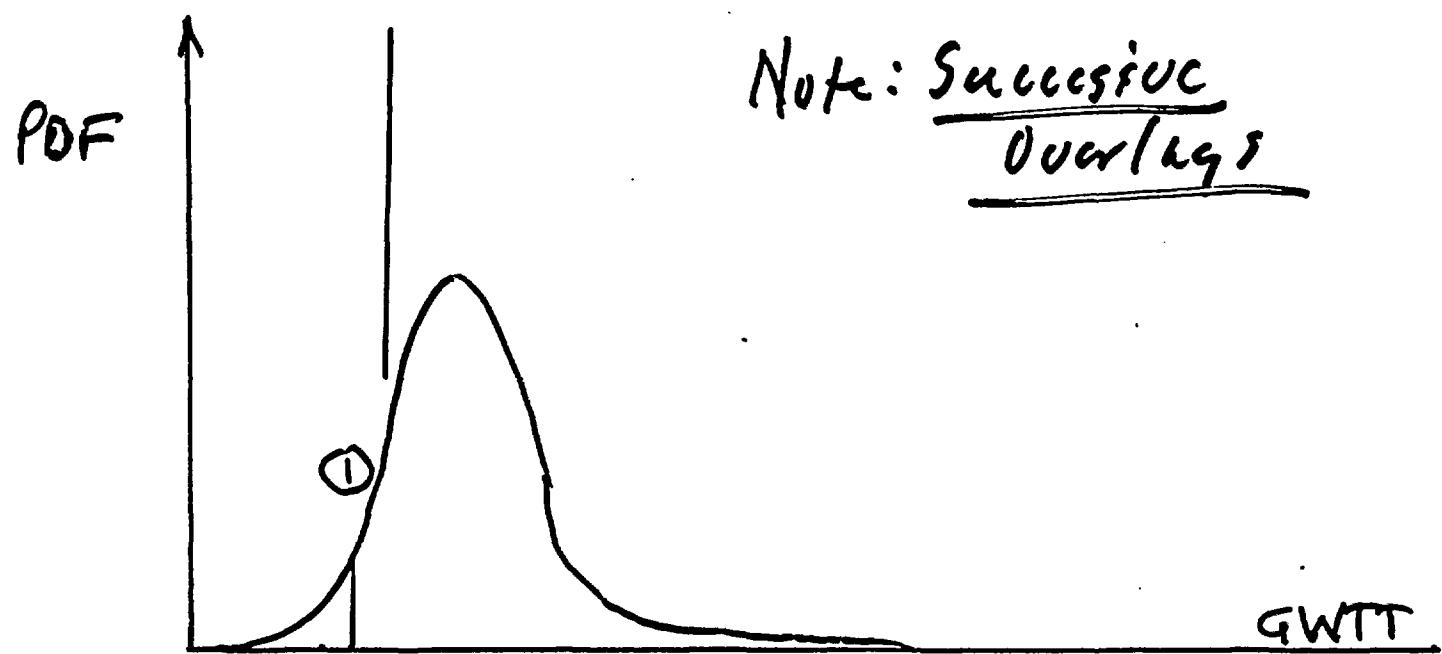
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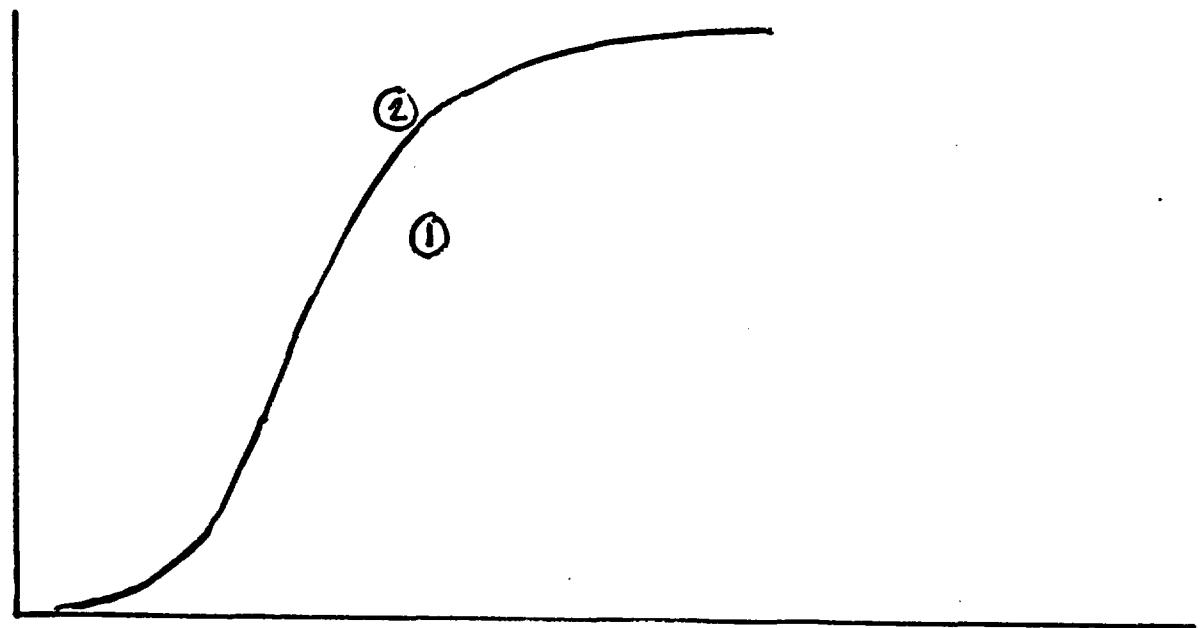
