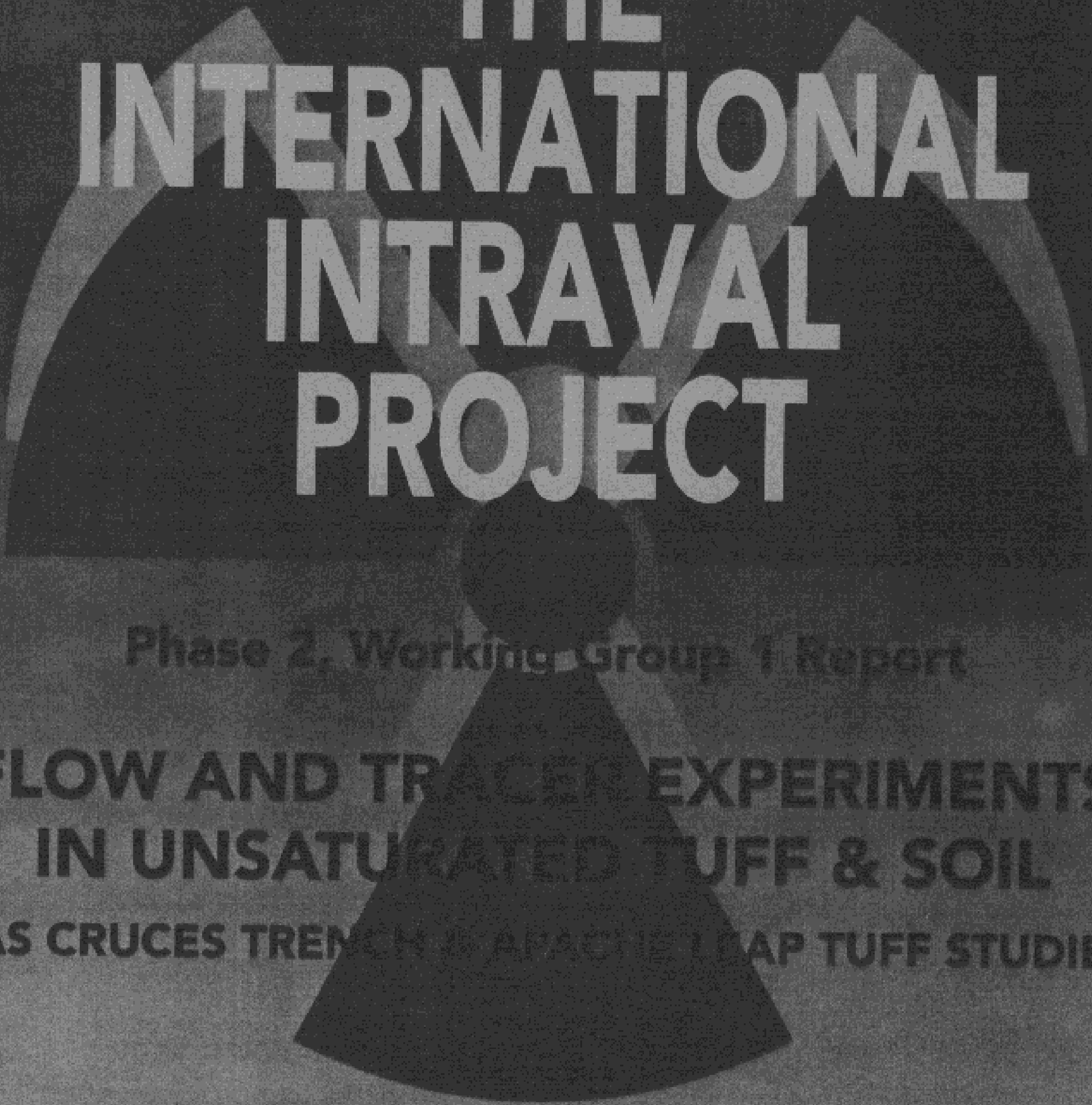

THE INTERNATIONAL INTRAVAL PROJECT

Phase 2, Working Group 1 Report

FLOW AND TRACER EXPERIMENTS IN UNSATURATED TUFF & SOIL

LAS CRUCES TRENCH & APACHE LEAP TUFF STUDIES

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THE INTERNATIONAL INTRAVAL PROJECT

TO STUDY VALIDATION OF GEOSPHERE
TRANSPORT MODELS FOR PERFORMANCE ASSESSMENT
OF NUCLEAR WASTE DISPOSAL

PHASE 2, Working Group 1 Report

Flow and Tracer Experiments in Unsaturated Tuff & Soil
Las Cruces Trench & Apache Leap Tuff Studies

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NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

Pursuant to Article 1 of the Convention signed in Paris on 14th December 1960, and which came into force on 30th September 1961, the Organisation for Economic Co-operation and Development (OECD) shall promote policies designed:

- to achieve the highest sustainable economic growth and employment and a rising standard of living in Member countries, while maintaining financial stability, and thus to contribute to the development of the world economy;
- to contribute to sound economic expansion in Member as well as non-member countries in the process of economic development; and
- to contribute to the expansion of world trade on a multilateral, non-discriminatory basis in accordance with international obligations.

The original Member countries of the OECD are Austria, Belgium,Canada, Denmark, France, Germany, Greece, Iceland, Ireland, Italy, Luxembourg, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, Turkey, the United Kingdom and the United States. The following countries became Members subsequently through accession at the dates indicated hereafter: Japan (28th April 1964), Finland (28th January 1969), Australia (7th June 1971), New Zealand (29th May 1973), Mexico (18th May 1994) the Czech Republic (21st December 1995), Hungary (7th May 1996), Poland (22nd November 1996) and the Republic of Korea (12th December 1996). The Commission of the European Communities takes part in the work of the OECD (Article 13 of the OECD Convention).

NUCLEAR ENERGY AGENCY

The OECD Nuclear Energy Agency (NEA) was established on 1st February 1958 under the name of the OEEC European Nuclear Energy Agency. It received its present designation on 20th April 1972, when Japan became its first non-European full Member. NEA membership today consists of all European Member countries of OECD as well as Australia, Canada, Japan, Republic of Korea, Mexico and the United States. The Commission of the European Communities takes part in the work of the Agency.

The primary objective of NEA is to promote co-operation among the governments of its participating countries in furthering the development of nuclear power as a safe, environmentally acceptable and economic energy source.

This is achieved by:

- *encouraging harmonization of national regulatory policies and practices, with particular reference to the safety of nuclear installations, protection of man against ionising radiation and preservation of the environment, radioactive waste management, and nuclear third party liability and insurance;*
- *assessing the contribution of nuclear power to the overall energy supply by keeping under review the technical and economic aspects of nuclear power growth and forecasting demand and supply for the different phases of the nuclear fuel cycle;*
- *developing exchanges of scientific and technical information particularly through participation in common services;*
- *setting up international research and development programmes and joint undertakings.*

In these and related tasks, NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has concluded a Co-operation Agreement, as well as with other international organisations in the nuclear field.

Foreword

Radioactive waste management programmes in OECD countries cover a wide range of activities in research and development with the common purpose to get the necessary scientific basis for disposal of various types of radioactive waste. The concern for the safety of final disposal is shared among the safety authorities and the radioactive waste producers, primarily the nuclear utilities. In some countries, site selection and characterisation programmes for high-level waste disposal are at a relatively advanced stage and several countries already have repositories for low-level waste in operation. Due to the difficulties involved and the amount of work necessary to get the required scientific information, the problems to be resolved have a high priority in national and international co-operative programmes.

INTRAVAL was set up as an international project concerned with the use of mathematical models for predicting the potential transport of radioactive substances in the geosphere. Such models are used to help assess the long-term safety of radioactive waste disposal systems. The INTRAVAL project was established by the Swedish Nuclear Power Inspectorate to evaluate the validity of these models. Results from a set of selected laboratory and field experiments as well as studies of occurrences of radioactive substances in nature (natural analogues) were compared in a systematic way with model predictions. Discrepancies between observations and predictions were discussed and analysed.

The project ran for six years, from 1987 to 1993. It was organised in two phases. The Swedish Nuclear Power Inspectorate (SKI) was managing participant during both phases and the OECD/Nuclear Energy Agency, Her Majesty's Inspectorate of Pollution (HMIP/DOE), United Kingdom, and Kemakta Consultants, Sweden took part in the project secretariat. The project had also observers from the International Atomic Energy Agency and from the State of Nevada.

The first phase of INTRAVAL was finished in 1990. Reports of the results from the first phase were issued in 1990, 1992 and 1993. A summary report of phase one of the project was published in the beginning of 1994.

The second phase of INTRAVAL was initiated in 1990 and finished 1993. Thirty-eight organisations from thirteen OECD countries participated in the second phase. Test cases were divided among four working groups which describe their findings in four separate reports. This report is one of them. In addition a summary report will be issued as well as a report from an independent subcommittee for integration.

Abstract

The Working Group 1 final report summaries two test case studies, the Las Cruces Trench (LCT), and Apache Leap Tuff Site (ALTS) experiments. These test cases were in the earlier Phase 1 effort and are discussed in the Phase 1 final report. For Phase 2 they were refocused to address field validation aspects building upon the accomplishments in Phase 1. The objectives of these two field studies were to evaluate models for water flow and contaminant transport in unsaturated, heterogeneous soils and fractured tuff. The LCT experiments were specifically designed to test various deterministic and stochastic models of water flow and solute transport in heterogeneous, unsaturated soils. Experimental data from the first two LCT experiments, and detailed field characterisation studies provided information for developing and calibrating the models. Experimental results from the third experiment were held confidential from the modellers, and were used for model comparison. Comparative analyses included: point comparisons of water content; predicted mean behavior for water flow; point comparisons of solute concentrations; and predicted mean behavior for tritium transport. These analyses indicated that no model, whether uniform or heterogeneous, proved superior. Since the INTRAVAL study, however, a new method has been developed for conditioning the hydraulic properties used for flow and transport modelling based on the initial field-measured water content distributions and a set of scale-mean hydraulic parameters. Very good matches between the observed and simulated flow and transport behavior were obtained using the conditioning procedure, without model calibration. The ALTS experiments were designed to evaluate characterisation methods and their associated conceptual models for coupled matrix-fracture continua over a range of scales (i.e., 2.5 centimeter rock samples; 10 centimeter cores; 1 meter block; and 30 meter boreholes). Within these spatial scales, laboratory and field tests were conducted for estimating pneumatic, thermal, hydraulic, and transport property values for different conceptual models. The analyses included testing of current conceptual, mathematical and physical models using the ALTS characterisation data. Conclusions drawn were: (1) wetting history has a significant influence on formulating the characteristic curve; (2) thermal conductivity is only poorly related in a linear fashion to water content; and (3) the fracture saturation behind the wetting front initially is very low, perhaps ten percent, but increases to complete saturation during the course of the block wetting experiment contrary to the modelling results which overestimated the fracture imbibition volume by a factor of twenty, and the fracture wetting front advance by a factor of eight. Both the LCT and ALTS studies have demonstrated the value of field-scale experiments and the importance of experimentalists and modellers working together to solve complex flow and transport problems.

