THE INTERNATIONAL INTRAVAL PROJECT

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

PHASE 2, Summary Report

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NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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Foreword

Radioactive waste management programmes in OECD countries cover a wide range of activities aiming at the gradual implementation of disposal concepts for various types of radionuclear waste. This concerns institutional and regulatory aspects as well as research and development activities related to the selection and characterisation of potential sites for radioactive waste disposal. Among these activities, safety issues are of particular interest and enjoy a high priority in international co-operative programmes.

The international study INTRAVAL addressed the validation of models of the transport of radioactive substances through groundwater in the geosphere. The project started in 1987 on the initiative of the Swedish Nuclear Power Inspectorate with the general support of the OECD Nuclear Energy Agency. The study was performed in two phases, of which the first was reported in 1993. The second and final phase is summarised in this report. Twenty-three organisations from thirteen countries have participated in INTRAVAL Phase 2. Details of the organisations are given in Appendix 1.

During the course of the INTRAVAL projects, many reports have been published, including progress reports, reports on test cases for the project, and reports on studies and results of the test cases. This report gives a summary of the work performed under Phase 2 of INTRAVAL. In addition to the information presented in this summary report, the interested reader is referred to a report on the final results from the entire INTRAVAL project, compiled by a subcommittee set up by the project, as well as to working group reports issued by the project.

This summary report is being published after approval by the Coordinating Group for the project. Neither the Coordinating Group nor the Project Secretariat takes any legal responsibility for results presented in this report or for their future use.

Abstract

The international project INTRAVAL addresses the validation of models of transport of radionuclides through groundwater in the geosphere. Such models are used in the assessment of the long-term safety of radioactive waste disposal systems.

INTRAVAL is the third in a series of international projects concerned with related issues. The INTRACOIN project (1981–1986) dealt with verification of geosphere transport models, involving checking of the accuracy of computer programs. The HYDROCOIN project (1984–1990) addressed verification, validation, and sensitivity and uncertainty analysis of groundwater flow models. The INTRAVAL study has to a large extent built upon the experiences gained from these previous projects.

The purpose of INTRAVAL was to increase the understanding of mathematical models that describe various geophysical, hydrogeological and geochemical processes of importance in the safety assessment of nuclear waste repositories. This has been dealt with systematically using information from laboratory and field experiments and from natural analogue studies. A wide range of processes on various length and time-scales have been studied. An essential objective of INTRAVAL has been the study of the process of validation of employed computer models.

The first phase of the INTRAVAL study started in 1987 and lasted for three years. During that period, the main emphasis of the work was put on identification of important processes in model validation, based on laboratory and field experiment test cases.

22 organisations from 12 countries took part in this first phase of INTRAVAL, including both organisations responsible for the disposal of radioactive waste and regulatory agencies. The Swedish Nuclear Power Inspectorate (SKI) was responsible for initiating the study and acted as managing participant. Reports from INTRAVAL Phase 1 were published during 1992 to 1994.

The second phase of INTRAVAL, which started in 1990, was concluded at the end of 1993. The objective of Phase 2 was to increase the understanding how various geophysical, geohydrological and geochemical phenomena of importance for radionuclide transport from a repository to the biosphere could be described by mathematical models and to study the model validation process. 23 organisations from 13 countries, mostly the same as in Phase 1, participated in this second phase of INTRAVAL.

As in Phase 1, each organisation set up one or more project teams responsible for work within the project. Kemakta Consultants Co. has acted as principal investigator and has provided the secretariat in collaboration with the OECD Nuclear Energy Agency and Her Majesty's Inspectorate of Pollution, UK.

Only field cases were included in INTRAVAL Phase 2. The cases treated different rock types that have been proposed as suitable for nuclear waste repositories, namely unsaturated rock (Las Cruces Trench, and Apache Leap in USA), saturated fractured rock (Finnsjön and Stripa in Sweden), salt (WIPP in USA and Gorleben in Germany) and clay (Mol in Belgium). In addition, the natural analogue at Alligator Rivers in Australia was included. Different models were studied,

including stochastic models. As was pointed out in the previous studies, it was difficult to find field studies that were particularly suited to the objective of INTRAVAL Phase 2. Nevertheless the project teams were provided with a wealth of data from the selected sites.

The modellers fitted the results of their predictions to the data obtained in the field and supporting laboratory data. It was found that often a simple model could give nearly as good results as a complicated model. This was partly explained by a lack of experimental data on input parameters for the complicated model.

Stochastic models were extensively tested in a couple of cases and provided interesting results when fractures and layering were only partly known, as is nearly always the case.

In some cases, it was found that 1-D modelling gave as good, or sometimes better, results than 2-D or 3-D modelling.

Only in one instance, at Las Cruces Trench, was it possible to test the ability of the models to predict the outcome of performed experiments.

The scale problem was also treated. Obviously, it is not possible to perform studies over time scales that are related to the real lifetime of a nuclear waste repository. However, some information might be found from comparisons with natural analogues, for instance from studies of the uranium deposits at Alligator Rivers in Australia. The two teams that treated this test case found that, with reasonable assumptions of the climate over the last million years, the uranium migration at Koongarra has continued over a time period from half a million up to a few million years. This result agreed reasonably well with results from independent geomorphological information.

In addition to the summarised results from Phase 2 of the INTRAVAL study, which are presented in this report, detailed reports are also available.

Contents

1. Introduction

The safety of repositories for radioactive waste is an issue of great concern to the different bodies and organisations dealing with nuclear power production and the handling of radioactive materials, as well as to the general public. Several repositories for low- and intermediate-level waste have been brought into operation during the last ten or fifteen years. A few repositories have been in operation for a substantial time and some of these have almost reached their full waste holding capacity.

No repositories for high-level waste have so far (1997) obtained an operating license. One important reason for this is public reluctance and anxiety, which are tied to the stringent safety precautions that must be attached to these repositories, due to the long-term hazards connected with high-level nuclear waste.

A comprehensive understanding of the processes that govern the fate of the disposed radionuclides over time will be required to evaluate the safety of a nuclear waste repository. To facilitate the understanding of these processes, it has proved useful to describe them in mathematical terms resulting in mathematical models. A number of such models have been developed and are now being applied to performance assessment exercises dealing with nuclear waste repositories. Of particular interest to the INTRAVAL study are models that depict the transport of radionuclides in the geosphere. How well such models describe what actually takes place in space and time is a question of major concern. The evaluation of the models in this respect is often called validation.

The Swedish Nuclear Power Inspectorate (SKI) in 1980 took the initiative to organise in international collaboration a study of the validation of models for transport of radionuclides in the geosphere. At first the aim was primarily directed towards obtaining an understanding of the possibilities and the limitations of the use of the different models rather than the validation of computer models. Later on, the main emphasis was put on the validation process itself, using the models and test cases as means to comprehend the factors influencing the validation.

The first project for the purpose, INTRACOIN, started in 1981 with the participation of organisations from several countries, including safety authorities and implementing bodies. SKI took upon itself to lead the project as managing participant. The INTRACOIN study specifically addressed the verification of geosphere transport models and the checking of the accuracy of the computer programs. The study was finished in 1986 *[1, 2]*.

The INTRACOIN study was followed by the HYDROCOIN project (1984–1990) which was directed towards verification and validation, as well as sensitivity and uncertainty of groundwater flow models *[3–7]*.

Already, at the end of the INTRACOIN study in 1986, the participants felt that a more conclusive study was needed to get a better understanding of the long-term processes which are acting upon a nuclear waste repository. Having finished INTRACOIN and HYDROCOIN, the Coordinating Group of HYDROCOIN decided to initiate to a study, INTRAVAL, which should more fully address the process of validation of computer models for hydrology and nuclide transport in the geosphere. Based upon the work of an ad hoc group *[8, 9]* SKI invited organisations which had participated in the INTRACOIN and HYDROCOIN studies to participate in INTRAVAL and, having got positive answers, the new study could start in 1987. The participants, including some new members, agreed to cooperate for three years with the possible extension for an additional three year period.

The reports of the first phase of the INTRAVAL project were published in 1992 and 1993 *[10–23]* and a summary report in the beginning of 1994 *[24]*.

In the summary report of INTRAVAL Phase 1 it was stated that the goal of INTRAVAL should be "to provide a framework for international cooperation that can meet some major demands on the development of strategies for the validation of performance assessment models". To meet this goal more fully, the participating organisations in 1990 decided to extend the study for a second three year term.

The overall objectives of INTRAVAL Phase 1 were carried over to Phase 2, and the goal of the second phase was defined as an attempt to "increase the understanding of how various geophysical, geohydrological and geochemical phenomena of importance for radionuclide transport from a repository to the biosphere can be described by mathematical models and to study the model validation process". The purpose of INTRAVAL was specified to cover both validation of models with regard to the processes and site-specific systems. As the emphasis of the work in Phase 1 had been put on the identification of processes, based on laboratory experiment test cases, the focus of Phase 2 was shifted towards identification of structures. This led to increased complexity due to the increase in the number of degrees of freedom in the interpretation of the experiments and also because the analysis was to be based entirely on field scale experiments.

2. Organisation

The structure of the organisation for INTRAVAL Phase 2 has essentially been the same as for the first phase. The study was directed by a coordinating group with one member from each participating party. The Swedish Nuclear Power Inspectorate (SKI) acted as managing participant and a project secretariat was set up by the Inspectorate in cooperation with Her Majesty's Inspectorate of Pollution (HMIP/DoE), UK, and the Organisation for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA). Kemakta Consultants was contracted by SKI to function as principal investigator within the project secretariat. Each party covered the costs for its participation and was responsible for the funding of its own project team or teams, including computer costs, travelling expenses, etc.

A pilot group was appointed for each test case in order to secure the necessary information transfer from the experimental work to the project secretariat and the project secretariat assisted in this information transfer. Workshops were held at suitable time intervals depending upon the progress of the study, normally in conjunction with meetings of the coordinating group. To facilitate the final reporting, four working groups were set up covering unsaturated rock, saturated rock, salt (including clay) and natural analogues.

The work of the VOIC committee, that had acted during Phase 1 of the study, was discontinued and a new committee, the INTRAVAL sub-committee for integration (ISI), was created to assist the secretariat and the working groups. The primary objective of the new committee was to integrate the findings of the different INTRAVAL test cases regarding validation issues and methodologies.

The structure of the INTRAVAL organisation is given in Figure 2.1 followed by a list of members of the central organisation. A list of the participating organisations is found in Appendix 1.

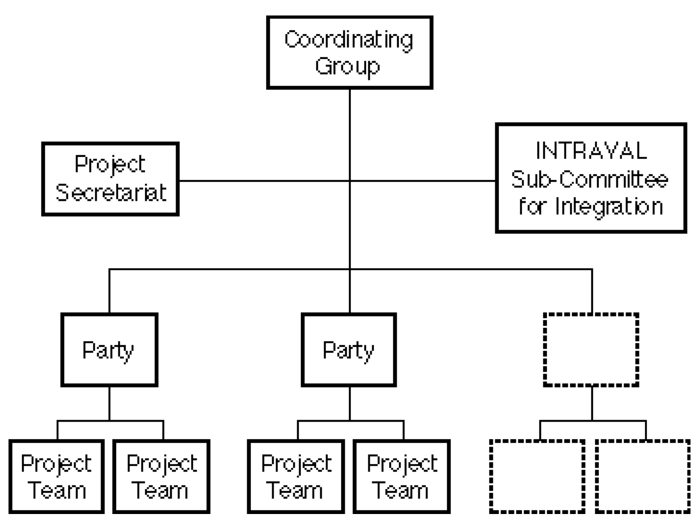


Figure 2.1. INTRAVAL organisational chart.

Chairmen, Vice Chairman and Secretaries of the Coordinating Group

Chairmen
A. Larsson, SKI/Kemakta (1987–1990)
K. Andersson, SKI (1990–1992)
J. Andersson, SKI (1992–1995)

Vice chairman
T. Nicholson, U.S. NRC

Secretaries
K. Andersson, SKI (1987–1990)
J. Andersson, SKI (1990–1992)
B. Dverstorp, SKI (1992–)

Members of the Project Secretariat (1992–)

J. Andersson, SKI
B. Dverstorp, SKI
M. Ericsson, Kemakta
P. Jackson, AEA Technology
A. Larsson, Kemakta
C. Pescatore, OECD/NEA
K. Pers, Kemakta
K. Skagius, Kemakta

Members of the INTRAVAL Subcommittee for Integration

T. Nicholson, NRC
N. Chapman, Intera
J. Andersson, SKI
P. Bogorinsky, GRS
J. Hadermann. PSI
P. Jackson, AEA Technology
I. Neretnieks, KTH
S. Neuman, UAZ
K. Skagius, Kemakta
C.-F. Tsang, LBL
C. Voss, GOLDER

3. Technical Realisation

The Coordinating Group decided that, for the second phase of INTRAVAL, essentially only field experiments should be used for the validation exercises. The test cases were selected taking this general criterion into account and also the objective of limiting the number of cases. Four different rock types were addressed, crystalline (fractured) rock, unsaturated rock, deposited salt and clay. In addition, the modelling and analytical work based on the Alligator Rivers natural analogue, already started during the first phase, was continued.

Following the established practice, workshops were held in connection with coordinating group meetings. During the course of the project, progress reports were issued, containing summaries of presentations made at the workshops relating to ongoing work on the different test cases. The progress reports also included lists of test case related presentations at INTRAVAL workshops.

Members of the ISI committee participated at the meetings. At the end of the project, the committee reviewed their findings and impressions. Their work resulted in a published report, in which the two phases of the INTRAVAL study were evaluated *[25]*.

Times and locations of the INTRAVAL Phase 2 meetings are shown in Table 3.1.

Table 3.1. Workshops and coordinating group meetings.