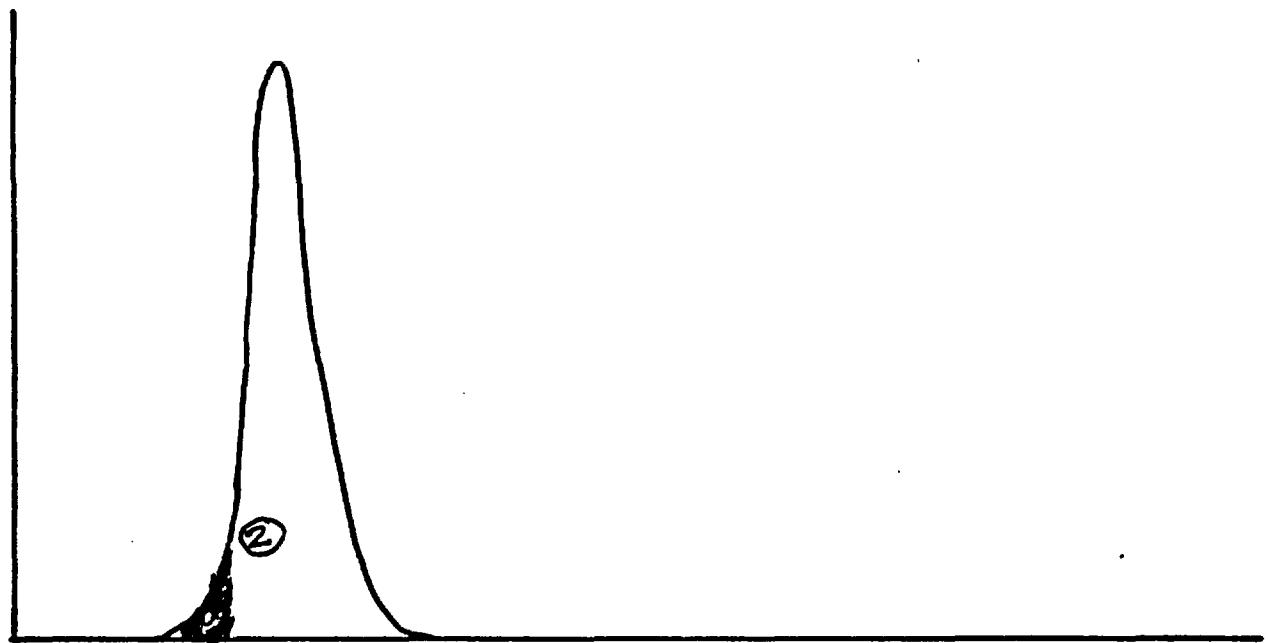
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Figure 6. A schematic illustration of the conditional simulation.