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1 Introduction

Phase 2 of the International INTRAVAL Project initiated in October 1990 was organised into four working groups. Working Group 1 (WG1) originally addressed the Las Cruces Trench, Apache Leap, and Twin Lake Test Cases. In April 1991 the Twin Lake Test Case was moved to Working Group 4, and later returned to WG1 prior to the completion of Phase 2. The Yucca Mountain Test Case, considered an auxiliary test case of the Apache Leap Test Case was added in 1992. At the final technical workshop of Phase 2 held in Stockholm in September 1993, members of WG1 met to organise the final reporting strategy. It was agreed that each test case would be documented in a final published report under the responsibility of the Pilot Team. The WG1 final report would contain summaries taken from the individual test case reports. To date only the Las Cruces Trench and Apache Leap Test Cases have been documented in final published reports, "INTRAVAL Phase 2 Modelling Testing at the Las Cruces Trench Site" by *Hills and Wierenga, 1993*, and "Apache Leap Tuff INTRAVAL Experiments: Results and Lessons Learned" by *Rasmussen et al., 1996*. Information on the Twin Lake and Yucca Mountain test cases are provided in the final INTRAVAL Progress Report 10 issued in 1993 prior to the completion of Phase 2. Therefore the WG1 final report is limited to summaries reporting on the Las Cruces Trench and Apache Leap Test Cases.

At the conclusion of Phase 1 of INTRAVAL, the NRC staff nominated two ongoing field studies for consideration in Phase 2 of the INTRAVAL Project. These experiments dealt with the testing and confirmation of water flow and contaminant transport models for unsaturated, heterogeneous soils and fractured tuff. In Phase 1 of INTRAVAL which focused on laboratory and field studies, the Las Cruces Trench studies were proposed by the NRC staff to examine issues of heterogeneity in unsaturated soils. Specifically, how to characterise it, model it, and assess uncertainty in simulated flow and transport results (the Phase 1 results are discussed in *Voss and Nicholson, 1993*). The Apache Leap Tuff studies were proposed by the NRC staff to examine issues of non-isothermal, multi-phase flow and transport in unsaturated, fractured tuff. Both projects were approved for continuation in Phase 2 which focused on field studies and natural analogues.

2 Test Case Summaries

The following test case summaries were developed from the final test cases reports ([*Hills and Wierenga, 1993*] for Las Cruces Trench; [*Rasmussen et al., 1996*] for Apache Leap). Data reports and peer-reviewed journal articles are cited throughout the test case summaries which further document modelling and experimental results, information and detailed datasets. Lessons learned from these two test cases were presented at the GEOVAL-94 symposium [*Nicholson et al., 1995*] using information from the WG1 final report.

2.1 Las Cruces Trench Studies

2.1.1 Background

The Las Cruces Trench (LCT) studies originated as a cooperative research effort between field experimentalists at New Mexico State University (NMSU), Pacific Northwest Laboratory (PNL), and modellers at the Massachusetts Institute of Technology (MIT)[*Wierenga et al., 1986*]. The field site was already part of a long-term environmental research study at the NMSU College Ranch (located 64 kilometres northeast of Las Cruces, New Mexico, USA) which was examining soil moisture processes in arid, cattle grazing land. The stated objective of the pre-INTRAVAL LCT study was "to collect a detailed data base for validating stochastic flow and transport models for unsaturated soils" [*Nicholson et al., 1989*]. The original objective went on to state "The theoretical stochastic method; the approach for selecting an adequate data base upon which stochastic models can be tested; and the details of the field program, including the plot design and initial test configuration of the field trench, are all integral parts of the validation process." Central to the LCT study was the need to determine the degree of heterogeneity at the field site, and how it should be represented (e.g., stochastic random fields characterised by means, variances and correlation scales) [*Nicholson et al., 1989*].

2.1.2 Experimental Objectives

For the INTRAVAL Project, the LCT studies were reformulated using the goal of rigorous model testing (both deterministic and stochastic models) to include multiple field tests. The experimental objectives were that:

- The hydraulic properties for the site should be characterised in sufficient detail so that the site can be modelled using deterministic and stochastic models;

- The boundary conditions on water flow and solute transport should be carefully controlled to minimise ambiguities associated with model testing; and

- The movement of water and solute through the soil profile during infiltration and redistribution should be monitored in sufficient detail so that the effect of spatial variability can be defined [*Hills and Wierenga, 1994*].

These experimental objectives were successfully met, due in part to the detailed instrumentation and monitoring activities which produced significant experimental datasets [*Wierenga et al., 1989 and 1990; and Hills and Wierenga, 1994*].

2.1.3 Experimental Design

Figure 2.1 illustrates the experimental design. Water was applied at a rate that would not create saturated conditions, but would enhance lateral spreading to magnify the lateral and vertical heterogeneities of the unsaturated soil profile. The facility was designed for monitoring the applied water and tracer movement at various depths. The field instrumentation consisted of numerous neutron access tubes, and tensiometers and solute samplers installed in the wall of the excavated trench. The trench face was exposed for the first experiment allowing visual observation of the wetting front advance. Water and tracers were applied to two different experimental plots.

A trench measuring 26.5 m long, 4.8 m wide, and 6.0 m deep was excavated through a series of soil horizons. The trench served as an observation, sampling and instrumentation facility. Earlier soil column and lysimeter experiments were important in defining the soil properties and for testing the horizontal versus vertical property differences for various infiltration rates [*Wierenga et al., 1986*]. This information was used to determine the irrigation application rate for the first wetting experiment (Plot 1) using the 4m wide by 9m long irrigation strip shown in Figure 2.1. The Plot 1 test can be viewed as an initial characterisation experiment which along with the earlier lysimeter and laboratory experiments defined the soil horizons, properties and ambient conditions [*Wierenga et al., 1989*]. The Plot 2a test was considered a dynamic experiment in which model calibration was possible [*Wierenga et al., 1990*]. Plot 2b was also a dynamic experiment but was performed as a validation experiment since the experimental results were not given to the modellers [*Hills and Wierenga, 1994*].

The first experiment used the 4.0 by 9.0 metre plot (Plot 1) with a water application rate of 1.82 cm/day. Tritium was applied with the irrigation water for the first ten days, followed by 76 days of irrigation without the tritium. The second (Plot 2a) and third experiments (Plot 2b) used the 1.22 m wide by 12 m long irrigation strip. The Plot 2a test in Phase 1 of INTRAVAL involved a reduced application rate (0.43 cm/day) with tritium and bromide tracers for 11.5 days followed by an additional 64 days of water application without tracers. The Plot 2b test, designed by scientists at the University of Arizona and NMSU in consultation with the modelling teams in INTRAVAL, used an application rate identical to the first experiment (1.82 cm/day) but used a different application schedule and tracers [chromium, boron, and pentafluorobenzoic acid (PFBA) initially, and tritium, bromide and 2,6-difluorobenzoic acid (DFBA) later] (see Figure 2.2).

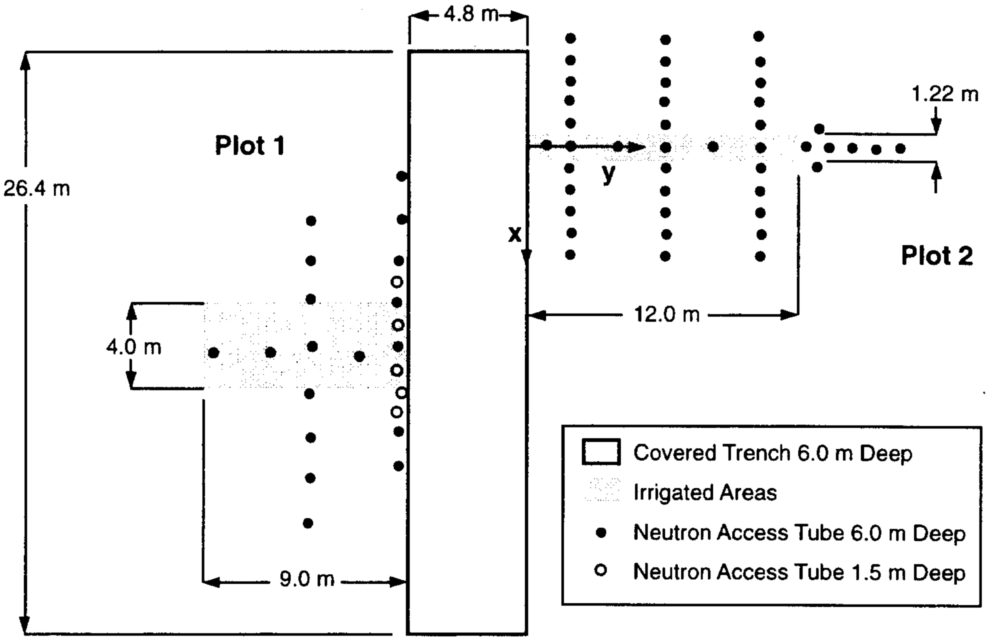


Figure 2.1 Plan view for the Las Cruces Trench Experiments (from Hills and Wierenga, [1994]).

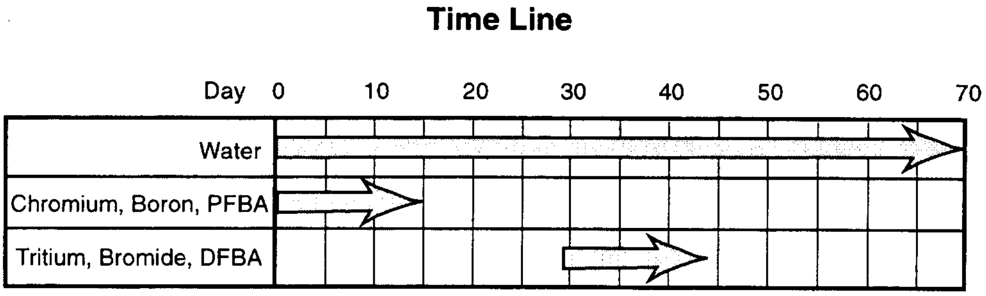


Figure 2.2 Plot 2b water and chemical tracer application schedule (from Hills and Wierenga, [1994]).

2.1.4 Experimental Analysis

The experiments were analysed by defining: (1) the characterisation and dynamic variable properties measured during the experiments (see Table 2.1); (2) the distributions of water contents using the neutron access holes taking readings at various depths; (3) the tracer plume concentration contours using collected water samples via the soil solution samplers in the face of the trench during the experiments, and destructive core samples collected at the end of the experiments; and (4) the wetting front positions for Plot 1 based upon photographs of the trench face over time.