Meeting	Location	Time
WS + CG	Cologne	October 1990
WS + CG	Seattle	April 1991
WS + CG	Sidney	February 1992
WS + CG	San Antonio	November 1992
CG	Stockholm	September 1993

WS = Workshops; CG = Coordinating group meetings

Ten test cases were included in Phase 2 of the study. The test cases were based on experimental programmes undertaken within national and international projects. The pilot groups had the responsibility to compile data and propose formulations of the test cases in such a way that it was possible to simulate the experiments with model calculations.

An overview of the treated test cases is found in Table 3.2. It should be noted that it has not been possible for the secretariat to obtain any information regarding Twin Lake, which was suggested as an additional test case. Furthermore, the change in organisation at ANSTO in Australia made it necessary for Kemakta Consultants to issue the final report regarding the Alligator Rivers test case.

Table 3.2. Test Cases.

Test case	General description
Las Cruces Trench	Flow and transport experiments in unsaturated porous media performed at Las Cruces, New Mexico, USA
Apache Leap	Flow and transport experiments in unsaturated fractured rock performed at Apache Leap Tuff Site, Arizona, USA
Yucca Mountain	Yucca Mountain experiments, Nevada, USA
Finnsjön	Tracer experiments in a fracture zone at the Finnsjön research area, Sweden
Stripa	Flow and tracer experiments in crystalline rock based on the Stripa 3-D experiments, Sweden
WIPP 2	Flow and transport experiments in heterogeneous fractured media performed at the Waste Isolation Pilot Plant (WIPP) in Carlsbad, New Mexico, USA
Gorleben	Saline groundwater movements in the vicinity of the Gorleben salt dome, Germany
WIPP 1	Brine flow through bedded evaporites at the Waste Isolation Pilot Plant (WIPP) in Carlsbad, New Mexico, USA
Mol	Migration experiments in the Boom clay formation at the Mol site, Belgium
Alligator Rivers	Natural analogue studies at the Koongarra site in the Alligator Rivers area of the Northern Territory, Australia

As for Phase 1, working group leaders were appointed to deal with groups of test cases and to compile final results from the cases. Four such groups were formed (Table 3.3) and group leaders were nominated.

Table 3.3. INTRAVAL Phase 2 working groups.

Working group	Test cases
1	Las Cruces Trench, Apache Leap
2	Finnsjön, Stripa, WIPP2
3	Gorleben, WIPP1, Mol
4	Alligator Rivers

4. Test Cases, Descriptions and Results

This chapter gives a general overview of the different test cases, the experimental designs, analyses, conceptual models for the analyses and general results. Detailed reports, generally compiled by the working group leaders and members of the working groups, are issued as separate documents *[26, 27, 28]*. It should be noted that for the test cases Mol (Chapter 4.6), Gorleben (Chapter 4.7) and WIPP 1 (Chapter 4.8) it has not been possible for the secretariat to obtain any working group report from the assigned working group leader. These chapters in the summary report are therefore solely based on a report by the working group leader to the Geoval '94 symposium in Paris, 1994 *[29]*.

4.1 Flow and Tracer Experiments in Unsaturated Soil Performed at Las Cruces Trench

4.1.1 Overview

This test case was based on a series of experiments performed at the New Mexico State University College Ranch, 49 km northeast of Las Cruces, New Mexico, USA. In the Las Cruces Trench studies, unsaturated flow and transport of water and solutes in porous media were examined using wetting-front and tracer migration and redistribution experiments in undisturbed soil profiles. The purpose of the experiments was to provide sufficient data to test the ability of stochastic and deterministic models to simulate flow and transport in spatially variable, unsaturated soils. The studies at Las Cruces site also formed part of a test case for INTRAVAL Phase 1.

To provide data for more rigorous model testing, a new series of experiments was performed at the site, which formed the basis for the test case included in Part 2 of the INTRAVAL project.

Five teams from the USA participated in the INTRAVAL Phase 2 Las Cruces Trench study: the Center for Nuclear Waste Regulatory Analysis (CNWRA), Massachusetts Institute of Technology (MIT), New Mexico State University (NMSU), the Pacific Northwest Laboratory (PNL), and the Bureau of Economic Geology (BEG).

4.1.2 Experimental Design and Analysis

Background and Objectives

The studies at Las Cruces Trench (LCT) originated as a cooperative research effort between field experimentalists at New Mexico State University (NMSU), the Pacific Northwest Laboratory (PNL), and modellers at the Massachusetts Institute of Technology (MIT). At the time, the field site was already part of a long-term environmental research study of soil-moisture processes in arid, cattle-grazing land at the NMSU College Ranch.

Originally, the objective of the LCT study was to collect a data base for validating stochastic flow and transport models for unsaturated soils. An additional objective was the integration of a stochastic method for modelling the site, the collection of an adequate data base upon which stochastic models could be tested, and a field programme, including plot design and initial test configuration of the field trench as part of the validation process. The need to determine the degree of heterogeneity at the site and how the heterogeneity should be represented, e.g. by stochastic random fields characterised by means, variances and correlation scales, was also regarded as important.

More specifically, the experimental objectives were the following:

- The hydraulic properties for the site should be characterised in sufficient detail that the site could 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.
- The movement of water and solute through the soil profile during infiltration and during redistribution should be monitored in sufficient detail that the effect of spatial variability could be defined.

For the INTRAVAL project, the studies at Las Cruces were reformulated, introducing a requirement of rigorous model testing, including deterministic and stochastic models as well as multiple field tests.

To handle the Las Cruces Trench test case within INTRAVAL Phase 2, a pilot group was set up within the University of Arizona (UA) and New Mexico State University (NMSU). The pilot group consisted of specialists in the areas of soil physics, soil chemistry, soil morphology, hydro-geology and numerical methods.

Experimental Setup

To characterise the hydraulic properties of the site, a 26.5 m long, 4.8 m wide, and 6.0 m deep trench was excavated to provide soil samples and horizontal access to the irrigated area through the trench face. The trench and adjacent area were covered to prevent surface runoff and infiltration due to rainfall, and to minimise evaporation. A 4 m by 9 m irrigated area was located on the south side of the trench for the Plot 1 experiment and a 1.2 by 12 m irrigated area on the north side of the trench for the Plot 2 a and Plot 2 b experiments. The facility was designed to make it possible to monitor the applied water and tracer movements at various depths. The site was heavily instrumented with a great number of neutron access tubes, tensiometers and solute samplers. The trench face was exposed for the first experiment, allowing visual observation of the wetting front advance. Figure 4.1.1 illustrates the experimental setup.

In the experiments, water was administered at a rate that would enhance lateral spreading to magnify the lateral and vertical heterogeneities of the unsaturated soil profile, but not create saturated conditions.

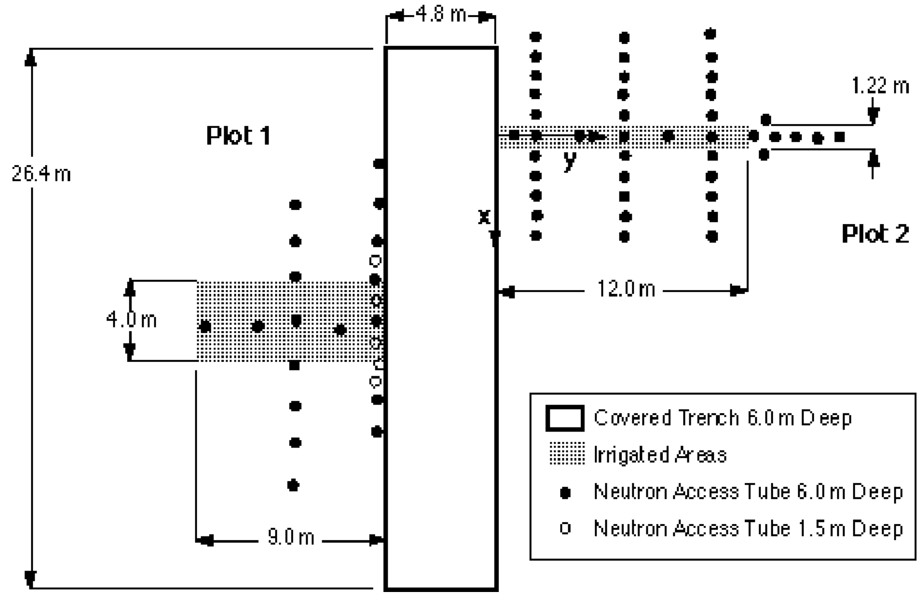


Figure 4.1.1. Plan view of the Las Cruces Trench experiments.

As was the case for the Plot 2a test in INTRAVAL Phase 1, Plot 2b which was a dynamic experiment, was treated as a blind modelling test, since the experimental results were not initially given to the modellers.

The Plot 2b test used a water application rate of 1.82 cm/day during a 70-day irrigation period. Chromium, boron and pentafluorobenzoic acid were applied during the first 15 days of irrigation, with tritium, bromide, and difluorobenzoic acid being applied during days 29 through 44 of irrigation (Figure 4.1.2).

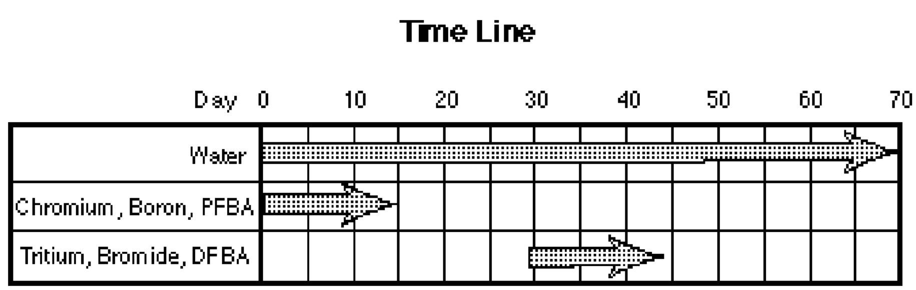


Figure 4.1.2. Plot 2b water and chemical tracer application schedule

Available Calibration Data

Although the Plot 2b experimental data were not provided to the modellers until blind model predictions were provided to NMSU, the data from the characterisation experiments and from the Plot 1 and 2a experiments were available. These data were accessible in both raw and processed form. The raw data included water-retention data, density profiles, particle size analysis data and saturated hydraulic conductivities measured in the laboratory and *in situ* during the characterisation experiments. Also water-content data, tensiometer data, solute concentrations and application rates measured during the Plot 1 and Plot 2a experiments were provided to the project teams. In addition, morphological mapping of the trench face, drip irrigation distribution tests and outflow and inflow measurements from large and small column tests using similar soils were on file at NMSU and at UA.

4.1.3 Conceptual Models

For INTRAVAL Phase 2, the dynamic models simulated flow and transport of the Plot 2b experiment. Table 4.1.1 summarises the models used and the manner in which they represented heterogeneities. A "blind model" was defined as one that was formulated before the modeller had seen the experimental results.

Table 4.1.1. Modelling of the Plot 2b experiment [30].

Group	Models	Comments
BEG	BEG1	**Not Blind**. Finite-difference code for two-phase flow and multi-component 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 nine 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-medium stochastic property model (homogeneous, anisotropic) in a 2-D simulation.
NMSU	NMSU1	**Not Blind.** Water-content using 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 the 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.

4.1.4 Results

Procedure for Model Testing

The modellers were provided with the initial conditions for water content in the y = 2, 6, and 10 m planes, and for tritium in the y = 0.5 m plane. Using the actual water/tracer application histories (Figure 4.1.2), the Plot 2b experiment was simulated. Model predictions were returned to NMSU 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 measured relative to the Plot 2b irrigation centre line and the value of the predicted variable. Since the model results were provided to NMSU without the modellers having access to the experimental data, these model predictions were considered blind (Table 4.1.1).

As shown in Figure 4.1.2, several chemical tracers 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 was deemed by the experimentalists to be the most reliable.

Preliminary comparisons between experimental data and model predictions were made and presented at an INTRAVAL workshop. The experimental data were then released to those modellers that had supplied the corresponding model predictions to NMSU. Additional model predictions were provided to NMSU after the above presentations were made. These later modelling predictions were considered non-blind (Table 4.1.1). 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.

Performance Measures

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

The point comparisons were:

- Contour plots of observed and predicted water contents and solute concentrations
- Scatter plots of observed and predicted water contents and solute concentrations
- First-arrival times of the water and solute plumes as a function of depth.

Contour plots were used as a first point-value comparison approach, because they were very useful in visualising the behaviour of the wetting front, moisture redistribution, and solute plume. However, contouring methods inherently, and sometimes intentionally, average data and the resulting contours can be very dependent on the analytical techniques and the contouring algorithm used to generate the contours. An example of contour plots for observed and simulated water-content distributions is given in figure 4.1.3.

The second point-value comparison approach used scatter plots of observed versus predicted volumetric water contents and normalised solute concentrations. The Pilot Group considered scatter plots to provide a more realistic assessment of point-value predictions than the contour plots. They also felt that scatter plots would have the added advantage of showing the scatter of the observations about the predictions, which would give a good indication of bias and uncertainty about the mean.

As the third point-value comparison approach, plots of first-arrival times of the water and solute plumes at various depths were used. The Pilot Group defined the time of arrival of the water plume as the 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.

The integrated quantities used for comparison were:

- First and second moments of the water and tritium plumes as a function of time
- The normalised change in total water volume below each of the z = 0, 1,..., 5 m horizontal planes as a function of time. The Pilot Group felt that the observed change in water volume below a horizontal plane was a good estimator of the water passing through that plane, while the plume remained fully observable.
- 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.