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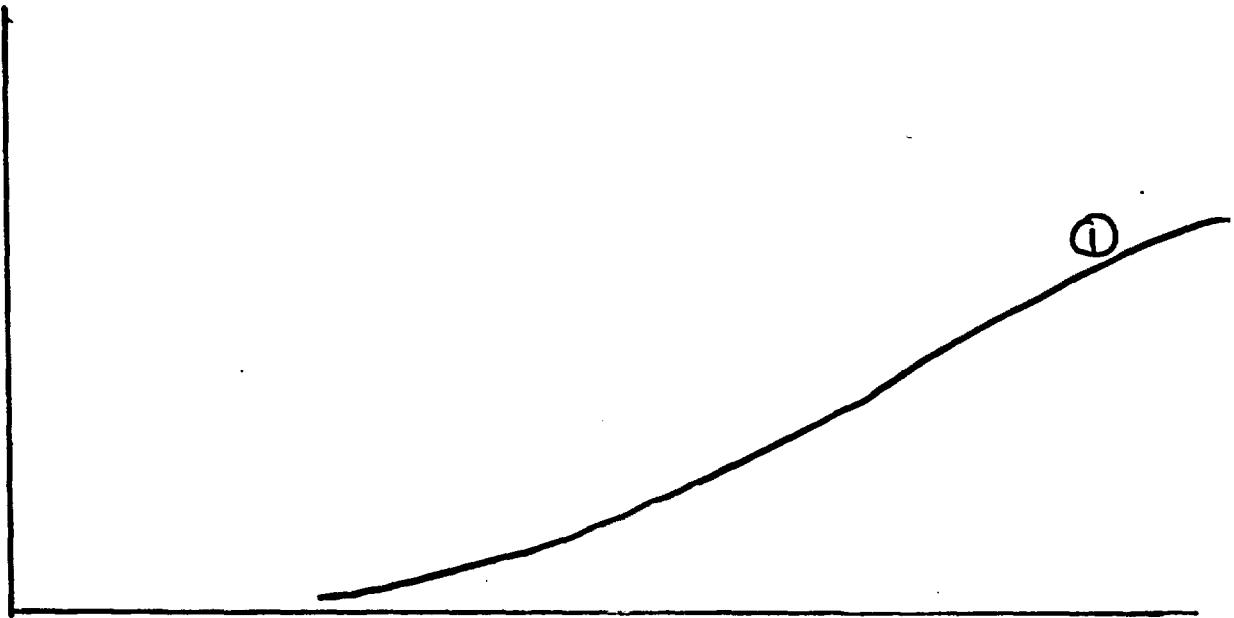
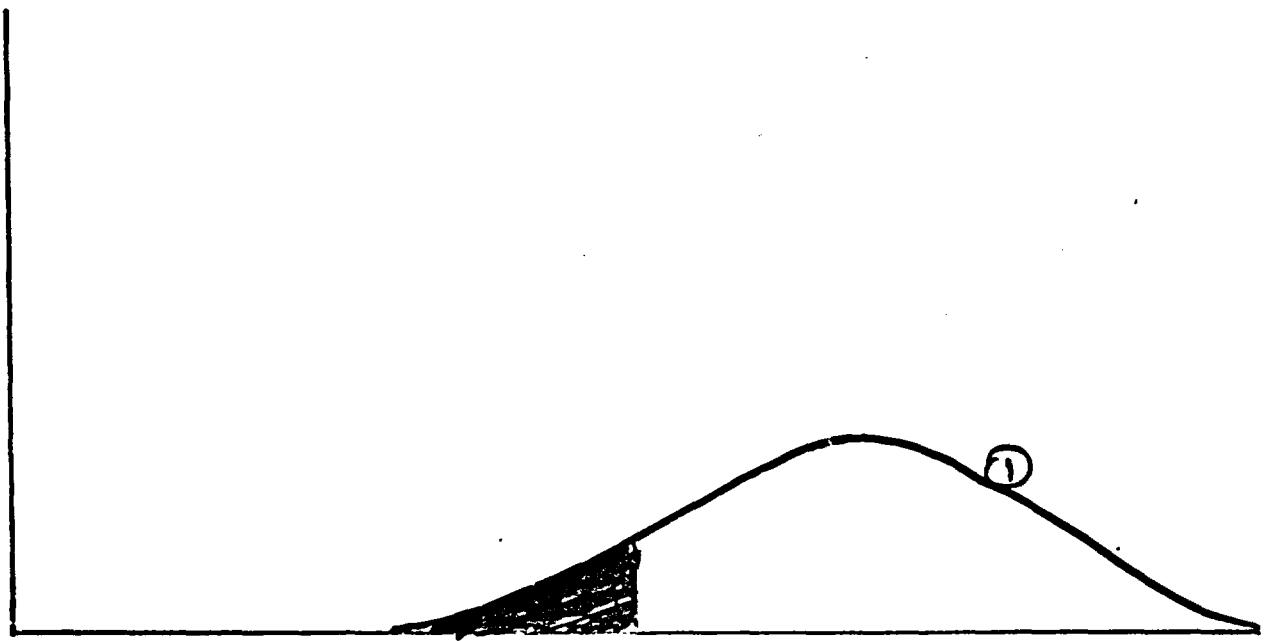
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