Table 2.1 also provides the scale and technique used to determine the characterisation and dynamic variables (where θ, θ_r and θ_s are the volumetric water content, residual water content, and saturated volumetric water content, α and n are parameters that define the shape of the van Genuchten model soil-water retention curves, and h is pressure head) measured during the experiments [*Hills and Wierenga, 1994*].

To characterise the transport parameters of the tracers (tritium, bromide, chromium, boron and chloride) a series of laboratory and field column studies were performed, and are reported in *Porro et al.* [*1993*], and *Porro and Wierenga* [*1992*]. PFBA and DFBA are non-reactive anions and are considered to have the same properties as bromide, and therefore were not tested.

2.1.5 Models Developed for Testing

During Phase 1 of INTRAVAL, the modelling teams consisted of: (1) the Bureau for Economic Geology, University of Texas (BEG); (2) the Center for Nuclear Waste Regulatory Analysis (CNWRA); (3) HydroGeologic Inc. (HGL): (4) Kemakta Consultants Co. (KKC); (5) Massachusetts Institute of Technology (MIT); (6) New Mexico State University (NMSU); (7) Pacific Northwest Laboratory (PNL); and (8) Sandia National Laboratory (SNL). In Phase 2 the groups included BEG, CNWRA, MIT, NMSU, and PNL.

Table 2.1 Parameters measured during the Las Cruces Trench experiments (from Hills and Wierenga, [1994]).

Parameter	Scale	Technique	Reference
		Characterisation Variables	
K_{sat}	8 cm	Measured flow through saturated cores	*Elrick et al.* [*1980*], *Wierenga et al.* [*1989a*]
K_{sat}	10 cm	Borehole permeameter	*Reynolds et al.* [*1984*], *Wierenga et al.* [*1989a*]
θ_r,θ_s,α,n	8 cm	Cores and constant pressure apparatus combined with parameter estimation	*Wierenga et al.* [*1989a*]
Particle size distribution	8 cm	Soil sieves and modified pipet method *Wierenga et al.* [*1989a*]	*Gee and Bauder* [*1986*].
		Dynamic Variables	
θ	50 cm	Neutron Probe	*Wierenga et al.* [*1990*]
h	2 cm	Tensiometer	*Wierenga et al.* [*1990*]
Concentration of tracers	2 cm	Solute samplers and soil sampling	*Wierenga et al.* [*1990*]

Table 2.2 lists the models that were developed and used to analyse the Plot 1 and 2a experiments both prior to and during Phase 1 of INTRAVAL. The models can be grouped into two categories, (1) *deterministic models* that represent heterogeneities as homogenous, uniform property values or as heterogenous with various approaches to portraying distributed property values, and (2) *stochastic models* using Monte Carlo methods or the techniques of *Mantoglou and Gelhar* [*1987*] to represent heterogeneities. The process models in Phase 1 focused on those used to characterise the soil hydraulic properties, and dynamic models used to simulate flow and transport for Plot 1 and 2a experiments as shown in Table 2.2. Details on the conceptual and numerical aspects of these models is provided in *Hills and Wierenga* [*1994*].

Table 2.2 Modelling of the Plot 1 and 2a experiments (from Hills and Wierenga, [1994]).

Group	**Model**	**Comments**
CNWRA	BIGFLOW	Finite difference code for high resolution water flow simulations. Modelled a 3-D, randomly heterogeneous and stratified soil with boundary conditions similar to Plot 1 but with wetter initial conditions.
HGL	VAM2D	Finite element code for water flow and transport. Modelled Plot 2a with several levels of heterogeneities (isotropic and anisotropic) in 2-D.
KKC	TRUST + TRUMP	Integrated finite difference code for water flow and transport. Modelled Plot 2a as a homogeneous and a layered soil in 2-D.
MIT		Finite element code for water flow using modified Picard Iteration. Modelled Plot 1 using 3-D effective media stochastic property models in a 2-D simulation.
NMSU		Water Content based finite difference code for water flow & transport. Modelled Plot 2a as a homogenous soil in 2-D.
PNL	UNSAT-H UNSAT2	One and two-dimensional finite difference and finite element codes for water flow. Modelled Plot 1 water flow with several levels of heterogeneities in 2-D.
SNL	VAM2D	Finite element code for water flow and transport. Monte-Carlo simulation of 2-D water flow using VAM2D with multiple realisations of a uniform soil model. Analytic 1-D models are used.

For Phase 2, the dynamic models simulated flow and transport of the Plot 2b experiment. Table 2.3 summarises the models used and the manner in which they represented heterogeneities. (Note: a "blind model" was defined as "one which was formulated before the modeller had seen the experimental results." The NMSU models could not be classified as blind since the modeller was also the party responsible for collecting and analysing the experimental results.) Detailed discussions of the models listed in both Tables 2.2 and 2.3 are provided in *Hills and Wierenga* [*1994*].

2.1.6 Model Comparison and Testing Strategy

The following procedure as discussed in *Hills and Wierenga* [*1994*] was developed and implemented by the LCT Pilot Team for the Phase 2 model comparison.

1. The water/tracer application rates, the initial volumetric water contents in the y = 2, 6, and 10 m planes (see Figure 2.1), and the initial normalised solute concentrations in the y = 0.5 m plane were provided to the modellers.

2. Using the actual water/tracer application histories (see Figure 2.2), the Plot 2b experiment was simulated by the participating modellers.

3. Several of the modellers provided NMSU with ASCII files of the predicted volumetric water contents and normalised solute concentrations at the measurement locations and times. Since this data was provided to NMSU without the modellers having access to the experimental data, these model predictions were considered blind (see Table 2.3).

4. Preliminary comparisons between experimental data and model predictions were made and presented at an INTRAVAL workshop. The experimental data was then released to those modellers that had supplied the corresponding model predictions to NMSU.

5. Additional model predictions were provided to NMSU after the above presentations were made. These later modelling predictions were considered non-blind (see Table 2.3). To be totally unbiased, the model predictions provided by NMSU were also considered non-blind since one of the NMSU personnel had access to the data.

Table 2.3 Modelling of the Plot 2b experiment (from Hills and Wierenga, [1994]).

Group	Models	Comments
BEG	BEG1	**Not Blind.** Finite difference code for two phase flow and multicomponent transport. Modelled water flow in 2-D assuming uniform, isotropic soil.
CNWRA	CNWRA1	**Blind.** Finite volume code for water flow. Modelled water flow in 2-D using a 9 layer, isotropic soil model.
	CNWRA2	**Blind.** Finite volume code for water flow. Modelled water flow using a 2-D, heterogeneous 121 zone (11 × 11 grid), isotropic soil model based on trench face characterisation.
	CNWRA3	**Blind.** Finite volume code for water flow. Modelled water flow using a 2-D, heterogeneous 3621 (51 × 71 grid), isotropic soil model based on trench face characterisation.
MIT	MIT1	**Blind.** Finite element code for water flow using modified Picard approximation. Modelled water flow using a 3-D effective media stochastic property model (homogeneous, anisotropic) in a 2-D simulation.
NMSU	NMSU1	**Not Blind.** Water content based finite difference code for water flow and tritium transport. Modelled water flow and tritium transport assuming soil is homogeneous and isotropic in 2-D.
	NMSU2-NMSU5	**Not Blind.** Water content based finite difference code for water flow and tritium transport. Modelled hydraulic properties of soil as heterogeneous, isotropic in 2-D using four property realisations sampled from the trench face characterisation. Transport properties were modelled as uniform, isotropic.
PNL	PNL1	**Blind.** Finite difference code for two-phase flow and transport. Modelled water flow and tritium transport in 2-D using a composite van Genuchten, uniform, isotropic soil model for the hydraulic properties. Transport properties were modelled as uniform and isotropic.
	PNL2	**Blind.** Finite difference code for two-phase flow and transport. Modelled water flow and tritium transport assuming the hydraulic properties of the soil were uniform, anisotropic, using modified parameters in the standard van Genuchten model. Transport properties were modelled as uniform and isotropic.
	PNL3	**Blind.** Finite difference code for two-phase flow and transport. Modelled water flow and tritium transport assuming the hydraulic properties of the soil were uniform, isotropic, and using van Genuchten parameters estimated from a 1-D inverse analysis of Plot 1 experiment. Transport properties were modelled as uniform and isotropic.
	PNL4	**Blind.** Finite difference code for two-phase flow and transport. Modelled water flow and tritium transport using the 2-D trench face characterisation of the water retention parameters and an isotropic, 2-D heterogeneous, conditioned realisation of the saturated hydraulic conductivity field. Transport properties were modelled as uniform and isotropic.

The modellers were periodically updated at Working Group 1 meetings by the Pilot Team who conducted the quantitative comparisons. As shown in Figure 2.2 several chemicals were applied during the execution of the Plot 2b experiment. However, only tritium was modelled since the data set from tritium proved to be the most complete, and deemed to be the most reliable by the experimentalist.

As discussed in *Hills and Wierenga* [*1994*] the initial conditions were provided to the modellers via ASCII files for water content in the y=2, 6, and 10 m planes, and tritium in the y=0.5 m plane. Model predictions were returned to NMSU in the same format for the measurement times and locations. Each record of the initial condition and model prediction files included a time (days since start of Plot 2b experiment), the x, y, z coordinates (m) measured relative to the Plot 2b irrigation centerline, and the value of the predicted variable.

2.1.7 Alternative Conceptual Models Tested and Assessed

As shown in Tables 2.2 and 2.3, a great variety of alternative conceptual models were tested and assessed. The alternatives ranged from uniform property to complex distributed property value models. The stochastic models considered spatial variability using spectral analysis approaches which related property distributions to tension dependency.