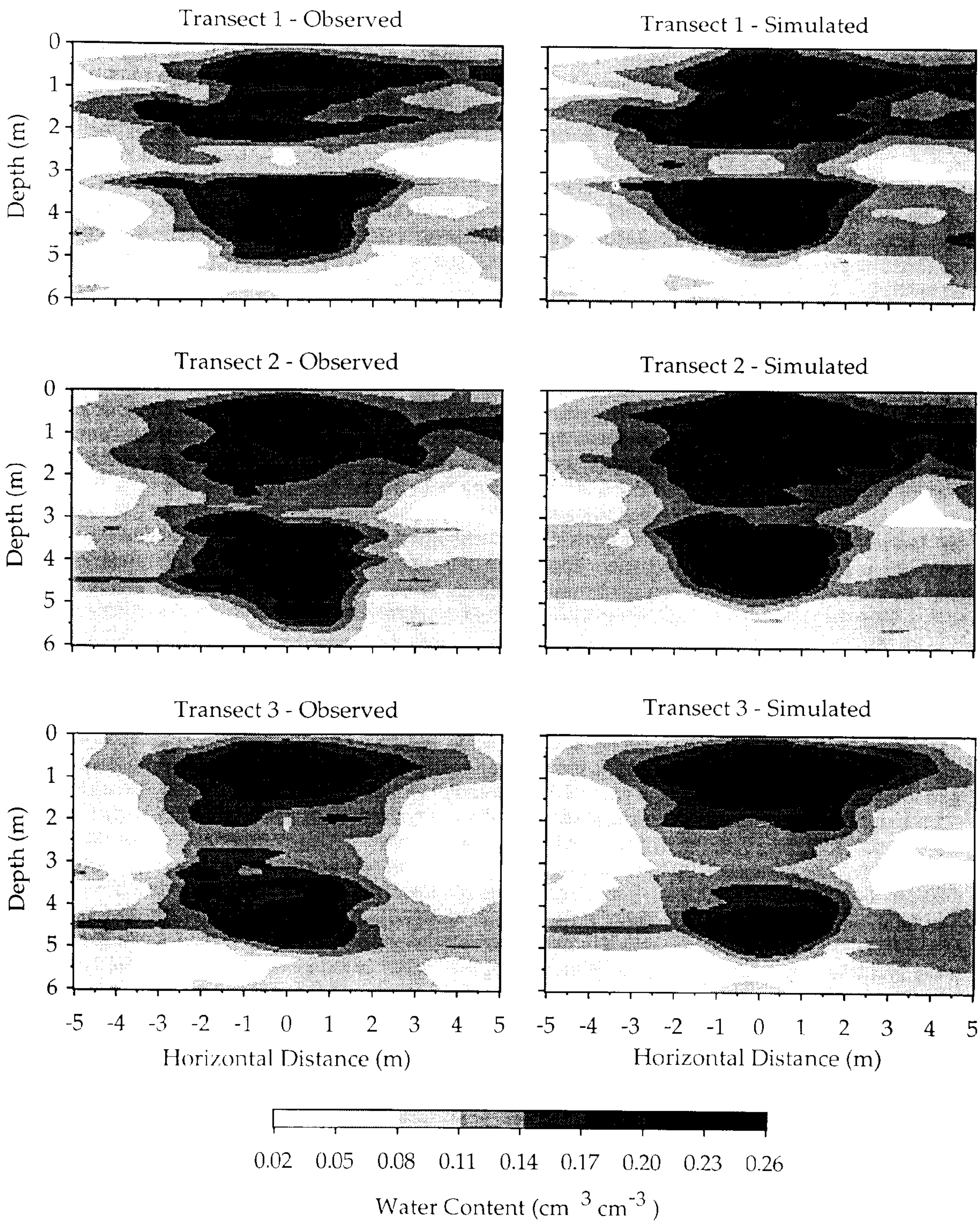


Figure 4.1.3. Observed and simulated water content distributions for day 70 [31].

Testing and Assessment of Conceptual Models

As shown in Table 4.1.1, various alternative conceptual models were tested and assessed. The alternatives ranged from uniform property to complex distributed-property models. The stochastic models considered spatial variability using spectral-analysis approaches that related property distributions to tension dependency.

Two measures were used to assess the effect of increased model complexity on the accuracy of the predicted water contents. 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 led 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. It was concluded 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, based on conditioning the soil hydraulic properties on the initial field-measured water content distributions and a set of scale-mean hydraulic parameters, was successfully applied to the data sets for the Plot 2b experiment. Very good matches between the observed and simulated flow behaviour were obtained, using the conditioning procedure without model calibration, as shown in Figure 4.1.3.

Another technological advancement derived from the LCT study 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.

4.1.5 Validation Issues

The results from the Las Cruces Trench test case in INTRAVAL Phase 2 have demonstrated one approach to validation through interactive laboratory and field experiments and modelling, using a quantitative model testing strategy with performance measures tied directly to regulatory significant criteria.

4.1.6 Conclusions

The assessment of success involved model testing and the repeated re-evaluation of the experimental results. Both field monitoring data and destructive core sampling were used in these re-evaluations.

The testing of models using data from dry, spatially variable soils involved fundamental difficulties. Not only was it difficult to characterise the site, but also to obtain sufficiently high quality solute samples to get good estimates of the movement of solute plumes as a function of time. In contrast, water flow in unsaturated soils was easier to monitor. Neutron probes allowed water to be monitored at many locations and the measurements were 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.

There were considerable differences in model predictions, even though all the modellers had access to the same very large characterisation data set for the experiments. Some of the models applied 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. Of the models considered, none stood out as clearly superior. All of the models underpredicted first arrival times of the water plume at depths greater than 4.5 m. 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 did 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. As a result of less powerful, non-parametric quantitative and graphical comparisons, several observations could be made.

The CNWRA and PNL models consistently provided better predictions of mean or median water contents (i.e. near zero mean or median prediction errors), which suggested a good accounting for the total mass in the system. This was probably 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 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.

First-arrival times of the water plume were greater for the experiment than predicted by any of the models, once the plume reached 4.5 m. Although this is expected for 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 was due to limitations in the experimental characterisation procedures, the inability of Mualem's model to predict unsaturated hydraulic conductivity for the soil layer given the van Genuchten retention model, 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. Although PNL3 overpredicted the change in water content at depth, the behaviour of water content 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 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 PNL2 and MIT1 models conceptualised the soil as anisotropic. MIT1 overpredicted the water-plume spreading and underpredicted the 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. However, most of the model comparisons made during the Plot 2a experiment were side-by-side comparisons of smoothed contour plots. More extensive comparisons 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 was 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 for water flow that appear superior or conservative from a regulatory point of view 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 the use of 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 were considerable differences in the way 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 the way the models conceptualise the soil.

4.2 Flow and Tracer Experiments in Unsaturated Tuff Performed at Apache Leap Tuff Site, Arizona

4.2.1 Overview

In the Apache Leap test case, two topics were primarily treated: how a thermal source will affect air, vapour, water and solute movement in geologic media, especially unsaturated fractured rock, and the water and air transport properties of fractures and rock matrix in unsaturated rock. The test case was based on field and laboratory experiments carried out in unsaturated welded and non-welded tuff at the Apache Leap Tuff Site, Arizona, USA. The case was included in both Phase 1 and 2 of the INTRAVAL study.

The experiments involving the Apache Leap were part of a continuing effort at the site and were only to a limited extent connected to INTRAVAL.

4.2.2 Background

The Apache Leap Tuff Site studies originated as a research programme carried out by investigators at the University of Arizona. Its purpose was to examine site characteristics and conceptual model issues associated with high-level radioactive waste repositories. More precisely, the objective was to examine models and strategies for obtaining characterisation data. To fully characterise fluid flow and solute transport through unsaturated fractured rock requires site-specific conceptual models to be defined, parameters for the models to be estimated using field and laboratory data, and also validation of the conceptual models. As the understanding of the fundamental processes and the development of conceptual models describing flow and transport in unsaturated, fractured rock was in its infancy, it was necessary to focus on a fundamental level of characterisation techniques and conceptual model development.

To meet the objectives of the INTRAVAL Project, the Apache Leap studies were reformulated to testing conceptual models and their linkage to characterisation approaches. The experimental plans were to verify the existence of proposed processes and the parametric form of hypothesised material properties and to examine conceptual models and characterisation approaches over a range of scales and processes. During Phase 1 of INTRAVAL, the modelling teams consisted of: the Bureau for Economic Geology, University of Texas (BEG); the Center for Nuclear Waste Regulatory Analysis (CNWRA); HydroGeologic Inc. (HGL); Kemakta Consultants Co. (KKC); Massachusetts Institute of Technology (MIT) New Mexico State University (NMSU); Pacific Northwest Laboratory (PNL); and Sandia National Laboratory (SNL). In Phase 2, the groups included BEG, CNWRA, MIT, NMSU and PNL.

The efforts were divided between laboratory and field experiments. In the laboratory experiments, large- and small-diameter bore cores from the site, as well as a larger block containing a persisting single fracture, were used. The experiments consisted of measuring the hydraulic, pneumatic and thermal properties of the rock, non-isothermal core experiments for coupled water, vapour and solute movements, and determining imbibition rates. Air-injection field experiments were undertaken to characterise the heterogeneity of fracture-related permeabilities.

4.2.3 Experimental Setup and Analysis

The Apache Leap experiments were designed to evaluate characterisation methods and conceptual models for coupled matrix-fracture continua over a range of scales up to 30 m. Within these spatial scales, laboratory and field tests were conducted to estimate pneumatic, thermal, hydraulic, and transport property values for different conceptual models.

Figure 4.2.1 illustrates the experimental setup for the core and block studies 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. The block contained a discrete fracture along the long axis.

The experimental setup for the core heater experiment 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. A one-dimensional thermal gradient, 5 to 45EC, was applied along the axis of the core. The core was hermetically sealed and insulated. Dual-gamma attenuation methods were employed to provide water content and solute concentration profiles. Temperatures along the core were also measured and solute concentrations were determined.

Figure 4.2.2 gives a three-dimensional portrayal of the 15 inclined and vertical boreholes at the Apache Leap site. Figure 4.2.3 shows a schematic representation of the air injection setup 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 at the injection interval. Atmospheric temperatures and pressures were also monitored.

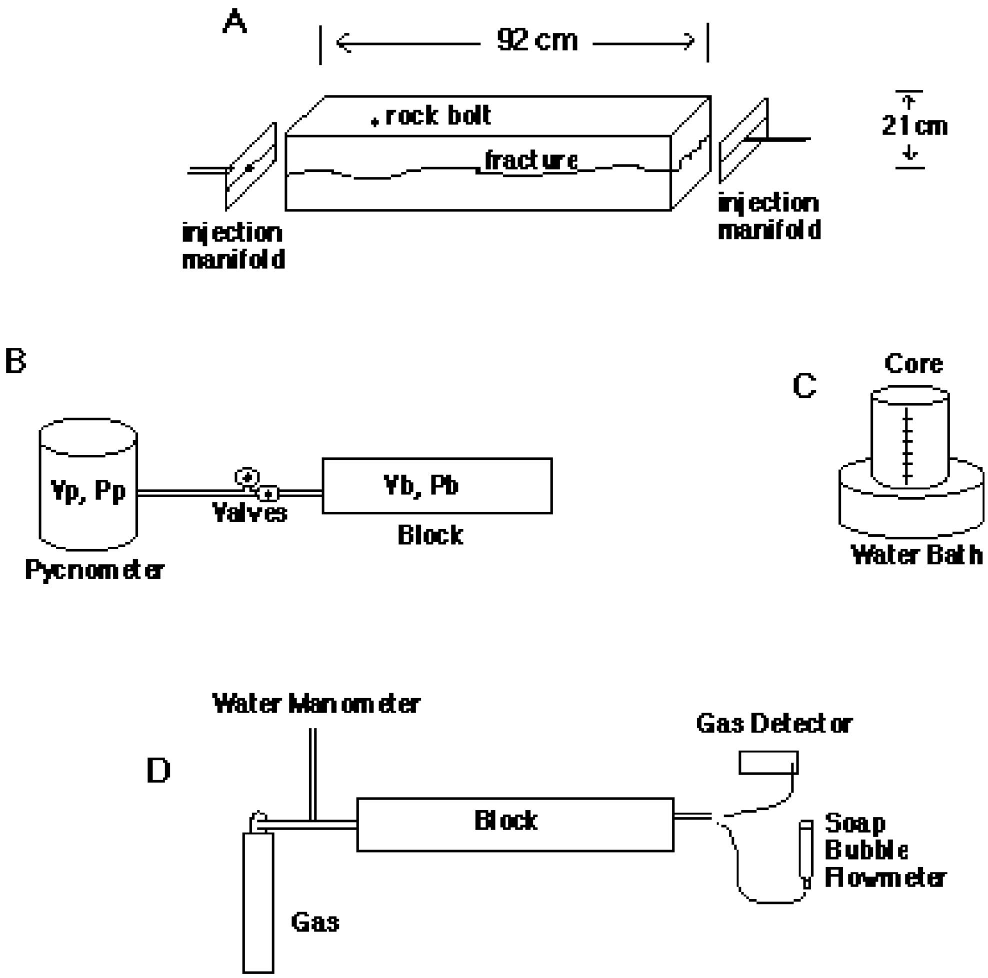


Figure 4.2.1. Experimental setup for: (A) the wetting-front experiment for the fractured block; (B) the rock porosity measurement experiments of the matrix using a pycnometer; (C) the hydraulic diffusivity coefficient measurement using a core imbibition experiment; and (D) the gas diffusion coefficient measurements and breakthrough curve experiment [32].