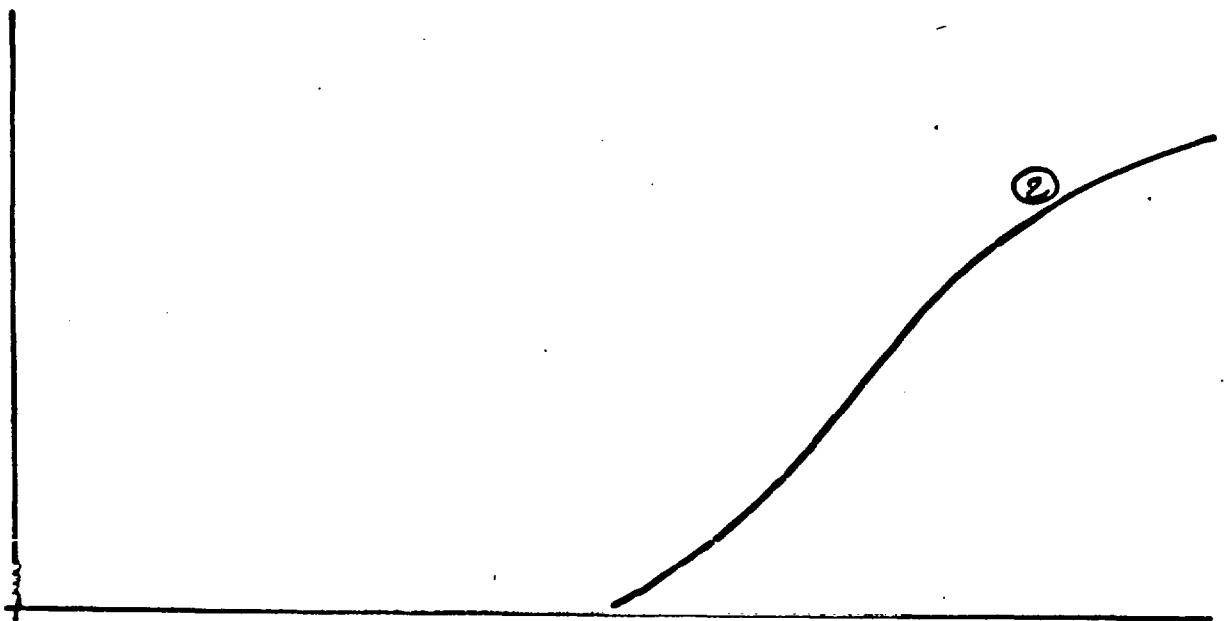
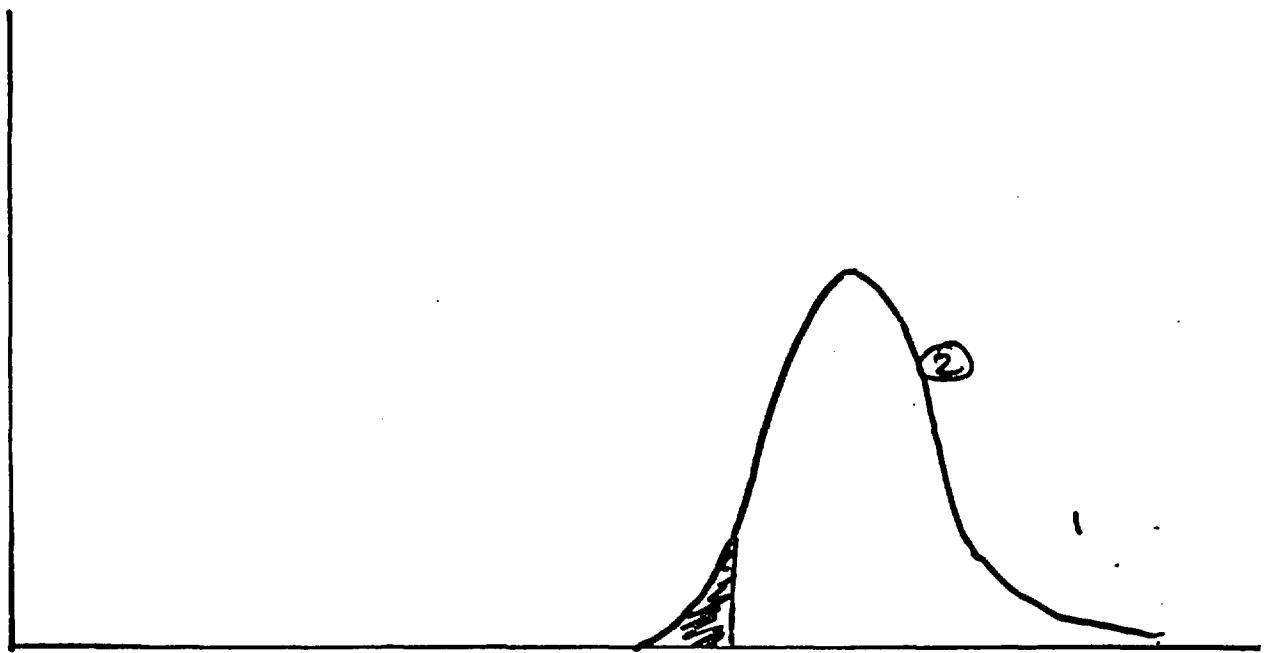
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11/15/86