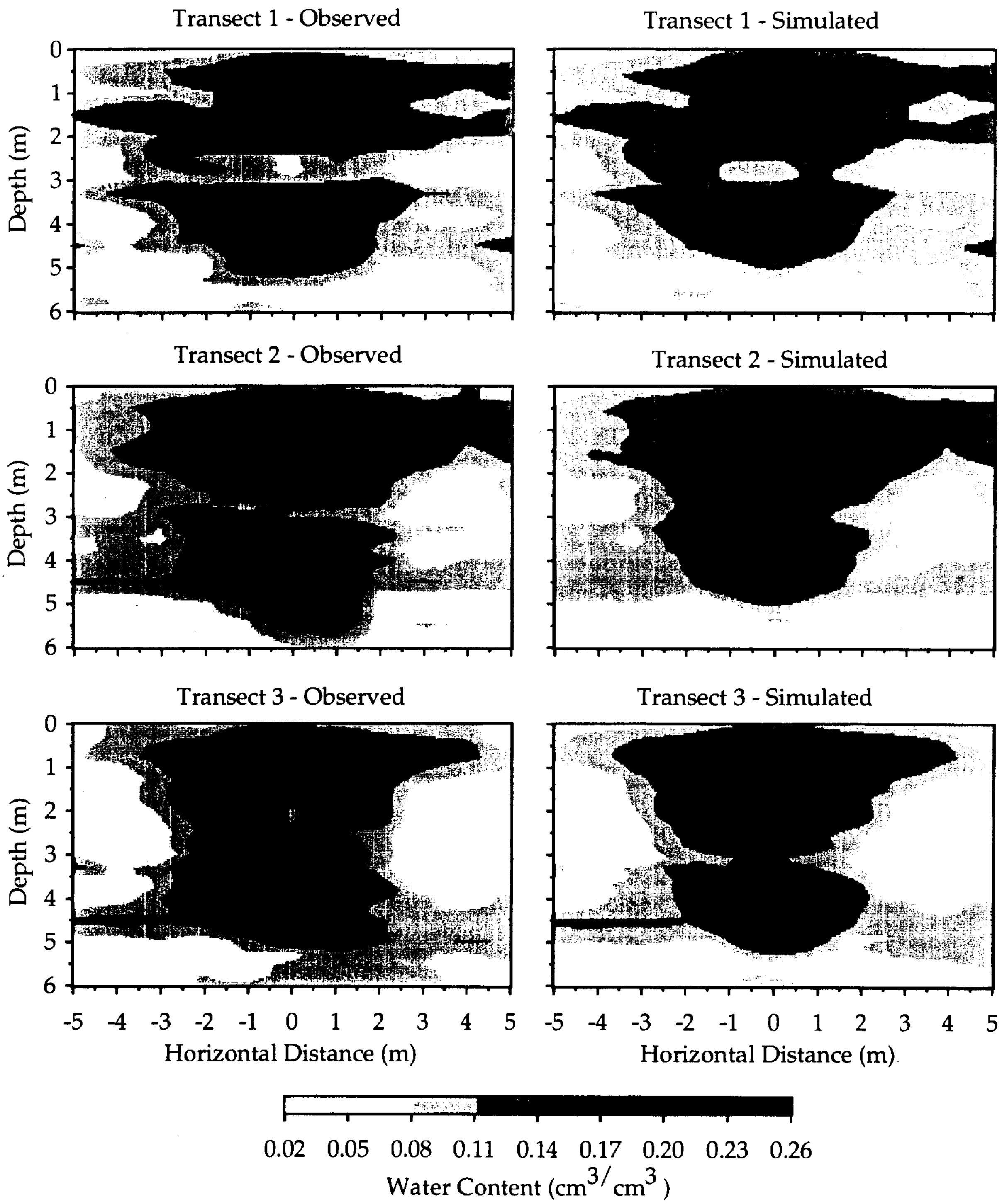
Wittmeyer and Sagar [*1993*] used the LCT data to assess the effect of increased model complexity on the accuracy of the predicted water contents using two separate measures. Based on the sum of squared differences between measured and predicted water contents, the most complex model (CNWRA3) produced the most accurate predictions. However, comparative analysis of the first and second moments of the water content distribution as functions of time lead to equivocal results; no one model was consistently better than the others. That there was less variation among the second moments predicted by the models than between the models and the experimental results suggested that there was a consistent source of bias in the models; an observation confirmed by visual inspection of the propagation of the predicted and observed wetting fronts. *Wittmeyer and Sagar* [*1993*] concluded from their study that while increased detail in model structure may indeed increase the accuracy of predictions, site characterisation efforts should focus on those specific geologic features whose presence dominates the flow regime.

Following the final modelling comparison studies, a newly developed method focusing on conditioning methods was successfully applied to the LCT datasets for the Plot 2b experiment. This method is based on conditioning the soil hydraulic properties on the initial field-measured water content distributions and a set of scale-mean hydraulic parameters [*Rockhold et al., 1994*; and *Rockhold et al., 1996*]. Very good matches between the observed and simulated flow and transport behaviour were obtained using the conditioning procedure, without model calibration as shown in Figure 2.3.

Another technological advancement derived from the LCT study, as presented in *Hills et al.* [*1994*], was the development of a flux-corrected transport based numerical algorithm to model solute transport in heterogeneous variably saturated soils. Application of this new algorithm to the LCT database indicated that the movement of the wetting front may be heavily influenced by the old water, whereas the new water tends to bypass much of the old water indicating preferential flow. Also developed during the INTRAVAL Project and documented recently, was a computer code, POLYRES, which uses a polygon-based solution technique to solve the governing Richards equation for partially-saturated flow conditions [*Hills et al., 1995*]). POLYRES has proven useful in simulating ground-water flow in complex, heterogeneous, unsaturated porous media.

2.1.8 Integration of Multi-Disciplines

The Pilot Team (University of Arizona and New Mexico State University investigators) consisted of specialists in the areas of soil physics, soil chemistry, soil morphology, hydrogeology and numerical methods. The modelling teams similarly brought varied expertise to the effort. The integration occurred through the four phases of the LCT studies: (1) the site characterisation stage in which the soil horizons were mapped in detailed; in situ saturated hydraulic conductivity tests were performed; core samples were collected and tested for hydraulic and transport properties; and particle size distributions were analysed [*Wierenga et al., 1989*]; (2) the design, construction and conducting of the Plot 1 experiment [*Hills et al., 1989a* and *1989b*]; (3) the design and execution of the Plot 2a experiment using information and analysis of the Plot 1 experiment [*Wierenga et al. 1990*]; and (4) the final design and execution of the Plot 2b experiment using the detailed monitored data and analysis from the Plot 2a experiment [*Hills and Wierenga, 1994*]. The integration is also reflected in the joint authorship of the numerous papers produced and the subjects discussed (e.g., field and laboratory studies as well as modelling). Ultimately the integration occurred in the analysis of the site characterisation, field experimental, and modelling results as discussed in *Hills and Wierenga* [*1994*].


Transect 1 - Observed

Transect 1 - Simulated

Transect 2 - Observed

Transect 2 - Simulated

Transect 3 - Observed

Transect 3 - Simulated

Figure 2.3 Observed and simulated water content distributions for day 70 (from Rockhold et al., [1994]).

2.1.9 Performance Measures Used to Assess Modelling Results

For the INTRAVAL Phase 2 analysis, the performance measures used to assess the simulation results consisted of both point comparisons, and integrated comparisons with the experimental data.

Point Comparisons

The point comparisons were;

1. Contour plots of observed and predicted water contents and solute concentrations,

2. Scatter plots of observed and predicted water contents and solute concentrations, and

3. First arrival times of the water and solute plumes as a function of depth.

Contour plots as presented in *Hills and Wierenga* [*1994*] were very useful in visualising the behaviour of the wetting front, moisture redistribution, and the solute plume. However, caution is advised in interpreting these plots since the contour results often are very dependent on the contouring algorithm.

Therefore, the second point value comparison approach used was scatter plots of observed versus predicted volumetric water contents and normalised solute concentrations. The LCT Pilot Team considered scatter plots to provide a more realistic assessment of point value predictions than the contour plots because contouring methods inherently (sometimes intentionally) average data and because the resulting contours can be very dependent on the analytical techniques used to generate the contours. It was also felt that scatter plots have the added advantage of showing the scatter of the observations about the predictions which give a good indication of bias and uncertainty about the mean [*Hills and Wierenga, 1994*].

The third point value comparison approach used plots of first arrival times of the water and solute plumes at various depths. The LCT Pilot Team defined the time of arrival of the water plume as that time when the volumetric water content increased by 0.03 from the initial conditions in any of the three measurement planes y = 2, 6, and 10 m [*Hills and Wierenga, 1994*].

Integrated Comparisons

The integrated quantities used for comparison as discussed in *Hills and Wierenga* [*1994*] were:

1. First and second moments of the water and tritium plumes as a function of time;

2. The normalised change in total water volume below each of the z=0, 1,..., 5 m horizontal planes as a function of time; (The LCT Pilot Team felt that the observed changes in water

volume below a horizontal plane was a good estimator of the water to pass through that plane while the plume remained fully observable.) and

3. The changes in the sum of relative tritium concentration below each of the z=0,1,..., 5 m horizontal planes as a function of time.

Implementation

The LCT Pilot Team wrote four FORTRAN programs to generate the desired data files, given the point values of the experimental data and model predictions [*Hills and Wierenga, 1994*]. Two programs processed the data for water flow and two processed the data for tritium transport for the point and integrated quantities outlined above.

2.1.10 Principal Findings

The assessment of success involved both model testing and the repeated reevaluation of the experimental results. Both field monitoring data and destructive core sampling were used in these reevaluations. The success was also measured by the advance in knowledge and datasets created [*Wierenga et al., 1993*]. The following observations as discussed in the final LCT INTRAVAL report [*Hills and Wierenga, 1994*] demonstrate this interrelationship between model testing and field analysis.

Sufficiency of Experimental Data

"The testing of models using data from dry, spatially variable soils is not a trivial task. Not only is it difficult to characterise the site, but it is difficult to obtain sufficient high quality solute samples to obtain good estimates of the movement of solute plumes as a function of time. In contrast, water flow in unsaturated soils is easier to monitor. Neutron probes allow water to be monitored at many locations and the measurements are very consistent day to day over periods of years. For the Plot 2b experiment, the total increase in water observed by the neutron probe just after irrigation was very close to the actual water applied (less than 1% error) suggesting that given the spatial variability of the site, the number and location of the neutron probe measurements were sufficient to resolve the water plume."

Differences in Model Predictions

The final LCT report goes on to indicate that "there are considerable differences in model predictions even though all the modellers had access to the same very large characterisation data set for the Las Cruces Trench experiments. Some of the models presented were fairly simple and assumed uniform soil hydraulic property fields while others conditioned the soil models on the observed two-dimensional spatial heterogeneities observed in the trench face. Even though many models were considered, none of the models stood out as clearly superior. All of the models under predicted first arrival times of the water plume at depths greater than 4.5 m and the models that tended to do well by one measure of mean behaviour would often perform poorly by another. Since the probability distributions of the prediction errors do not appear to be well defined and were not clearly distributed as normal or log-normal for all of the models considered, parametric statistical tests were not performed. Less powerful non-parametric tests were used. As a result of these quantitative and graphical comparisons, several observations can be made:

The CNWRA and PNL models consistently provided better predictions of mean or median water contents (i.e., near zero mean or median predictions errors) which suggested a good accounting for the total mass in the system. This was likely due to the extra care CNWRA and PNL exercised in modelling the actual spatial distribution of the initial water contents. However, the improvement in mass balance that resulted did not necessarily lead to a reduction in the spread of the population prediction errors (i.e. RMS error) about zero relative to the other models. NMSU1, for example, showed a lower RMS than the CNWRA models. Thus accurately modelling the initial conditions does not, in itself, always lead to improved predictions for water flow.