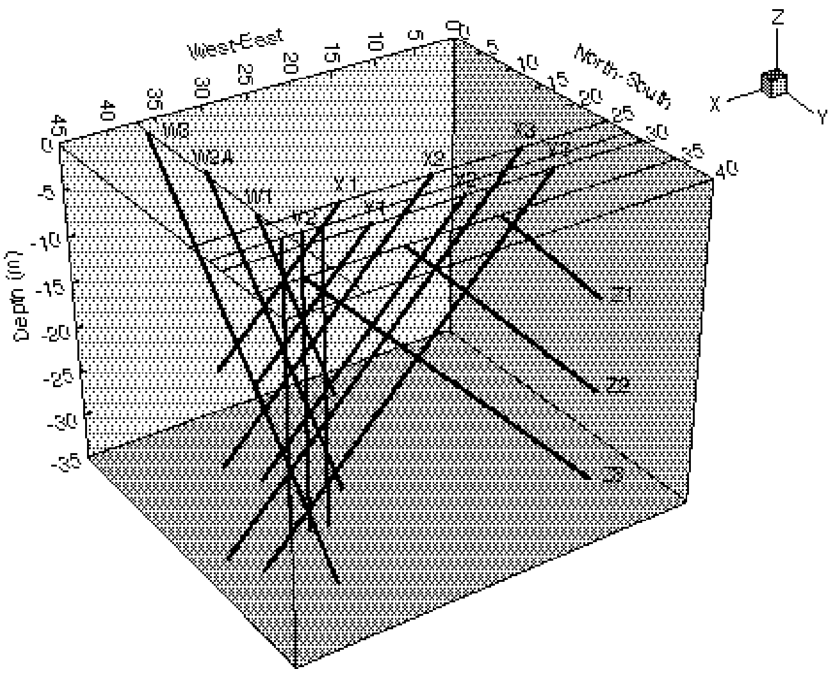


Figure 4.2.2. Borehole locations at the Apache Leap test site [33].

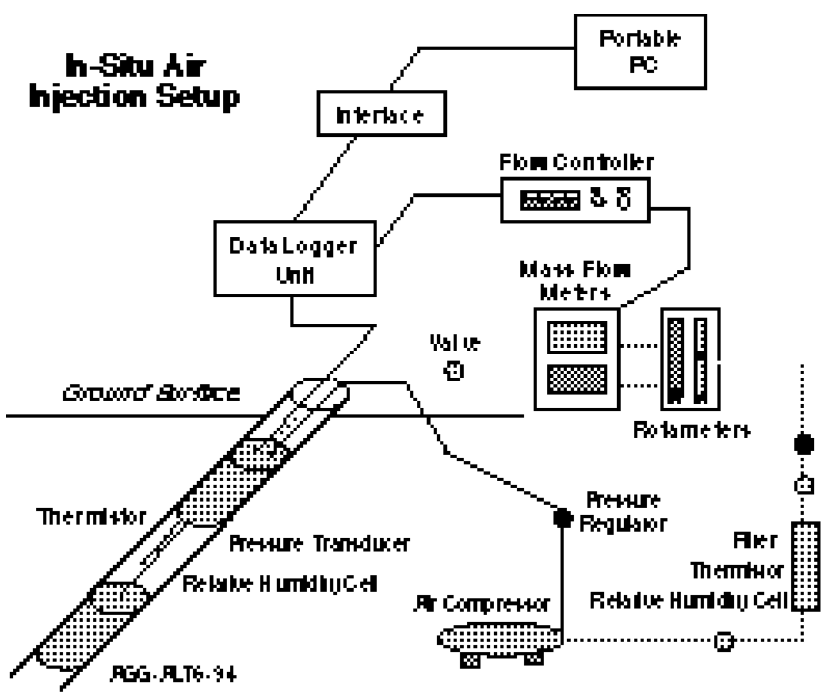


Figure 4.2.3. Schematic representation of the air injection system at the Apache Leap test site [33].

Laboratory analyses of small core samples from the site provided characterisation data on porosity, characteristic curves, hydraulic conductivity, air permeability and thermal conductivity. The effects of variable water content, hysteresis, and temperature on the physical parameters were examined, as well as the effects of solute concentration on ambient matric potential.

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 heat transport was insignificant compared to the conductive heat transport in this experiment. When a soluble salt (NaI) was introduced into the core, the heat-pipe phenomenon was not as effective 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.

The studies conducted on the fractured rock block provided information on the physical properties of the block. Equivalent fracture apertures were obtained using six types of experiments: three volumetric fracture aperture values obtained by using a pycnometer, tracer breakthrough volumes and the ratio of fracture transmissivity to fracture hydraulic conductivity; two Poiseuille apertures from the use of a cubic aperture equation applied to gas and water flow rates and applying quadratic-aperture-equation gas-breakthrough velocities; and a final estimate of fracture aperture using the air-entry potential of the saturated fracture.

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

The field air-injection data sets 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, different sets of data could be used to determine the air permeability of the rock surrounding the tested interval: transient sets during injection, steady-state sets, and one recovery set. The data sets consisted of air-permeability measurements at different scales and at multiple-injection rates in six of the boreholes.

4.2.4 Models Developed for Testing

The following models were developed for testing:

- Characterisation models used to define the porosity, characteristic curves, hydraulic conductivity, air permeability and thermal conductivity for the rock matrix using small cores. The models were studied to determine how sensitive they were to a range of water content, hysteresis and temperature.
- Conceptual models describing flow through a single fracture tested using the large block experiment. Values for the matrix and fracture apertures were measured and compared to the model estimates.
- An approximate analytic model of Nitao and Buscheck. The model was evaluated for its ability to predict the behaviour of water imbibition into initially dry fractured rock and its applicability

to unsaturated flow.

- C Conceptual models dealing with scale effects and spatial distribution of heterogeneities. The models were tested using data sets from the *in situ* air-injection studies.

The models were tested by estimating the physical, hydraulic, pneumatic, and thermal properties for the discrete fracture, and then making forecasts using alternate conceptual and mathematical models. The forecasts for each conceptual model include a forecast of the 95% confidence interval about the forecast, thus allowing an assessment of the accuracy of the forecast compared against the experimental result. The confidence intervals were generated by measuring the uncertainties in the input parameters and propagating those input parameter uncertainties through the model using a Taylor-series expansion. The model outputs were then compared against experimental results.

4.2.5 Results

Model Comparison and Testing

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 shown to have a large influence on the moisture-retention characteristic curve. 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 fopr the range of volumetric water contents from 0 to 0.0876. The effect of solute concentrations on the ambient matric potential was investigated. It was concluded that accumulation of saturated salt solution 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 determined volumetric aperture, using the ratio of fracture transmissivity to hydraulic conductivity, was least, 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 applied, a horizontal fracture imbibition experiment was conducted using water as a fluid imbibed into an initially dry, fractured rock. The model reproduced the imbibition rate. The form of the model prediction 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 reduction in water inflow may be due to phenomena neglected in the theoretical model, such as fracture surface coatings or enhanced surface wetting, or the inability to accurately determine fracture physical properties *a priori*, for instance the fracture water diffusivity. It was shown that fracture saturation behind the wetting front initially was very low, perhaps ten percent, but increased to complete saturation during the course of the experiment. This may indicate that fingers of saturation exist within the fracture during early time, and that these fingers expand laterally and dissipate over time.

Data from the imbibition experiment confirm the second imbibition phase hypothesised by the analytical model used. The experimentalists were not able to identify the first or the third imbibition phases of their model. However, a new imbibition phase was observed that resulted from the finite length of the fracture within the tuff. The analytical model should be modified to incorporate the finite extent of discrete fractures. A concern raised by the experiment was the failure to properly estimate fracture hydraulic properties. It was observed that laboratory estimates of rock fracture hydraulic properties, when used with the analytical 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 parameters were substantially less than the characterisation values. An additional shortcoming of the model was 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-injection tests were performed over a range of scales up to 3.0 m and at multiple-injection rates. Field data indicate that the air permeability determinations were 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. These measurements seemed to indicate some dependency of the mean permeability on measurement support (length of test interval), a "scale effect". Upscaling by weighted arithmetic averaging of the smaller measurement support data produced better estimates than geometric-weighted averaging. However, high permeability values were slightly underpredicted by either upscaling approach.

Although the observed variability of air permeabilities at the Apache Leap was over 3.5 orders of magnitude, the data were amenable to classical geostatistical analysis and yielded well-defined semivariograms. The omni-directional semivariogram exhibited a nested structure with two distinct plateaus and correlation scales and an additional correlation structure, whose sill and range were undefined due to the limited extent of the experimental site. It was observed that the increase in the variance and correlation scale grew with the scale. The available fractured rock permeability data may be viewed as a sample from a random (stochastic) field defined over a continuum with multiple scales of heterogeneity.

Laboratory Experimental Results

Results of laboratory experiments conducted to characterise the fluid and thermal flow parameters of unsaturated Apache Leap tuff indicated that hysteresis influenced the moisture characteristic curve. Wetting and drying characteristic curves were markedly different, with the wetting curve consistently showing higher matric potentials at equivalent water contents. To identify the matric potential from the water content of unsaturated rock, knowledge of the water content history of the site is needed. The application of osmotic solutions to maintain constant matric potentials was successfully demonstrated. Saturated salt solutions present in the geologic environment may affect the observed matric potential. Near a repository, accumulations of soluble salts may influence 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 a waste repository.

Temperature was shown to affect the characteristic curve. Both reduced and increased temperatures caused substantial shifts in the characteristic curve, attributable to change in the temperature dependence of the fluid surface tension.

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.

Laboratory experiments conducted to observe thermal, liquid, vapour, and solute transport through variably saturated, fractured Apache Leap tuff demonstrated that conduction was the dominant heat transport mechanism, even when a significant heat-pipe effect was present. The water content increased away from the heat source due to vapour-driven advection and condensation. Solutes accumulated near the heat source, but the accumulation of solutes increased the osmotic potential, which decreased the heat-pipe phenomenon. Solute transport was substantially affected by the heat-pipe phenomenon, resulting in accumulation of significant solutes nearer the heat source, than would have occurred, if the heat pipe had not been present. Models of solute transport should incorporate the heat-pipe phenomenon and should also consider the effects of osmotic potential on liquid and vapour transport.

Additional laboratory and computer simulation experiments would have to 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 would require examination. It is possible that processes not yet considered may significantly affect the migration of radionuclides in the region immediately adjacent to a waste repository. Field and laboratory-scale experiments would be necessary to identify such unknown processes.

Uncertainty Assessments

Table 4.2.1 presents estimated characterisation properties of the rock matrix and the embedded fracture. The values for several parameters, including fracture porosity and liquid saturation changes across the wetting front in the fracture and rock matrix, are assumed. Table 4.2.1 also presents uncertainties in characterisation parameters. Uncertainties in the derived parameters were estimated by propagating parameter uncertainties using first-order Taylor-series approximations.

Table 4.2.1. Fractured block characterisation parameters [34].

Properties		Mean	± std dev.
Rock Matrix:			
V	rock volume	39.240	± 0 cm^3
zV_t	pore plus fracture volume	4.635	± 120 cm^3
V_m	matrix pore volume	4.493	± 127 cm^3
2_m	porosity	0.115	± 0.003
$)S_m$	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:			
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
2_f	porosity	1	± 0 (1)
$)S_f$	liquid saturation change	1	± 0 (1)
K_f	hydraulic conductivity	9650	± 504 cm
T_f	transmissivity	490	± 25.2 $cm^2\ hr^{-1}$
D_f	water diffusivity coefficient		

(1) Assumed value

It was 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.
It was 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.

Estimates of the uncertainty in the measured parameter are required to evaluate the uncertainty in predictions based upon the parameter. Forecasts of flow and transport require measures of the uncertainty in the forecast. Uncertainties in estimated parameters may contribute to large errors in forecasts.

Field Experimental Results

The following conclusions were drawn based on an extensive data set consisting of steady-state apparent-air-permeability values. The air permeability obtained from straddle-packer tests was strongly dependent on the applied pressure. Computer simulations confirmed that the changes in air permeability with pressure were due to two-phase flow and, in some cases, to inertial flow. Upscaling of the apparent permeability was best accomplished by weighted arithmetic averaging. Geostatistical and statistical analyses indicated that the apparent-permeability field from the Apache Leap studies behaved as a stochastic multi-scale continuum with an echelon and power-law (fractal) structure. The latter was 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.

Results from the analysis strongly suggested that site characterisations should be based on hydrogeologic data collected on a spectrum of scales relevant to performance assessment. They further indicated 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 investigators reported that inverse methods have promise here.

4.2.6 Conclusions

The Apache Leap 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 characterisation strategies, methods and instrumentation.

A variety of conceptual models founded on flow processes were evaluated against experimental data. From this evaluation, it was concluded that the wetting history has a significant influence on the formulation of the characteristic curve, but a linear relationship between the thermal conductivity and the water content could not be clearly demonstrated. The fracture saturation behind the wetting front was initially very low, perhaps ten percent, but increased to complete saturation during the course of the block wetting experiment. The modelling results overestimated the fracture imbibition volume by a factor of twenty and the fracture wetting front advance by a factor of eight.

4.3 Tracer Experiments in a Fracture Zone at the Finnsjön Research Area

4.3.1 Overview

The test case was based on three hydraulic interference tests and two tracer experiments performed in a major low-angle fracture zone at the Finnsjön research area located in central Sweden. The main objective of the experiments was to determine parameters important for the understanding of radionuclide transport in major fracture zones and to utilise the results for calibration and verification of radionuclide transport models. The experiments were designed to study phenomena, such as advection, dispersion, channelling, dilution, matrix diffusion, and heterogeneity on a large geometric scale.

Studies during INTRAVAL Phase 1 showed that tracer data from one or two tests at a site were not sufficient to discriminate between different models or different active processes. One important objective of including this test case in INTRAVAL Phase 2 was to investigate, if further studies could give results regarding discrimination different to the results obtained during Phase 1.