"11"

Dan Stephens - Multiple
Approach Concept to Treat
Uncertainty

1. Physical Approach - current efforts

Darcy Eqn \rightarrow flow velocity

Deterministic / Stochastic Analyses

2. Hydrochemical Approach

"Age" / residence time

Origin & travel path

Integration of ambient processes

A. If physical/chemical convergence,
support for conceptual & math.
models

B. If diverge \Rightarrow lack of information
or theory (conceptual/model)

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Table 1. Uncertainty in Ground Water Travel Time,
Deaf Smith County Site (Bedded Salt)

Source of Uncertainty	Relative Contribution to Total Uncertainty (%)	Methods to Reduce Uncertainty
Conceptual Model Errors	20	Focus on salt interbeds and Wolfcamp; Borehole shut-in pressure vs. depth, geochemistry (stable isotopes, noble gases, chlorine-36, iodine-129), down-hole camera and core inspection for fractures; Convergence of multiple hypotheses
Incomplete Knowledge of Data	30	Measurements and sampling in Boreholes along transect (E-W) across the basin, mostly within accessible environment; Conduct numerical experiments to assess sensitivity and to determine data collection requirements
Measurement Errors	25	Improve field technique for hydraulic testing low K rocks; Determine the zone of influence represented by the measurement or sample in heterogeneous systems; QA program
Modeling Errors	25	Comparative model studies Sensitivity analyses of physical properties and parameters; Estimate spatial correlation structure; Numerical experiments (e.g. conditional simulations) in heterogeneous and equivalent homogeneous systems; Model verification tests



11/15/86 Dave McWhorter - Treating¹¹²
Model Uncertainty

$$\frac{\partial}{\partial z} \left\{ K \left(\frac{\partial P}{\partial z} + \rho g \right) \right\} = \frac{\partial \theta}{\partial t} \quad (1)$$

low prospects for determining
functions for $K(P)$, $\theta(P)$

Alternatives? :

1. Synthesize $K(P)$, $\theta(P)$ from theoretical considerations
2. Use an alternative calculational model with at least these characteristics:
 - a) yields bWTT this is conservative
 - b) consistent with "best guess" model (1) in limiting circumstances
 - c) contains coefficients that are subject to measurement

Alternative Calculational model (con.)