Time of first arrival times of the water plume were greater for the experiment than for any of the models once the plume reached 4.5 m. This indicates that none of the models provided conservative estimates for these travel times from a regulatory point of view since they all over-predicted these times. While this is expected for the uniform soil models since they predict mean behaviour, this was not expected to be always true for the heterogeneous soil models. Contour plots of experimental water contents show that a dry layer extends throughout the measurement domain. This layer was not well-predicted by any of the models. It is not clear whether this is due to limitations in the experimental characterisation procedures, the inability of *Mualem's model* [*1976*] to predict unsaturated hydraulic conductivity for this soil layer given the *van Genuchten retention model* [*1980a*], or simply due to differences between the soil properties at and away from the trench face.

The observed change in the volume of water below all depths greater than 3 m was significantly greater than that predicted by all of the models except for PNL3. While PNL3 was conservative from a regulatory point of view in the sense that it overpredicted the change in water content at depth, its behaviour during redistribution was considerably different from that observed in the experiment. The predicted water plume was much more diffuse than the observed plume and more horizontal spreading was predicted. The hydraulic parameters used by PNL3 were obtained with a 1-D inverse procedure [*Rockhold, 1993*] using the experimental observations obtained during infiltration for the Plot 1 experiment. In contrast, the soil characterisation used by the other models was based on outflow data obtained from core and disturbed soil samples. This may explain why the other models (except MIT1) performed better during redistribution.

The two models, PNL2 and MIT1, conceptualised the soil as anisotropic. MIT1 overpredicted the water plume spreading and underpredicted vertical plume movement as did PNL2. PNL2 assumed that the horizontal hydraulic conductivity was twice the vertical whereas MIT1 used a tension dependent anisotropy derived from stochastic theory. For the first 310 days of the experiment, neither model seemed appropriate. The more conventional isotropic models performed as well or better. However, significant heterogeneity induced anisotropy may be present later in redistribution when the plume becomes larger and when the gravitational forces become less important relative to the matric potential forces.

The initial water contents used in the BEG1 model were significantly larger than those observed in the field. While this had the effect of accelerating the downward motion of the water plume which gave good first arrival time estimates, BEG1 performed poorly by many of the other measures.

Results from Phase 1 of INTRAVAL for the Plot 2a experiment suggested that water movement was easier to model than tritium transport [*Voss and Nicholson, 1993*]. However, most of the model comparisons made during the Plot 2a experiment were side by side comparisons of smoothed contour plots. The more extensive comparisons made here do not support this hypothesis. Tritium transport predictions for the Plot 2b experiment were more acceptable than the corresponding water flow predictions in the sense that the observed tritium behaviour (first arrival times, change in tritium concentrations below a horizon) was bounded by the various model predictions whereas the observed water flow was not. It is not clear if this is because tritium transport occurs in the wetter portion of the water plume or simply because the tritium plume did not pass through the anomalous dry layer at 3 m.

The present results indicate that models that appear superior or conservative (from a regulatory point of view) for water flow do not necessarily lead to superior or conservative predictions for tritium transport. For example, the PNL models generally gave better predictions of mean or median water contents while the NMSU models generally gave better predictions of mean or median solute concentrations. Only PNL4 provided conservative estimates of first arrival time down to 4 m for the water plume. In contrast, only the heterogeneous NMSU3 and NMSU4 models provided conservative estimates of first arrival times for the tritium plume introduced during the Plot 2a experiment whereas the heterogeneous models NMSU3 and NMSU5 and the uniform soil model PNL1 provided conservative estimates of arrival time of the plume introduced during the Plot 2b experiment. These results support the idea that using multiple realisations of heterogeneous soil models (i.e., NMSU2-NMSU5) is an appropriate way to bound contaminant plume behaviour.

Overall, the results of the present work show that for this particular experiment, traditional uniform soil or heterogeneous soil models conditioned on detailed site characterisation data can predict the overall features of water flow and tritium transport. Even though there are considerable differences in how the models conceptualised the soil profile, no model was clearly superior overall. Superior models by one measure were not always superior by another. This suggests that the effect of characterisation uncertainty, even when the site is characterised as thoroughly as the Las Cruces Trench Site, may have a greater impact on model predictions than differences in how the models conceptualise the soil.

The LCT studies and the model testing demonstrated one approach to validation through interactive laboratory and field experiments and modelling using a quantitative-based model testing strategy with performance measures tied directly to regulatory significant criteria.

2.2 Apache Leap Tuff Site Studies

2.2.1 Background

The Apache Leap Tuff Site (ALTS) studies originated as a research effort by investigators at the University of Arizona to examine site characterisation and conceptual model issues associated with high-level radioactive waste repositories. As discussed in *Yeh et al.,* [*1987*] the objective of this pre-INTRAVAL study was to examine models and strategies for obtaining characterisation data. Specifically, the design document stated that "Characterisation of fluid flow and solute transport through unsaturated fractured rock requires that site-specific conceptual models be defined, parameters for the models be estimated using field and laboratory data, and validation of the conceptual models be performed" [*Yeh et al., 1987*]. The great difficulty was that an understanding of the fundamental processes, and the development of conceptual models describing flow and transport in unsaturated, fractured rock was in its infancy. As opposed to the Las Cruces Trench studies, the focus needed to be on a much more fundamental and primitive level in which characterisation techniques and conceptual model development was very much in question.

2.2.2 Experimental Objectives

For the INTRAVAL Project, the ALTS studies were reformulated to meet the goal of testing conceptual models and their linkage to characterisation approaches. The experimental objectives were: (1) to verify the existence of proposed processes, and the parametric form of hypothesised material properties; and (2) to examine conceptual models and characterisation approaches over a range of scales and processes using the following approaches;

1. Rock matrix characterisation experiments for hydraulic, pneumatic and thermal properties using small (2.5 x 6.0 cm), and large (12 x 10 cm) cores;

2. Non-isothermal core experiments for coupled water, vapour and solute movement using (9.6 x 12 cm) core;

3. Rock fracture characterisation studies and analyses of water and gaseous flow properties using a (20 x 21 x 93 cm) block with persistent single fracture;

4. Fracture imbibition experiments for determining imbibition rates and related properties using a (20 x 21 x 93 cm) block with persistent single fracture; and

5. Field air injection experiments for characterising the heterogeneity of fracture-related permeabilities, and for examining dependency of measured pneumatic properties on measurement support (length of test interval) using inclined 30 m boreholes intersecting fractures.

These experimental objectives were addressed through numerous laboratory and field experiments, and are discussed in detail in *Rasmussen et al.* [*1994*], *Bassett et al.* [*1994*], and *Rasmussen et al.* [*1990*].

2.2.3 Experimental Design

Figure 2.4 illustrates the experimental design for the core and block studies (numbers 1, and 3 above) used to determine hydraulic, pneumatic, and gaseous transport property values for the matrix and fractures. The core and block specimens used were taken from the Apache Leap Tuff (white unit). The block contained a discrete fracture along the long axis. Details are provided in *Rasmussen et al.* [*1990*].

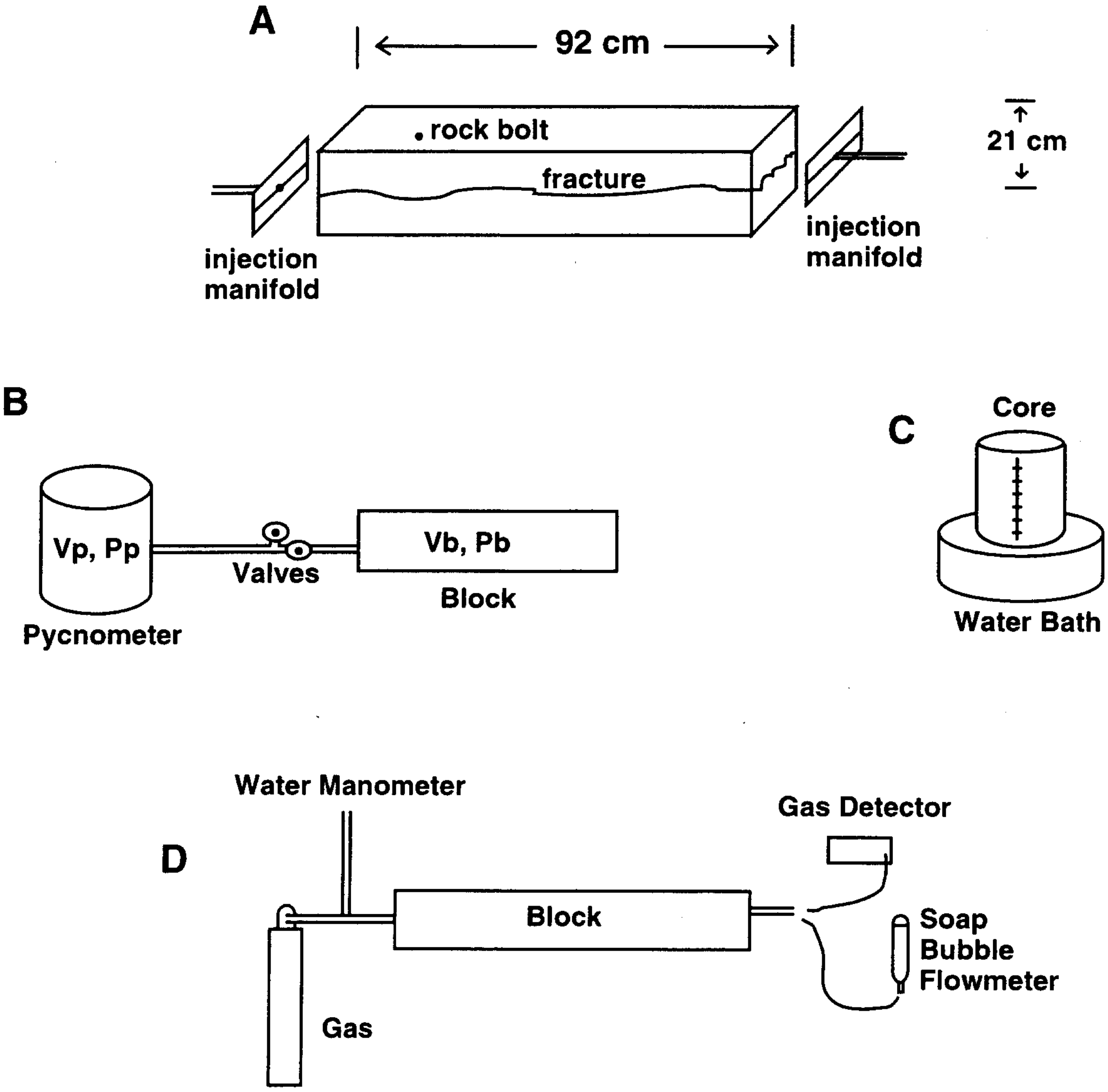


Figure 2.4 Experimental setups for (A) the wetting front experiment for the fractured block; (B) the rock porosity measurement experiments of the matrix using a pycnometer; (C) hydraulic diffusivity coefficient measurement using a core imbibition experiment; and (D) gas diffusion coefficient measurements and breakthrough curve experiment. (from Bassett et al., [1994]).