Nine project teams from seven countries applied a total of ten different models ranging from advection–dispersion models to complex fracture-network approaches. Most of the models used in the Phase 2 studies were two-dimensional porous models, although some project teams applied one-dimensional and sometimes, for large-scale modelling, even three-dimensional models. A comparative study based on a hypothetical natural-gradient experiment was initiated at the end of Phase 2 to illustrate the predictive uncertainty of the different modelling concepts.

4.3.2 Site Description and Experimental Design

Two major fracture zones have been identified at the Finnsjön study site as shown in Figure 4.3.1, a steep fracture zone (Zone 1) and a low-angle zone (Zone 2). The geohydrology of the site is dominated by these two highly conductive zones. Zone 2, which was the zone used for the tracer tests, consists of sections with high fracture frequency and tectonisation. The zone is well defined in seven boreholes located within an area of about 500×500 m. The upper surface is located between 100 and 240 m below ground surface. The zone consists of three subzones with transmissivities in the order of 10^{-5} to 10^{-3} m^2/s. Between the subzones the transmissivities are similar to the country rock. The hydraulic gradient in the zone is about 0.3%.

The water above Zone 2 is a fairly young near-surface water. Below the zone the water consists of an old saline water characterised by a high content of species in solution, such as sodium, calcium and chlorine. The water within the zone is a mixture of these two kinds of water.

Three hydraulic interference tests and two large-scale tracer tests were performed in Zone 2. The interference tests were carried out by withdrawing water from different isolated intervals of Zone 2 in borehole BFI02. Tracers were injected as pulses in the upper highly conductive subzone of Zone 2 in boreholes BFI01, KFI06 and KFI11. Tracer breakthroughs were monitored in the pumping well BFI02. The location of the boreholes is seen in Figures 4.3.1 and 4.3.4.

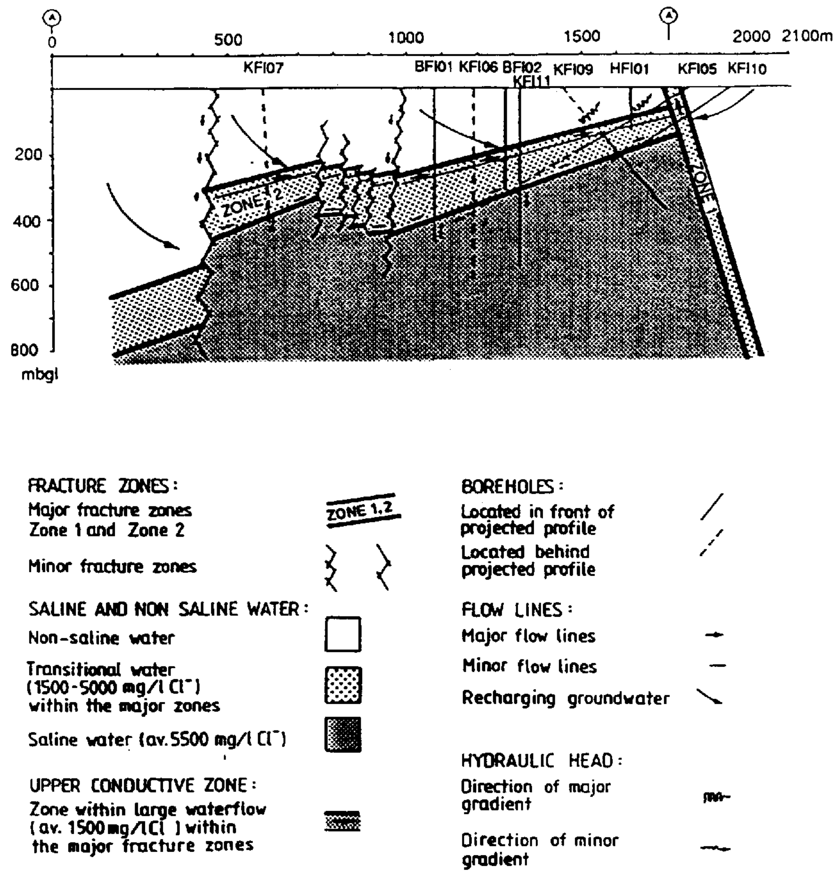


Figure 4.3.1. Cross-section of the Finnsjön site.

A radially-converging tracer experiment was performed by pumping in borehole BFI02 and injecting tracers into Zone 2 in three peripheral holes, BFI01, KFI06 and KFI11. Eleven different tracers were injected, eight of them continuously for 5–7 weeks, and three as pulses.

A dipole tracer experiment was performed in a recirculating system between BFI01 (injection) and BFI02 (withdrawal). Boreholes KFI06 and KFI11 were used as observation holes. 15 tracer injections, including both non-sorbing and sorbing species, were made in BFI01. Two tracer injections were also performed in the upper section of the observation hole KFI11.

4.3.3 Models and Processes

The conceptual approaches, modelling objectives and processes used by the nine teams are summarised in Table 4.3.1

Table 4.3.1. Conceptual approaches, modelling objectives, and processes considered by the teams modelling the Finnsjön test case.

Modelling team	Conceptual approach	Modelling objectives	Processes considered
Hazama Corp., Japan	crack-tensor theory	flow and transport analysis using REV approach	advection
Conterra/Water Res. Eng., KTH, (SKB), Sweden	stochastic continuum multiGaussian	test on a large scale of a stochastic continuum flow model calibrated on a local scale	advection
BRGM (ANDRA), France	continuum model	evaluation, comparison between analytical and numerical modelling, effect of boundaries and layering	advection–dispersion, kinematic dispersion, radioactive decay
GEOSIGMA/ (SKB) Sweden	continuum model	comparison of prediction and experimental data (2-D), evaluation and comparison of transport parameters (1-D)	advection–dispersion, diffusion, sorption, matrix diffusion, radioactive decay
VTT (TVO), Finland	non-interacting varying aperture channel model	realistic description of flow and transport in rock, relative weight of processes, parameter consistency	advective diffusion, matrix diffusion, generalised Taylor dispersion, multiple flow paths
PNC, Japan	dual-porosity continuum model with mixing zone, stream tube concept	effect of heterogeneity on advection–dispersion, transport	multiple flow paths
UPV (ENRESA), Spain	stochastic continuum multiGaussian, non-multiGaussian	impact on travel times of low continuity of extreme values	advection
PSI (NAGRA), Switzerland	single and dual porosity continuum model	identification of dominant transport processes, effect of varying flow boundaries	advection–dispersion, multiple flow paths, sorption, matrix diffusion
U. of New Mexico, USA	single and dual porosity continuum model	model discrimination	advection–dispersion, molecular diffusion, matrix diffusion

The conceptual models applied by the modelling teams in Phase 1 of INTRAVAL focused on porous media approaches. Seven of nine teams used this concept in Phase 2. The VTT team applied a network of channels, for which transport was assumed to take place in a few non-interacting channels and the Hazama team used a concept based on a representative elementary volume (REV) obtained by applying crack-tensor theory.

In comparing different conceptual models, the PNC team used two different approaches to determine the hydraulic conductivity distribution. They applied a one-dimensional stream tube as well as a two-dimensional finite-difference methods to analyse the transport. The UPV team compared Gaussian and non-Gaussian stochastical models, and the PSI team applied fracture and vein flow models. The U. of New Mexico team compared single versus double porosity models. Some of the teams used the comparisons to judge which conceptual approach gave the best correlation to the experimental data and which of the models could be more or less rejected.

Although two-dimensional models were generally used, which was a natural choice given the two-dimensional character of flow in Zone 2, a few teams used one-dimensional transport concepts and two teams used three-dimensional approaches. If all the tracer tests were to be considered, a three-dimensional model might be needed, especially if large-scale head responses were to be incorporated. Experimental evidence of vertical interconnections between different subzones and leakage from the bedrock below the zone also speaks in favour of three-dimensional approaches.

Four modelling teams, Conterra/KTH-WRE, UPV, Hazama, and PNC used geostatistical methods to obtain transmissivity or aperture distributions for stochastic travel time analysis.

4.3.4 Results

Models and Processes

The dimensionality of the models did not seem to be decisive for the ability to accurately reproduce the field responses at Finnsjön. The relatively simple one-dimensional approach seemed to be very useful in some cases. For example, in the analysis of the radially converging test the effects of variations in source terms and influences of multiple flow paths and matrix diffusion could be effectively simulated.

The four teams that used geostatistical methods demonstrated that stochastic approaches may be used within the context of a validation process, although the question remains of how to formally validate a stochastic continuum model.

In INTRAVAL Phase 1, it was concluded that the tracer experiments performed at Finnsjön were insufficient to discriminate between different models of advection. The studies during Phase 2 seemed to confirm this judgement.

The GEOSIGMA and PSI teams were the only teams that considered sorption. The reason for this was probably that no independent laboratory or field data existed for the weakly sorbing tracers used in the dipole test. It should be noted that the PSI team used a different data set. Their data set, which also came from Finnsjön, had previously been used in INTRACOIN, and especially addressed sorption processes. The PSI team concluded that sorption parameters determined from these tests agreed well with literature data.

The PSI team analysed the effect of matrix diffusion and concluded that matrix diffusion had a small, but non-negligible, effect. The U. of New Mexico team calculated the ratio of matrix to fracture porosity and arrived at a figure of 10^{-2}, and suggested that matrix diffusion is an important process at Finnsjön. The GEOSIGMA team drew the opposite conclusion based on the same ratio and they did not consider matrix diffusion at all in their analysis.

Another result by the GEOSIGMA team was that the one-dimensional analysis showed that the transport between the injection hole and observation borehole KFI11 could be well described with a single flow path model (Figure 4.3.2).

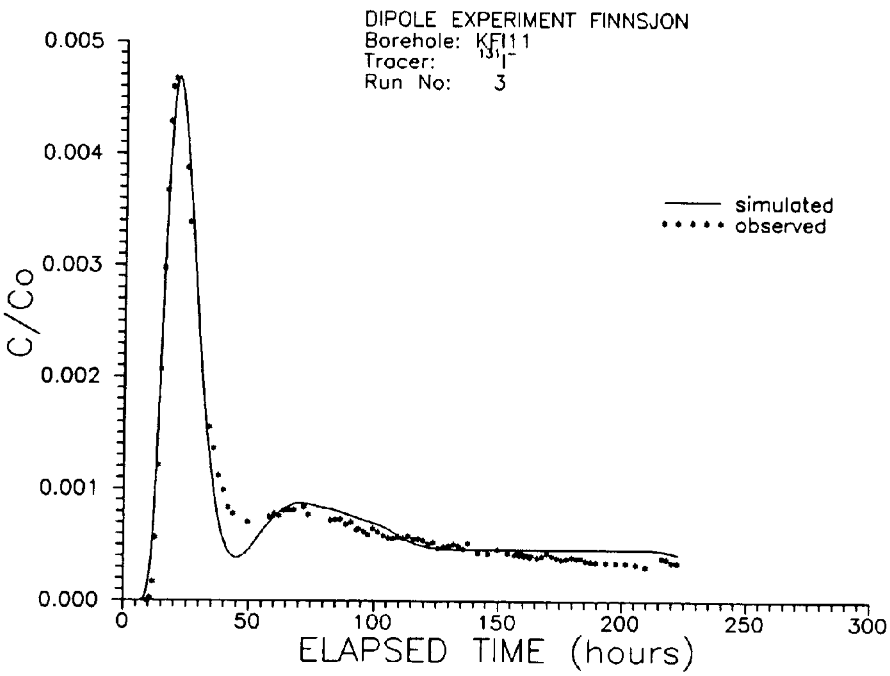


Figure 4.3.2. GEOSIGMA/SKB. Simulated and observed breakthrough of iodide in borehole KFI11.

All teams concluded that flow and transport in Zone 2 is governed by advection and that hydrodynamic dispersion is needed to explain the breakthrough curves. Most teams agreed that matrix diffusion has no or only a very small effect in the experiments, given the high induced velocities and the corresponding short travel times.

Validation Aspects

During Phase 2, various validation aspects were considered (Table 4.3.2). Five groups addressed the general approach to validation, e.g., calibration of a set of model parameters against a given experimental geometry for a specific stress of the geological system. Two groups, utilising the stochastic continuum approach, addressed other validation aspects.

The modelling teams from GEOSIGMA and VTT studied parameter consistency between all the three tracer tests performed at Finnsjön. The results showed that the average transport behaviour of the system can be acceptably described with one single set of transport parameters. However, the parameters have to be adjusted for different flow geometries to give a good understanding of individual transport paths.

Table 4.3.2. Phase 2 analysis of tracer tests at Finnsjön. Scale of problem and validation aspects.

Modelling team	Scale of problem	Validation aspects of problem
GEOSIGMA/SKB, Sweden	2500×1500 m (far-field) 500×500 m (local scale) 10×10 m discretisation	Same conceptual model used for all analysed tracer tests. Checking the possibility of simulating tracer tests results in various geometries with equal transport parameters
VTT/TVO, Finland	< 200 m	Testing if the same conceptual model can explain all tracer test results
PNC, Japan	< 200 m	Testing of the calibrated dipole model by simulating the radially-converging tracer test
PSI/NAGRA, Switzerland	~ 30 m	Consistency in evaluated transport parameters. Comparison between laboratory test results and field test results performed at different sites in granitic rock in various geometries
U. of New Mexico, USA	~ 200×200 m	Model(s) calibrated using the radially-converging tracer test tested by simulating the dipole tracer test
Hazama Co, Japan	1000×1000×100 m (far-field) 300×300×100 m (local scale) 20×20×20 m discretisation	Use of the REV concept in the analysis of flow and transport in fractured rock
Conterra/ICIH/SKB,	1200×1200 m (far-field) 200×200 m (local scale) 10×10 m discretisation	Extrapolation of a model, calibrated on a Sweden local scale, to a larger far-field scale
BRGM/ANDRA,	2500×1200×100 m	Consistency in evaluated flow and transport France parameters
UPV/ENRESA, Spain	1000×1000 m 20×20 m discretisation	Testing if the use of a Gaussian model is a conservative choice

Applying a porous medium, double porosity model, the PNC team calibrated the transport parameters for the dipole tracer test. The validity of the model was subsequently checked by simulating the radially converging test. The results showed good predictive capability for early times, whereas tails in the breakthrough curves were poorly represented (Figure 4.3.3). The latter discrepancy was dealt with by introducing a mixing zone between the modelled high-conductivity layer and an overlying low-conductivity layer.