The experimental setup for the core heater experiment (number 2 above) used a large core measuring 9.6 cm in diameter and 12 cm in length that was subjected to a series of coupled heat, water, vapour and solute transport experiments. These experiments involved the use of a one-dimensional thermal gradient (5 to 45 °C) applied along the long-axis of the core. The core was hermetically sealed and insulated to provide a closed system for air and water. Dual-gamma attenuation methods were employed to provide water content and solute concentration profiles along the length of the core. Coincident temperatures along the core using thermocouple ports were also measured. Solute concentrations at the end of the experiment were determined [*Rasmussen et al., 1994*].

Figure 2.5 provides a three-dimensional portrayal of the 15 inclined and vertical boreholes at the ALTS. Figure 2.6 provides a schematic representation of the air injection setup (number 5 above) for determining the apparent permeabilities along the borehole intervals. The permeability tests consisted of imposing a sequence of increasing flow rates (a minimum of three), each of which was continued until a steady state pressure response was attained. Air pressure, temperature and relative humidity were measured at the surface and the injection interval. Atmospheric temperature and pressure were also monitored. The flow rate was preset at the surface with the aid of electronic mass flow controllers.

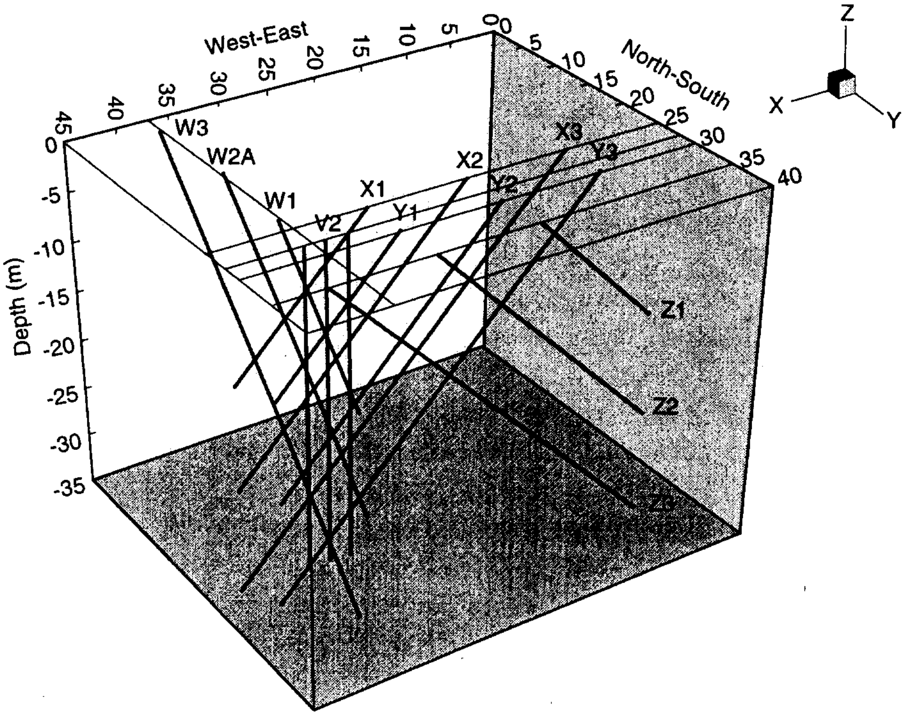


Figure 2.5 Borehole location at the Apache Leap Tuff Site (from Guzman-Guzman and Neuman, [1994]).

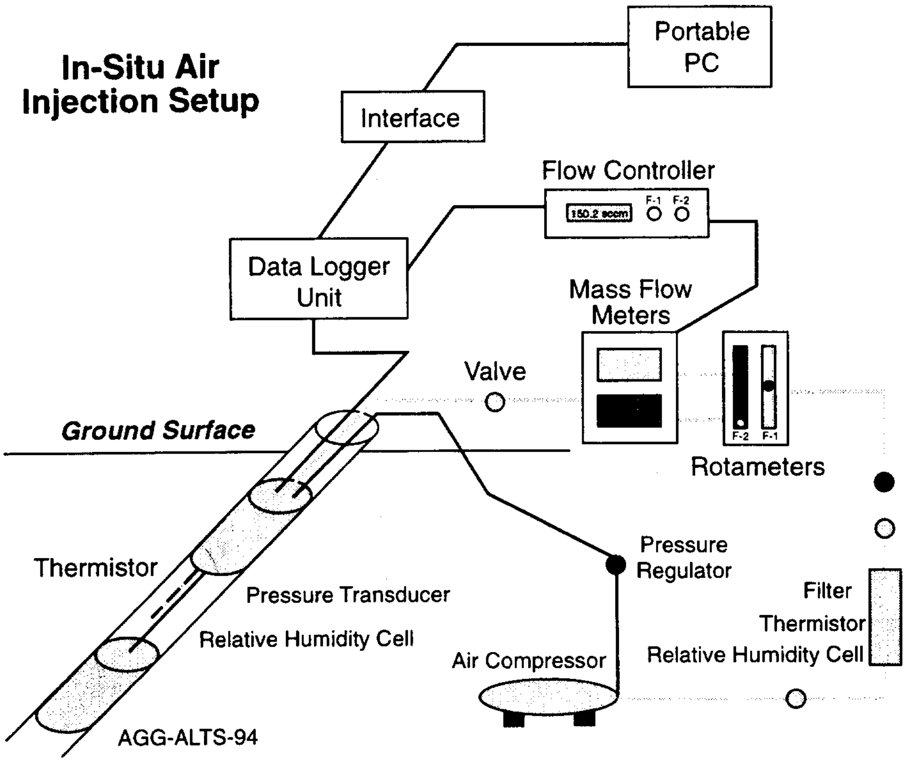


Figure 2.6 Schematic representation of the air injection system (Guzman-Guzman and Neuman, [1994]).

2.2.4 Experimental Analysis

The five distinct groups of studies (see above) produced significant datasets as discussed in *Rasmussen et al.* [*1994*]. The information produced, and the analysis of these datasets have been summarised in the final INTRAVAL report [*Rasmussen et al., 1994*] as follows:

1. Laboratory analyses of the first set of experiments on the small core samples provided characterisation data related to porosity, characteristic curves, hydraulic conductivity, air permeability and thermal conductivity. The effects of variable water contents, hysteresis and temperature on the physical parameters were examined, as well as, the effects of solute concentrations on ambient matric potential.

2. The core heater experiment demonstrated the presence of an active heat pipe which was observed when the core was brought to an intermediate water content. The resulting latent heat transport was insignificant in comparison to the conductive heat transport in this experiment. When a soluble salt (NaI) was introduced into the experiment, the heat pipe phenomenon was not as active due to the increased osmotic potential near the warm end of the core. The increased osmotic potential lowered the vapour pressure near the warm end and reduced the vapour phase transport of water.

3. The third set of studies conducted on the fractured rock block provided information to characterise the physical properties of the block. Equivalent fracture apertures were obtained using six types of experiments. Three volumetric fracture aperture values were obtained by using a pycnometer, tracer breakthrough volumes, and the ratio of fracture transmissivity to fracture hydraulic conductivity. Two Poiseuille apertures were obtained using a cubic aperture equation applied to gas and water flow rates, and using a quadratic aperture equation gas breakthrough velocities. A final estimate of fracture aperture was obtained using the air-entry potential of the saturated fracture.

4. A horizontal fracture imbibition experiment was conducted using water as a fluid imbibed into an initially dry fractured rock to obtain values of cumulative water imbibition volume, and to examine visible wetting front positions.

5. The field air-injection datasets consisted of *in-situ* air-permeability measurements obtained from straddle-packer tests on selected intervals of the boreholes. At the completion of each injection test, there were at least seven different sets of data that could be used to determine the air permeability of the rock surrounding the interval tested; three transient sets during injection; three steady state sets and one recovery set. The datasets consisted of air-permeability measurements at different scales (0.5, 1.0 and 3.0 m) and at multiple-injection rates in six of the boreholes [*Guzman-Guzman and Neuman, 1994*].

2.2.5 Models Developed for Testing

The following models were developed for testing:

1. Characterisation models used to define the porosity, characteristic curves, hydraulic conductivity, air permeability and thermal conductivity for the rock matrix using small cores were tested. The models were examined to determine how sensitive they were to a range of water contents, hysteresis and temperatures.

2. Conceptual models describing flow through a single fracture were tested using the large block experiment. Property values for the matrix and fracture apertures were measured repeatedly and compared to the model estimates.

3. The approximate analytic model of *Nitao and Buscheck* [*1991*] was evaluated for its ability to predict the behaviour of water imbibition into initially dry fractured rock. The model was evaluated to determine its suitability for use in understanding unsaturated flow.

4. Conceptual models dealing with scale effects (i.e., that due to the growth of permeability and dispersivity with support scale), and spatial distributions of heterogeneities were tested using datasets from the *in situ* air-injections studies [*Guzman-Guzman and Neuman, 1994*].

2.2.6 Model Comparison and Testing Strategy

For the characterisation models, the experimental data indicated that variations in temperature affect the shape and position of the moisture-retention curve, and by inference, the shape and position of the relative permeability curve. The wetting history was also shown to have a large influence on the moisture-retention characteristic curve. Thermal conductivity was shown to be only poorly related in a linear fashion to water content. The effects of solute concentrations on ambient matric potential are also demonstrated. It can be concluded that accumulations of saturated salt solutions will increase the osmotic potential which in turn affects the total potential observed under non-isothermal conditions.

For the fracture flow conceptual models, the volumetric apertures estimated using the pycnometer and the tracer breakthrough volumes were closely related. The volumetric aperture determined using the ratio of fracture transmissivity to hydraulic conductivity was less, followed by the apertures determined using the cubic and quadratic equations, respectively. The smallest aperture observed was the capillary aperture. This progression is consistent with the hypothesis that fracture roughness will decrease the effective flow area for the Poiseuille flow, and induce an ink bottle effect at fracture constrictions.