The BRGM team succeeded in predicting late interference-test results based on calibration to early interference tests.

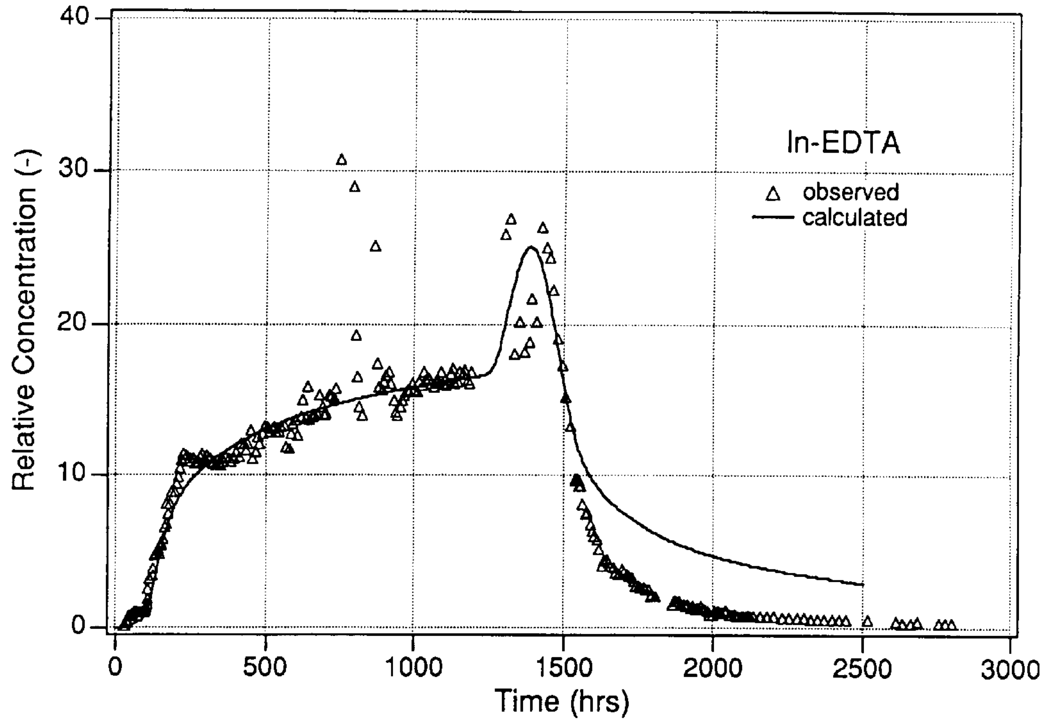


Figure 4.3.3. PNC. Comparison between simulations and experimental data for In-EDTA in the radially converging test based on dipole data.

The U. of New Mexico team used a single/double porosity 2-D model to predict the converging test and checked the validity of their models by simulating the dipole test. They concluded that a reasonable agreement between measured and simulated breakthrough could be obtained.

The Conterra/KTH-WRE team addressed a performance assessment issue, namely, extrapolation of transport models, calibrated on a small scale, to larger transport scales. Using an extensive reference library of transmissivity fields and a stochastic continuum approach, they showed that a model calibrated on an experimental scale is not validated on a larger far-field scale when being subjected to extrapolation and simulation of a far-field natural gradient test. The reason is that local-scale conditioning data do not suffice to describe far-field scale heterogeneity.

The UPV team raised an important issue related to the choice of statistical model when generating transmissivity fields in stochastic continuum applications. The UPV work showed that if the multiGaussian model is used instead of a non-multiGaussian model, this should be preceded by a check whether the data also are bivariate Gaussian, with the understanding that the multiGaussian approach intrinsically suppresses connectivity of extreme values. The latter is of paramount interest from a performance assessment perspective, since an unwarranted use of the multiGaussian model may lead to an incorrect assessment that a site is “safe”.

4.3.5 Comparative Study of a Synthetic Case

The fact that the Finnsjön experiments cannot be used to discriminate between different conceptual models should not constitute a problem from a performance assessment perspective if differences between predictions based on the models were negligible. To illustrate the relative predictive uncertainty amongst the different models, a synthetic natural-gradient tracer test was conceived, to which all INTRAVAL modelling teams were invited to apply their calibrated models *[35]*. In order to facilitate the analyses by the different modelling teams, two transport scales were defined: 500 m (Case A) and 1000 m (Case B). The layout of the test cases and the positioning of tracer line sources and line collectors are shown in Figure 4.3.4.

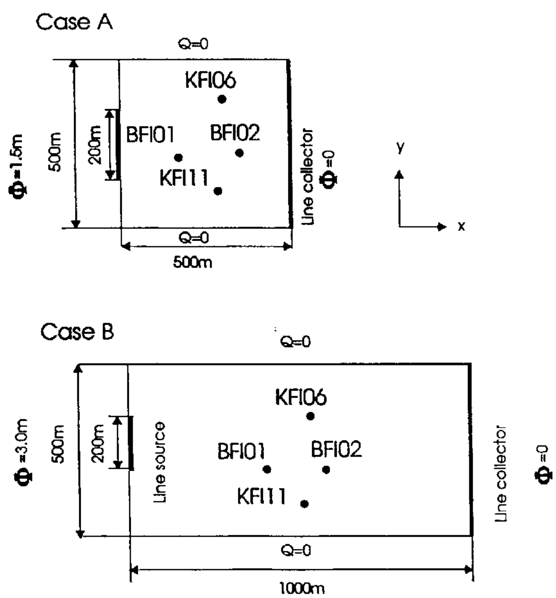


Figure 4.3.4. Layout of the synthetic tracer test used in the comparative study.

Tracer is introduced as a pulse over a period of 1 hour under a uniform gradient of 0.3%. The mass arrival (breakthrough) as a function of time is monitored along the respective sampling lines. A distribution coefficient, $K_d = 1.0\ m^3/kg$, is defined to address sorption. Representative input data used by the five modelling teams addressing the comparative study are shown in Table 4.3.3.

Table 4.3.3. Comparative study of synthetic model cases based on the Finnsjön test case. Selected input parameters used by the modelling teams.

Modelling team	Material property representation	Mean T (m^2/s)	B (m)	N (-)	$"_L$ (m)	$"_I$ (m)	R_d (-)
EdM	K, effective	$1.3 \cdot 10^{-3}$	5	$1.4 \cdot 10^{-3}$	A:50 B:100	–	–
JAERI	2b, stochastic	$6.3 \cdot 10^{-4}$	5	$3 \cdot 10^{-4}$	–	–	–
VTT	channels, number of	$1 \cdot 10^{-3}$	–	–	–	–	–
PNC	T, stochastic	$5.2 \cdot 10^{-4}$	5	$8 \cdot 10^{-3}$	–-	–	$3.3 \cdot 10^{5}$
GEOSIGMA	K, effective anisotropic	$T_{max}=1.5 \cdot 10^{-3}$ $T_{min}=1.8 \cdot 10^{-4}$	0.5	0.01	A:5	A:0.2	$2.7 \cdot 10^{5}$

T= transmissivity, B= fracture thickness, N = porosity, " = longitudinal dispersivity, $"_T$ = transversal dispersivity and R_d = retardation factor

Figure 4.3.5 shows breakthrough curves for Case A.

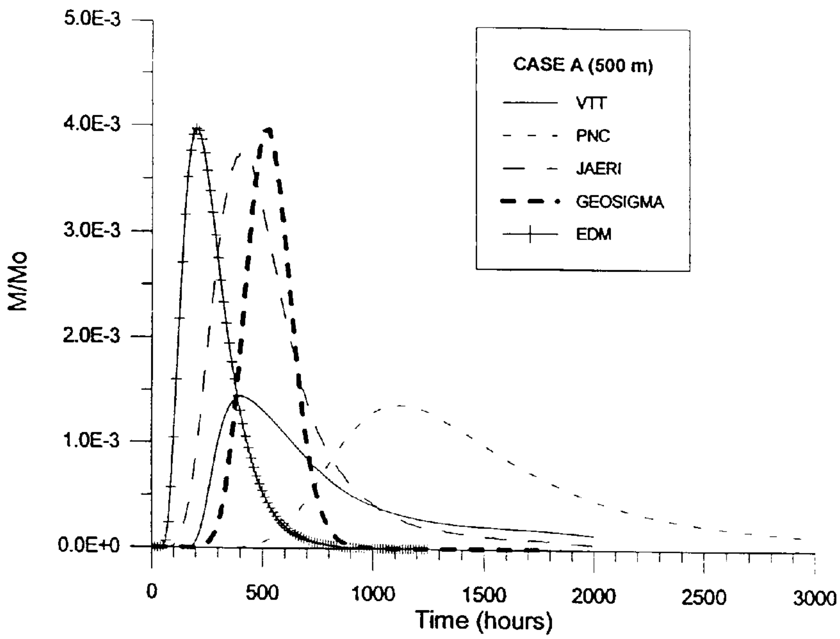


Figure 4.3.5. Predictions for the natural gradient tracer test, Case A (500 m).

The following performance measures were evaluated from the breakthrough curves: first arrival time $t_{5\%}$, the peak arrival time t_{peak}, the maximum relative concentration $(M/M_o)_{max}$ and an index of tracer spreading """ defined as $t_{90\%}$-$t_{10\%}$ (Table 4.3.4).

Table 4.3.4. Comparative study of synthetic model cases based on the Finnsjön test case. Measures from the calculated breakthrough curves.

Modelling team	$t_{5\%}$ (h)	t_{peak} (h)	M/M_o (max) (-)	""" (h)
CASE A (500 m)				
VTT	205	405	$1.4\cdot10^{-3}$	1731
PNC	520	1125	$1.4\cdot10^{-3}$	2350
JAERI	140	405	$3.8\cdot10^{-3}$	863
EdM	75	200	$4.0\cdot10^{-3}$	450
GEOSIGMA	295	520	$4.0\cdot10^{-3}$	440
CASE B (1000 m)				
VTT	470	890	$8.0\cdot10^{-4}$	3497
PNC	2050	3600	$4.4\cdot10^{-4}$	7710
JAERI	290	810	$2.2\cdot10^{-3}$	1420
EdM	150	400	$2.0\cdot10^{-3}$	900
GEOSIGMA	–	–	–	–

The results for Case A showed that the breakthrough curves obtained by most teams exhibited similar characteristics, the exception being the PNC breakthrough curve which was more smeared and delayed compared to the other breakthrough curves. This discrepancy was explained by the combined effect of the mixing zone introduced and matrix diffusion. The GEOSIGMA breakthrough curve showed the smallest dispersion. This was attributed to the lower values of dispersivity applied (Table 4.3.3).Similar behaviour was obtained for Case B with the exception of the PNC curve, for which the time dependency of matrix diffusion became more pronounced.

4.3.6 Conclusions

A variety of different conceptual approaches were applied in the analysis of the Finnsjön test case. The results show that the different approaches could be used to successfully model the experiments. A comparative study, aimed at quantifying the predictive uncertainty when extrapolating the calibrated models to larger transport scales, demonstrated that four out of five models provided results which were fairly similar on the two transport scales considered. The exception was a model incorporating a pronounced effect of matrix diffusion.

The work on the test case was dominated by porous media approaches in two dimensions, although some project teams applied one-dimensional and even three-dimensional approaches. As in INTRAVAL Phase 1, it was shown that tracer test data from one or two tests at a given site are not sufficient to discriminate between models or active processes. The dimensionality employed did not appear to be decisive for the ability to reproduce the field responses.

It was demonstrated that stochastic approaches could be used in validation processes. Flow and transport in the fracture zone studied are apparently governed by advection. However, hydrodynamic dispersion is needed to explain the breakthrough curves. Matrix diffusion seemed to have only a small effect on tracer transport.

The approaches to the validation of the models were versatile and addressed more issues than just the classical validation issue. Apart from improving the predictive capability of solute transport phenomena in crystalline rock, the additional knowledge obtained may be equally important for performance assessment. It was shown that the classical approach to validation of models can be successfully applied using a number of conceptual strategies.

One of the stochastic analyses showed that a heterogeneous model, calibrated on a local transport scale, will not necessarily be validated on a larger scale. Another stochastic approach showed that the choice of distribution model for material properties has implications for the continuity of extreme values and for travel time distributions.

4.4 Flow and Tracer Experiments in Crystalline Rock Based on the Stripa 3-D Experiments, Sweden

4.4.1 Overview

The Stripa 3-D migration experiment was based on the three-dimensional tracer tests that were performed in the Stripa mine in Sweden. The experiment formed part of the OECD/NEA International Stripa Project. The main purpose of the 3-D experiment was to investigate the spatial distribution of water flow paths in a large block of rock. The experiment gave an opportunity to validate geosphere transport models in terms of dispersion, channelling and geometrical factors in fractured crystalline rock over distances up to 50 m.

The test case was studied by two teams during INTRAVAL Phase 2. The first team comprised the Technical Research Centre of Finland (VTT) and the Industrial Power Company Ltd, Finland (TVO), and the second team BRGM/4S, France (BRGM), Itasca Consultants S.A., France (ITASCA) and the French Agency for Nuclear Waste Management (ANDRA).

4.4.2 Site Description and Experimental Design

The Stripa mine is a disused iron mine adjacent to a body of granite. There are several mine galleries at depths down to 410 m. The 3-D experiments were performed within the granite body at the 360 m level. The 3-D drift is a 75 m long test drift provided with two 12.5 m long side-arms that was excavated for experimental purpose.

Water emerging in the 3-D drift was collected in plastic sheets glued onto the ceiling and the upper parts of the walls. In total about 375 sheets, each having a surface area of about 2 m^2, served as sampling areas (Figure 4.4.1).

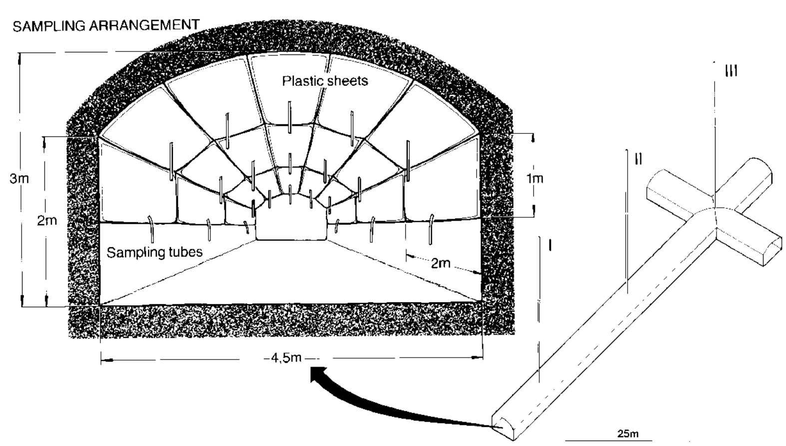


Figure 4.4.1. Layout of experimental 3-D drift at Stripa and sampling arrangement.

Monitoring showed that the water flow into the drift was very unevenly distributed and localised to certain wet areas with large dry areas in between. Measurable amounts of water emerged in 145 of the 375 sampling sheets. The sum of the 145 water inflow rates added up to about 600 ml/h. About 50% of the total water inflow occurred in approximately 3% of the covered area. The sheet with the largest inflow of water represented about 10% of the total inflow. The mapping of the major 100 fractures in the test site indicated that the areas having a higher number of fracture intersections also had higher water flow rates. This finding is in accordance with observations elsewhere.

For the tracer tests, three vertical holes for injection of tracers were drilled upwards with lengths of 70 m. Tracers were injected in nine highly permeable zones of the boreholes, located between 10 and 55 m above the test drift. The tracers were Uranine, Eosin B, Eosin Y, Phloxine B, Acid Red Y, Elbenyl, Duasyn, bromide, and iodide. The injections were carried out at constant pressure. The concentrations of the injected tracers varied between 1000 and 2000 ppm, and the flow rates fluctuated between 1 and 20 ml/h. The tracers were injected continuously over nearly two years.

Water entering the 3-D drift was sampled for tracers during the injection time of 20 months and during an additional 6 months after the end of injection. Tracers from at least six of the nine injection zones could be found in significant concentrations in about 35 sampling sheets. A seventh tracer was found in low concentrations in some of the sampling sheets at the end of the sampling period. No tracers were found in the right part of the arm, which is the area with the highest water inflow rates. The right arm is also closest to the injection zones in hole III, but the tracers injected at these zones emerged at the central part of the main drift. Figure 4.4.2 shows the locations where the individual tracers emerged. About 200 different tracer breakthrough curves were obtained from the experiments. Each curve was typically based on more than 1000 individual measurements.

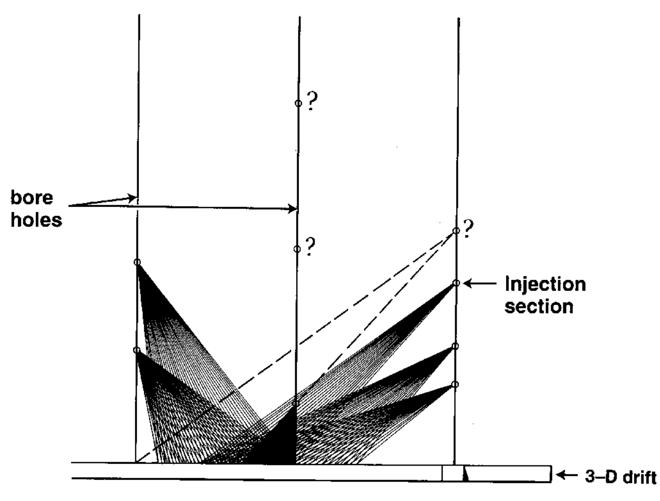


Figure 4.4.2. Areas in the test site where the different tracers emerged. "?" marks injection sections from which tracers were not found in the 3-D drift.

The experimental findings from the experiment demonstrated that the water flow into the drift was very unevenly distributed. There seemed to be a correlation between fracture intersections and high water flow rates. The tracers occurred unevenly distributed in the drifts. Experimental breakthrough curves in adjacent sheets for the same tracer were in many cases quite dissimilar.

4.4.3 Conceptual Models and Modelling Approaches

The conceptual approaches applied were mainly focused on the effect of channelling. A summary of the approaches in both Phase 1 and Phase 2 is given in Table 4.4.1.

Table 4.4.1 Conceptual approaches, modelling objectives and processes considered by the teams modelling the Stripa 3-D test case in Phase 1 and 2 of INTRAVAL.

Modelling Team	Conceptual model	Modelling objectives	Processes considered
Phase 1			
KTH/SKB	Combinations of 1-D fractures with advection–dispersion, advective channelling, matrix diffusion	Employ range of models	Advection–dispersion, matrix diffusion
LBL/USDOE	Solute transport in 2-D planes with variable aperture embedded in a 3-D space	Use multiple-variable aperture channel model to explain multiple-peak breakthrough	Advection–diffusion
KTH/SKI	Discrete fracture network	Calibrate network model. Employ different flow channel geometries	Advection–dispersion
INTERA/AEA/ NIREX	Pore-fracture-fault network is represented by a self-similar fractal structure	Apply fractal approach to model self-similar property of the rock	Advection–diffusion
Phase 2			
VTT/TVO		Use deconvolution technique to analyse experimental tracer breakthrough	
BRGM/ITASCA/ ANDRA	Solute transport in 3-D network of interconnected 1-D channels	Calibrate computer models and calculate tracer breakthrough	Advection–dispersion

The two Project Teams in Phase 2 used different modelling approaches to analyse the experimental data. The BRGM team considered a network of one-dimensional channels located in a three-dimensional network of interconnected disc-shaped fractures. The team considered a channel geometry, where flow was assumed to occur through ?bonds” joining the centre of each disc to the centre of the adjacent disc (the Simplified Disc Model, SDM). The team also used a model, where one-dimensional channels were randomly located on the fracture discs and where fracture intersections may or may not be considered as channels (Random Channel Model, RCM).

The VTT team applied a deconvolution technique to analyse the experimental breakthrough curves. The team focused on the detailed analysis of the impulse responses given by deconvolution of the experimental breakthrough curves and injection pulses, taking into account the effects of measurement errors and other disturbances on the deconvolution results. The team obtained impulse responses containing various peaks. This method, the Extreme Value Estimation method (EVE), estimates the lower and upper bounds of the unknowns or any user-defined linear expression formed from them.

The main data used for fitting transport parameters were the tracer breakthrough curves. However, the variation over time of the tracer injections posed a problem. While analytical or semi-analytical solutions of the 1-D convective–dispersive solute transport equation for simple injection histories exist, it is necessary to resort to numerical schemes when studying more complex injection patterns like the Stripa 3-D injections. The alternatives are the following:

- From the real data estimate what the response would have been, if a simple (pulse) injection had been performed. It is then possible to fit a model to the "simplified" breakthrough curves. Finding the impulse response necessarily involves a deconvolution technique.
- The response of the system to the time-varying injection is computed, using a convolution technique, and the parameters are fitted directly without an intermediate step of deconvolution.

The first approach was used by the VTT team and the second by the BRGM team.

The channel network employed by the BRGM team was based on a model in which the solute transport takes place in a three-dimensional network of interconnected one-dimensional channels located in disc-shaped fractures. A description of a channel network requires specification of many geometric parameters, such as the size density and orientation of fracture sets. For the RCM, several extra parameters are needed to define the geometry of the channel network on the discs. In addition, channel conductance distributions, as well as single-channel transport properties, are required. Fracture orientations were defined by the peak density value observed on the Schmidt diagram from the fracture mapping of the 3-D drift. The fracture radii distribution was derived from observed trace-length distributions taking into account biases affecting the experimental histogram. Log-normally distributed fracture radii were assumed for the derivation of the fracture size distribution. The team conditioned the disc network geometry to the actual fracture traces observed in the ceiling and walls of the experimental drift. The team found that the connectivity of the simulated Stripa network was not significantly changed when fractures with a radius below 2.0 m were removed. This simplified the fracture network and saved computer effort.

The objective of the calibration of the flow model was to determine the "channel transmissivity distributions" of the SDM and RCM channel networks. The hydraulic properties of the channels were assumed to be log-normally distributed. The criterion for calculation was matching flow rates into the drift. The flow was simulated in a 190×160×150 m volume having the 3-D drift located at the centre.

The team fitted the SDM and RCM channel-network transport models to the experimental breakthrough curves that had been obtained for Eosin B, Eosin Y, Uranine, and Elbenyl. The time-varying injection flow rates were explicitly treated in the calibration. Two parameters were used to calibrate the models. The first was a microdispersivity coefficient, ", which accounted for the local dispersion in the flow channels. The second was a shape factor, C_f, which was used to calculate the volume available for transport. The shape factor was determined on the basis that the width of the "parallel plate channel" was proportional to its length. Thus, using the cubic law, the calibration of C_f enabled the distribution of apertures and widths characterising the transport model to be determined. " and C_f were assumed to be constant over the whole network.

The VTT team used the Extreme Value Estimation method to perform the deconvolution. EVE is a general purpose tool for solving a linear set of equations in cases where all the unknowns have to be non-negative. It estimates the lower and upper bounds of the unknowns or any user-defined linear expressions formed from them. The equation solved is $y = \mathbf{M}\ a + e$, where the vector y contains the measured breakthrough curve pulse of the tracer, $\mathbf{M}$ is a kernel matrix formed from the injection pulse (a Toeplitz type lower triangular matrix), and a is the impulse response. Measurement errors associated to y are represented by e, assuming that they are independent random variables with known standard deviations. The basic assumption inherent in this technique is that the system under study is linear and time-invariant. Also, the technique must be constrained to yield only non-negative "pulse" breakthrough curve concentrations, since "perfect" measurements would lead to non-negative concentrations.

The team used a deconvolution technique to analyse the experimental breakthrough curves. The team focused on the detailed analysis of the impulse responses given by deconvolution of the experimental breakthrough curves and injection pulses, taking into account the effects of measurement errors and other disturbances on the deconvoluted results. The impulse responses obtained contained various peaks. The VTT team did not fit a given transport model to the estimated impulse responses.

4.4.4 Results

The BRGM began by evaluating a channel microdispersivity, ", assumed to be constant over the whole network, from the calibration of the channel-network models to the experimental breakthrough curves. In a second stage, Peclet numbers were estimated by fitting a continuum model to the simulated curves. "Global" dispersion lengths could be estimated from the Peclet numbers obtained by these fits. The ratio between the dispersivity obtained by this method and the microdispersivity introduced to calibrate the models could be used to evaluate the importance of network effects. Ratios between 1.1 (Elbenyl, SDM) and 18 (Uranine, RCM) were obtained with a mean of 4.6 for the SDM and 6.6 for the RCM. These results show that the transport pathways were reduced to only one or a few poorly connected channels in some realisations and a high channel microdispersivity was required in attempts to reproduce the dispersion revealed by the experimental curves.

Figure 4.4.3 shows the results obtained with the SDM for the four tracers and the "Eosin Y fits" obtained with the RCM. An example of fit of the analytical solution to a simulated curve is also given in the figure.