For the approximate analytic model of *Nitao and Buscheck [1991]*, a horizontal fracture imbibition experiment was also conducted using water as a fluid imbibed into an initially dry fractured rock. The imbibition rate was reproduced using a model developed by *Nitao and Buscheck [1991]*. The form of the model was found to provide a good fit to the shape of the observed data, but the model overestimated the fracture imbibition volume by a factor of twenty and the fracture wetting front advance by a factor of eight. The noted reduction in water inflow may be due to phenomena neglected in the theoretical model, such as fracture surface coatings or enhanced surface weathering, and the inability to accurately determine fracture physical properties *a priori*, such as the fracture water diffusivity. It was shown that fracture saturation behind the wetting front initially is very low, perhaps ten percent, but increases to complete saturation during the course of the experiment. This may indicate that fingers of saturation exist within the fracture during early time, and these fingers expand laterally and dissipate over time.

Data from the imbibition experiment reported here confirm the second imbibition phase as hypothesised by the Nitao and Buscheck model. The experiment was not able to distinguish either the first or third imbibition phase of their model. A new imbibition phase was observed, however, which resulted from the finite length of the fracture within the tuff. The Nitao and Buscheck model should be modified to incorporate the finite extent of discrete fractures. Another concern raised by the experiment was the failure to properly estimate fracture hydraulic properties. It is observed that laboratory estimates of rock fracture hydraulic properties, when used with the Nitao and Buscheck model, substantially overestimated the cumulative imbibition rate, and the rate of advance of the wetting front in the fractured block. Calibrated values of the fracture hydraulic parameter are substantially smaller than the characterisation value. An additional shortcoming of the model is the inability to reproduce the observed fingering of water within the fracture, although the fingering was limited only to the early fracture imbibition period. Fingering may be more important when vertically oriented fractures are present.

For the conceptual models dealing with scale effects and spatial distributions of heterogeneities, *in situ* air-injections tests were performed over a range of scales (i.e., 0.5, 1.0 and 3.0 m) and at multiple-injection rates. Field data indicate that the air permeability determinations are strongly affected by two-phase interaction between air and pore water, and in higher permeability zones by inertial flow effects. A 45-degree, 30-metre deep borehole was tested for permeability at three different scales to study the effect of measurement support on permeability estimates and their statistics [*Guzman-Guzman and Neuman, 1994*]. These measurements seem to indicate some dependency of the mean permeability on measurement support (length of test interval), a phenomenon known as "scale effect." Upscaling by weighted arithmetic averaging of the smaller measurement support data produces better estimates than geometric weighted averaging. High permeability values are, however, slightly underpredicted by either upscaling approach. Although the observed variability of air permeabilities at the ALTS is over 3.5 orders of magnitude, the data are amenable to classical geostatistical analysis and yield well-defined semivariograms. The omni-directional semivariogram.exhibits a nested structure with two distinct plateaus and correlation scales, and an additional correlation structure whose sill and range are undefined due to the limited extent of the experimental site [*Guzman-Guzman and Neuman, 1994*]. It was also observed that the increase in the variance and correlation scale which grew with the scale, is consistent with the multi-scale continua concept discussed by *Burrough* [*1983*], and *Neuman* [*1987, 1990, 1993, 1994*]. The available fractured rock permeability data can be viewed as a sample from a random (stochastic) field defined over a continuum with multiple scales of heterogeneity [*Guzman-Guzman and Neuman, 1994*].

2.2.7 Alternative Conceptual Models Tested and Assessed

The alternative conceptual models considered were an equivalent porous medium model and a model that considered the discrete fracture network embedded in a porous matrix. The models were tested by estimating the physical, hydraulic, pneumatic, and thermal properties for the discrete fracture, and then forming forecasts using the alternate conceptual and mathematical models. The forecasts for each conceptual model includes the 95% forecast confidence interval about the forecast, thus allowing assessment of the accuracy of the forecast when compared against the experimental result. The confidence intervals were generated by first measuring the uncertainties in the input parameters, and then propagating those input parameter uncertainties through the model using a Taylor series expansion. The model outputs were then compared against experimental results. Because the experimental results also contain uncertainties, the observed confidence intervals were also generated.

2.2.8 Integration of Multi-Disciplines

The test program utilised expertise from various disciplines as consultants. The core personnel were hydrologists, with support from individuals trained in geology, engineering (civil, chemical, mechanical, nuclear and geological), rock mechanics, and chemistry. The integration occurred through experimental design meetings and reports, discussions of experimental and modelling results, and joint field trips for examining and collecting flow and transport property measurements.

2.2.9 Evaluation Criteria

Success in experimental design and model performance was evaluated in two ways, heuristically and statistically. The models were tested heuristically by noting whether reasonable relationships between inputs and outputs were observed. Input parameters were varied and outputs were examined to survey the trend in response to combinations of inputs. The experiments were examined heuristically to note whether the measured responses were consistent with *a priori* estimates of system responses. Several defective experiments were found using this method.

The statistical evaluation consisted of comparing model forecast confidence intervals with the experimental results. If the experimental results were found to lie within 95% confidence region for the model forecast, then the model could not be rejected.

2.2.10 Principal Findings

The accomplishments of the test case were: (1) development of characterisation and calibration datasets that are useful for testing and evaluating conceptual and numerical models; (2) development of new characterisation techniques suitable for field-scale characterisation of unsaturated fractured rock; (3) development of new analytical techniques for analysing field tests (e.g., air permeability testing at various scales); and (4) estimation of parameter uncertainties in the characterisation experiments to quantify prediction accuracy.

Laboratory Experimental Results

Results of laboratory experiments conducted to characterise fluid and thermal flow parameters of unsaturated Apache Leap Tuff indicate that hysteresis influences the moisture characteristic curve. Wetting and drying characteristic curves are markedly different, with the wetting curve consistently showing higher matric potentials at equivalent water contents. Efforts to identify the matric potential from water contents of unsaturated rock will require knowledge of the water content history of the site. The successful application of osmotic solutions to maintain constant matric potentials was demonstrated. Saturated salt solutions present in the geologic environment may affect the observed matric potential. Near a repository, accumulations of soluble salts may affect the migration of liquid and vapour due to the osmotic potential induced at high salt concentrations. Coupling of salt concentrations with water activity should be an integral component of simulation models of fluid flow near the waste repository.

Temperature is shown to affect the characteristic curve. Both reduced and increased temperatures cause substantial shifts in the characteristic curve, attributable to the change in the temperature dependence of the fluid surface tension. Coupling of hysteresis effects with temperature changes was not evaluated, nor were changes in the characteristic curves evaluated as a function of dynamic temperature changes. Additional characterisation studies will be required to address the effects of temperature fluctuations on characteristic curves.

The relative permeabilities for air and water were determined using rock cores. Estimates of permeabilities were obtained under isothermal conditions. Additional experiments will be required to evaluate the importance of temperature on water and air relative permeability functions.

The influence of water content on the thermal conductivity was examined using a one-dimensional heat cell. A linear relationship between water content and thermal conductivity was not clearly demonstrated. Observed mean thermal conductivities were less than expected for the range of volumetric water contents from 0 to 0.0876. Additional studies will be required to investigate the nature of the unsaturated thermal conductivity relationship, and the influence of hysteresis on the relationship.

Laboratory experiments conducted to observe thermal, liquid, vapour and solute transport through variably saturated, fractured Apache Leap Tuff demonstrate that:

1. Conduction is the dominant heat transport mechanism even when a significant heat pipe effect is present.
2. Water contents increase away from the heat source due to vapour driven advection and condensation.
3. Solutes accumulate near the heat source, but the accumulation of solutes increases the osmotic potential which decreases the heat pipe phenomenon.
4. The heat pipe process may not significantly affect thermal or liquid flow in materials similar to the Apache Leap Tuff samples examined.
5. Solute transport was substantially affected by the heat pipe phenomenon, resulting in the accumulation of significant solutes nearer the heat source than would have occurred if the heat pipe had not been present.
6. Models of heat and liquid flow near high level waste repositories may not need to incorporate heat pipe effects.
7. Models of solute transport should incorporate the heat pipe phenomenon, and should also consider the effects of osmotic potential on liquid and vapour transport.

These observations may only be relevant to the conditions examined. Additional laboratory and computer simulation experiments should be conducted to evaluate the effects of coupled thermal, liquid, vapour and solute transport over a wider range of material properties. Also, the effects of thermomechanical, geochemical, biogeochemical, and radiation-induced changes will also require examination. It is possible that processes not yet considered may significantly affect the migration of radionuclides in the region immediately adjacent to the waste repository. Field and laboratory-scale experiments are necessary to identify these unknown processes.

Uncertainty Assessments

Table 2.4 presents estimated characterisation properties of the rock matrix and the embedded fracture. Several parameters, including the fracture porosity, liquid saturation changes across the wetting front in the fracture and rock matrix are assumed values. Table 2.4 also presents characterisation parameters with their uncertainties. Uncertainties in the derived parameters were estimated by propagating parameter uncertainties using first-order Taylor series approximations.

Table 2.4 Fractured block characterisation parameters (from Rasmussen et al., [1994]).

		mean ± std. dev.
Rock Matrix Properties:		
V	rock volume	39,240 ± 0 cm^3
V_t	pore plus fracture volume	4,635 ± 120 cm^3
V_m	matrix pore volume	4,493 ± 127 cm^3
θ_m	porosity	0.115 ± 0.003
Δs_m	liquid saturation change	1 ± 0 (1)
D_m	water diffusivity coefficient	3.61 ± 0.28 $cm^2\ hr^{-1}$
D_g	argon gas diffusion coefficient	31.0 ± 0.94 $cm^2\ hr^{-1}$
Rock Fracture Properties:		
V_f	volume	142.3 ± 41.7 cm^3
w	width	20.2 ± 0 cm
a	fracture-boundary distance	10.5 ± 3 cm
b	half-aperture	381 ± 11 μm
L	length	92.5 ± 0 cm
θ_f	porosity	1 ± 0 (1)
Δs_f	liquid saturation change	1 ± 0 (1)
K_f	hydraulic conductivity	9650 ± 504 cm hr^{-1}
T_f	transmissivity	490 ± 25.2 $cm^2\ hr^{-1}$
D_f	water diffusivity coefficient	

Note: (1) Assumed value.

A first-order approximation of parameter uncertainty propagation was estimated using the Taylor series expansion of the input errors.

Characterisation techniques which demonstrate promise for estimating material properties on field scales include the use of a pycnometer to measure fracture and matrix porosities, and gas-phase tracer experiments to estimate the fracture/matrix porosity ratio, the permeability distribution, and the porosity-length distribution. While these indices are only strictly appropriate for gas-phase transport, inferences to liquid phase transport may be derived if relationships between gas and liquid phase transport are known. It is anticipated that gas-phase testing using tracers will become a rapid and effective tool for characterising macropores on field scales. The interactions between matric storage and advection through fractures have been demonstrated in the laboratory, and field scale experiments are being explored to apply this new technique.

Interpretation of fracture aperture estimates is complicated by the observation that the estimated value is a function of the method employed to provide the estimate. Six measures of fracture aperture were developed and comparisons were made between methods. It was observed that volumetric measures of fracture aperture yield the highest values, with lower estimates provided by measures using Poiseuille's law. The lowest estimate was obtained using capillary theory. It can be concluded that when fracture aperture measurements are reported, the method employed to provide the estimate should also be indicated.

Uncertainty measures of characterisation parameters are also presented in *Rasmussen et al.* [*1994*]. The uncertainty in the measured parameter are required to evaluate the uncertainty in predictions based upon the parameter. Forecasts of flow and transport will require measures of uncertainty in the forecast. Uncertainties in estimated parameters may contribute to large errors in forecasts.

Field Experimental Results

Based on an extensive data set consisting of steady state apparent air permeability values, the following conclusions are presented in *Guzman-Guzman and Neuman* [*1994*]. The apparent air permeability from straddle-packer tests is a strong function of the applied pressure. Changes in air permeability with pressure are due to two-phase flow and, in some cases to inertial flow. Computer simulations confirmed the two-phase flow explanation. Upscaling of the apparent permeability is accomplished best via weighted arithmetic averaging. Geostatistical and statistical analyses indicate that the apparent permeability data from ALTS behave as a stochastic multiscale continuum with an echelon (see Figure 2.7), and power-law (fractal) structure as shown in Figure 2.8. The latter is associated with a Hurst coefficient $w = 0.28$ to 0.29 which is remarkably close to the generalised value $w = 0.25$ predicted by *Neuman* [*1990, 1994*]. Additional permeability tests spanning larger rock volumes at ALTS would help to determine whether the seemingly fractal behaviour extends beyond the scales already tested.

As presented in *Guzman-Guzman and Neuman* [*1994*] analysis results strongly suggest that site characterisations must be based on hydrogeologic data collected on a spectrum of scales relevant to performance assessment. They further point out the need to consider two-phase flow and inertia effects in the interpretation of air injection tests. The transient part of these tests may hold the key to site evaluation of functional relationships between rock permeability, fluid pressure and saturation. The ALTS investigators report that the inverse methods hold a promise in this regard, and propose to use them in the context of their ALTS data.

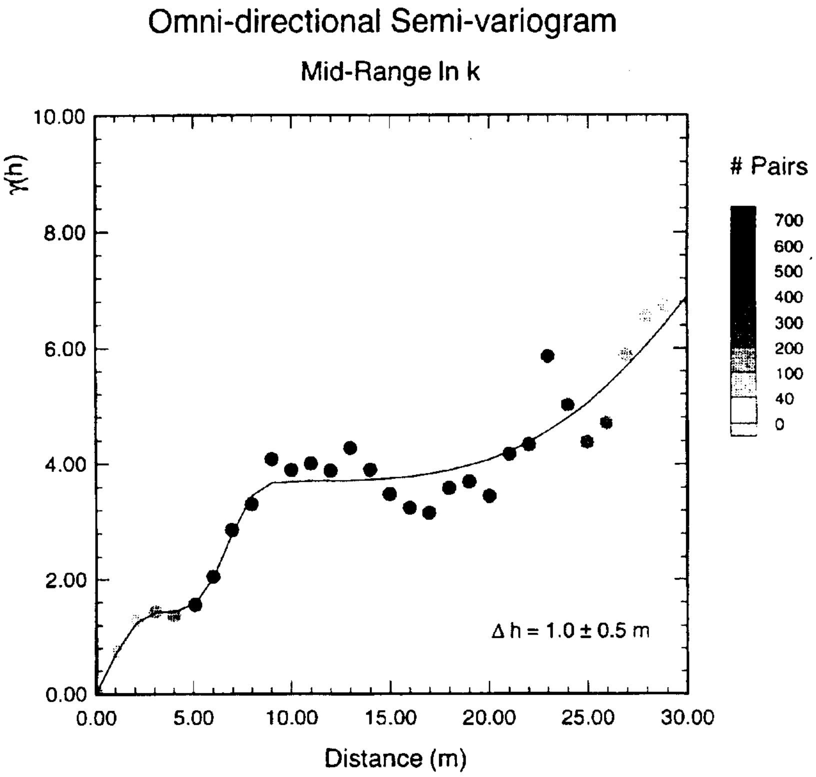


Figure 2.7 Three-dimensional omni-scale directional semivariogram of ln k 1-m scale (from [Rasmussen et al. 1996]).

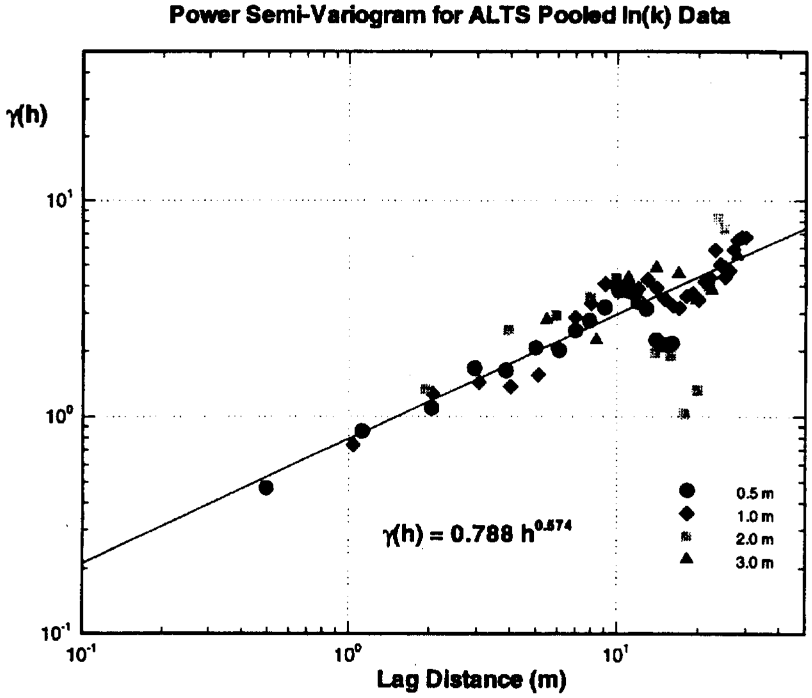


Figure 2.8 Log-Log semivariogram of ln k of the pooled data from the 0.5-, 1.0-, and 3.0-m scales.

3 Significant Lessons

During the Phase 2 effort significant accomplishments were realised. The LAS Cruces Trench (LCT) Test Case studies created the definitive field dataset for testing water flow and solute transport models as applied to variably saturated conditions in heterogeneous soils. The detailed LCT datasets provided greater information on spatial heterogeneity, moisture migration and redistribution, and coincident tracer movement than was previously available. The modellers had sufficient detailed information to conduct their simulations over a wide range of possible conceptual models. The use of sophisticated model comparison strategies was possible due to the extensive LCT experimental data available for three distinct field experiments. An iterative approach to modelling the three experiments (i.e., conceptualisation, characterisation, calibration and validation) was realised.

For the Apache Leap Tuff (ALT) Test Case, the accomplishments included: (1) development of characterisation and calibration datasets that are useful for testing and evaluating conceptual and numerical models; (2) development of new characterisation techniques suitable for field-scale characterisation of unsaturated fractured rock; (3) development of new analytical techniques for analysing field tests (e.g., air permeability testing at various scales); and (4) estimation of parameter uncertainties using the characterisation experiments to quantify prediction accuracy.

3.1 Characterisation Instrumentation & Methods

Both the LCT and ALT studies provided new characterisation strategies, methods and instrumentation. For example, the LCT studies used a combination of solution samplers and destructive core sampling to map the tracer movement during the "2b experiment". The ALT studies developed new methods for conducting air permeability testing and analyses in unsaturated fractured rock. Another major technical difficulty was overcome with the development of a vacuum distillation method for obtaining water and gas samples from rock core collected at the ALT site.

3.2 Conceptual Model Development

A significant accomplishment for both the LCT and ALT studies was the pursuit of alternative conceptual models. The testing strategy reflected a wide range of conceptual alternatives for characterising and modelling the experiments. For example the LCT models cover the range of uniform property to detailed discretised spatial property values (both deterministic and stochastic) based upon site data.

For the ALT studies, a variety of conceptual models dwelling on fundamental flow processes were evaluated against experimental data. Conclusions drawn were: (1) wetting history has a significant influence on formulating the characteristic curve; (2) thermal conductivity is only poorly related in a linear fashion to water content; and (3) the fracture saturation behind the wetting front initially is very low, perhaps ten percent, but increases to complete saturation during the course of the block wetting experiment contrary to the modelling results which overestimated the fracture imbibition volume by a factor of twenty, and the fracture wetting front advance by a factor of eight. Another example was the examination of conceptual models dealing with scale effects and spatial distributions of heterogeneities using datasets from the *in situ* air-injection studies.

3.3 Comparison Strategies and Measures

The LCT studies developed a very sophisticated approach to model comparison using both point (e.g., contour plots, scatter plots, and first arrival times) and integrated (e.g., first and second moments, normalised change in total water volume, and changes in the sum of relative tritium concentrations at specific horizons) measure comparisons coupled to a "blind" testing method. Detailed comparisons cover the entire range of the experiment (both early and later time horizons for the water and tracer movement). The LCT Test Case was the only test case to develop the validation experiment (i.e., "2b experiment") during Phase 2 (not *a priori*) using the model comparison strategy.

3.4 Acceptance Criteria

Again, the LCT test case was unique in developing detailed quantitative acceptance criteria based upon both statistical measures using the experimental data, and uncertainty information for the alternative conceptual models. The ALT acceptance criteria were generally qualitative focusing on characterisation and conceptual model testing.

4 Conclusions

Both the LCT and ALT studies contributed significantly to the field of characterisation strategies, methods and instrumentation. The field and earlier laboratory studies provided a wealth of data and practical experience in applying their innovative characterisation strategies, methods and instrumentation. Questions addressed included how to represent hydrogeologic heterogeneities over a range of scales, over what time-space continuum did the field methods, experimental data and numerical models function, the role of persistent discontinuities (e.g., macro-pores, faults and major fractures) in developing preferential infiltration and flow paths, and in estimating the scale effect by understanding the relevant test interval length or "support scale" for the field data. The LCT Test Case proved to be the best example of how to conduct a validation experiment for testing site specific conceptual and numerical models. Specifically, the LCT validation experiment ("2b experiment") was designed using the input from the modellers, and tailored to the performance measures and acceptance criteria. The field experimentalists and modellers worked together through all phases of the testing program.

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