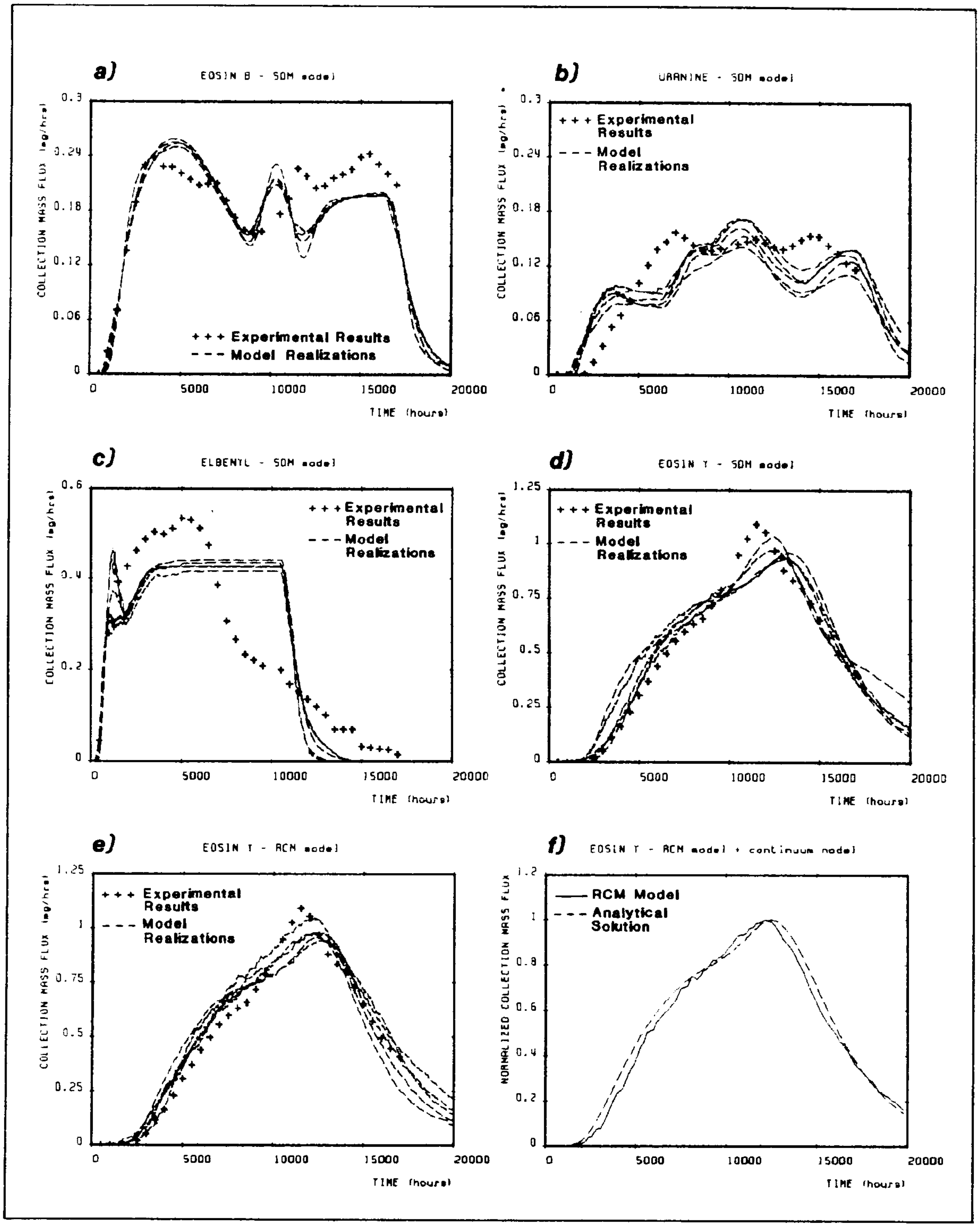


Figure 4.4.3. BRGM. Fit of the result of the channel-network models to the mass collection rates. a), b), c) and d) = simplified disk model, e) = random channel model, f) = fit of the analytical solution.

The results from the model fits indicated that:

C The fits were generally good for Eosin Y; satisfactory fits of the first behaviours were obtained for Eosin B; the beginning of the build-up was only well reproduced for Elbenyl; fits showed poor agreement for Uranine.

C The variation of the two calibrated parameters between realisations was by a factor 10, at the most.

C In most cases, the best-fit dispersivity "-values were not negligible. The highest values of " were obtained for the tracer Elbenyl, whereas the smallest ones were obtained for Uranine.

C the best-fit shape factor C_f-values were generally low with a mean around 0.7 for the SDM and 1.2 for the RCM. Considering the mean channel length in both models, such values would correspond to channel widths equal to 10 m on the average for the SDM and 0.8 m for the RCM.

The BRGM team did not consider matrix diffusion when simulating transport in the channel networks, but estimated the "geometric channel surface area per volume of rock". Obtained values ranged from about 0.5 m^2/m^3 for the RCM to about 5 m^2/m^3 for the SDM.

The team estimated porosity using the results of the calibration of their transport models to the total breakthrough curves. The calibrated SD flow model was used for this calculation. In this case, it was found that the flow porosity could vary by a factor 2 or 3 depending on the orientation of the gradient. Values obtained with the RCM were 5 to 7 times lower than the values obtained with the SDM.

The BRGM analysis also showed that the scale of the experiment, about 100 m, was not large enough for a porous medium to be a valid equivalent.

The VTT team analysed six tracers: Eosin B, Iodide, Bromide, Elbenyl, Eosin Y, and Uranine. Injection flow rates were discretised into constant time intervals of a length of 125 hours. The impulse responses were estimated using the rates of mass accumulation. For Eosin B, both concentrations and rates of mass accumulation were applied. Figure 4.4.4 displays representative responses obtained for Eosin B. The impulse responses are presented as confidence bands. In each case, the plot on the right-hand side indicates the goodness of the fit to the measurements (shown as stars) of the convolution of the the impulse response with the injection (shown as a solid curve). The impulse responses were computed using the 125 h discretisations of the measured pulses. As the kernel had a high condition number, the estimated functional was chosen to be the sum of the components of the impulse response in a window 1000 hours wide, moved in steps of 250 hours. A smoothed solution was then obtained.

The bands shown in Figure 4.4.4 were based on the assumption that the standard deviation of the errors was always 10 % of the breakthrough. Each impulse response was represented by two confidence bands. The wider band was plotted with solid double lines and corresponds to value 4.0 of a confidence parameter D, defined by the team. The narrower band, whose individual intervals are the vertical segments between the stars, corresponds to value 2.5 for D. The analysis was also performed with a 500 h discretisation of the initial data and a step of 500 h instead of 250 h for the window. It was found that the density of discretisation seemed to have very little effect upon the results. In the same way, it was observed that the shape of the band was not substantially changed by the value of the confidence parameter.

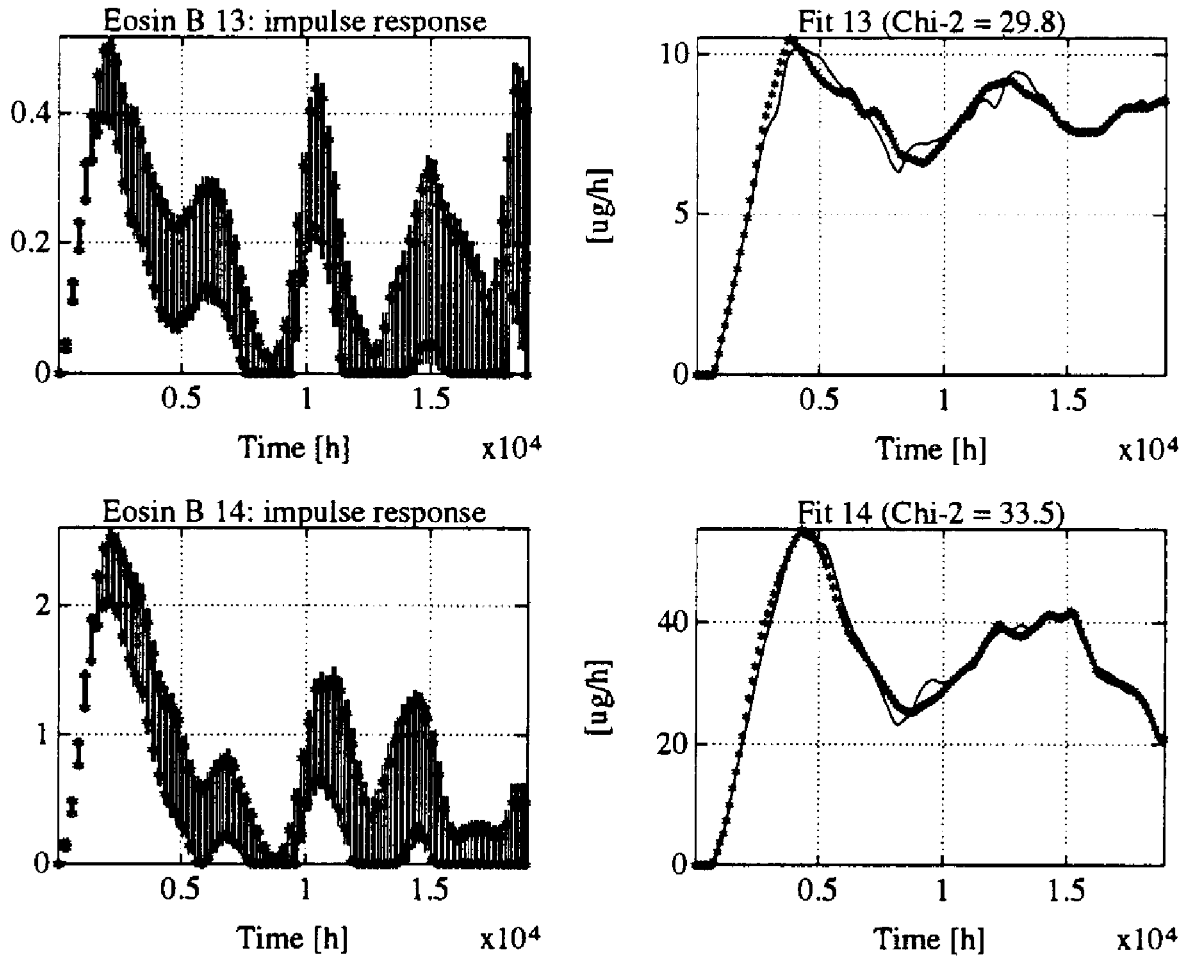


Figure 4.4.4. VTT. Representative results of EVE analysis method for Eosin B.

VTT also performed a sensitivity analysis in order to study the physical relevance of the multiple peaks identified from the impulse responses. It was concluded that interpretation of the impulse responses should be made with great care and the following points were emphasised:

- In the Stripa 3-D experiment, it is not known whether the assumptions made in the deconvolution procedure (linearity and time-invariance of the system) are valid.
- The basic properties of the solutions may be changed by quite minor changes in the injection functions.
- The available data are not sufficient to discriminate between various possible solutions.

- The physical relevance of multiple peaks appears rather uncertain in some cases, especially for Eosin B, and the apparent peaks are probably due to the mathematical appearance of the injection flow rate data.

The VTT team analysed the "dispersive powers" of hydrodynamic dispersion and matrix diffusion in order to study, whether matrix diffusion effects could be identified from the breakthrough curves. The analysis was based on the comparison of a 1-D analytical solution for the advection–dispersion equation to the corresponding solution for the advection–matrix diffusion equation. The team concluded that matrix diffusion did not seem to play an important role in the Stripa 3-D experiments. Consequently, the team could explain the experimental breakthrough data by hydrodynamic dispersion.

4.4.5 Validation

All of the teams validated highly-channelled flow path models. The INTERA/AEA/NIREX project team provided an independent validation of the one-dimensional flow path approach.

The assumptions used by the project teams were in some cases quite different, but nevertheless the various channel models were able to reproduce most of the trends observed in the experiment. This outcome would indicate that the experimental data could not be used to discriminate between the various channel models.

One problem remained unsolved. It was not understood why low recovery rates, and sometimes complete loss of tracers, were observed. Possible explanations were given, for instance by the KTH/SKB team, such as diffusion into the matrix or into stagnant water or flow paths leading away from the experimental drift. Unfortunately, data needed to evaluate these hypotheses were lacking. Although the models applied were able to reproduce some of the field observations, it was difficult to see how the observations could be predicted by the models. To overcome these difficulties, future tracer transport experiments should include more detailed investigations of flow conditions.

4.4.6 Conclusions

The Stripa 3-D experiments provided a good opportunity to study the advective flow and dispersion of soluble tracers through saturated fractured rock. The use of a multitude of plastic sheets in a long underground drift allowed a detailed survey of the spatial and temporal variability of flow and transport. Notably the investigations showed:

- an uneven distribution of water inflow rates into the drift
- a relationship between areas having a higher number of fracture intersections and areas having higher water flow rates
- an uneven distribution of tracer concentrations, underlined by the fact that experimental curves in adjacent sheets for the same tracer in many cases were quite dissimilar.

The uneven distribution of flow and tracer paths indicated one difficulty with the experiment, namely, the lack of knowledge of the flow patterns in the volume under study.

The observation that flow and tracer transport seemed to be located to a few preferential flowpaths or channels resulted in the project teams paying special attention to the definition and incorporation of channels and channel properties. Although the teams made quite different assumptions, the various channel models were able to reproduce most of the trends observed in the experiment. However, the experimental data could not be used to discriminate between the various channel models.

The calibration strategies used by the project teams were designed to estimate the effective parameters representing the Stripa flow system. The time-varying injection flow rates made the interpretation difficult in some cases. Deconvolution techniques appeared to be an interesting tool to treat such data, although, as noted by the VTT team, physical interpretation of the deconvoluted results should be made with great care. Considering only the fitting of the experimental breakthrough curves, the use of sophisticated numerical transport models with a large number of parameters did not improve fits obtained with simple analytical models. However, in a sparsely-fractured medium, conditioning appeared to be a potential tool to improve the calibration of stochastic transport models, as was noted by the BRGM team.

4.5 Flow and Transport Experiments in Heterogeneous Fractured Media Performed at the Waste Isolation Pilot Plant (WIPP) in Carlsbad, New Mexico

4.5.1 Overview

The INTRAVAL WIPP-2 test case was based on data from site investigations carried out at the Waste Isolation Pilot Plant (WIPP) near Carlsbad in New Mexico, USA. The site has been chosen as a potential location for a radioactive waste repository in a salt formation. At the site, a number of tunnels have been excavated. Some of the tunnels are used only for research purposes, while other tunnels have been excavated as proposed deposit tunnels.

Extensive investigations have been carried out at the site. For the purpose of INTRAVAL, the attention was mainly focused on groundwater flow and transport in the Culebra Dolomite. This is a thin horizontal formation extending for many kilometres, which is considered to form the main pathway for transport of radionuclides off the site by groundwater.

The test case was studied by the following five teams:

- AEA Technology, UK, on behalf of United Kingdom Nirex Limited, (AEA)
- Universidad Politécnica de Valencia, Spain (UPV)
- Bundesanstalt für Geowissenschaften und Rohstoffe, Germany (BGR)
- Sandia National Laboratory, USA (SNL)
- Atomic Energy Control Board of Canada (AECB).

During the course of the INTRAVAL project, the participants were given the opportunity to comment on design for a proposed new experiment at the WIPP site. The proposed experiment was intended to examine transport of both reactive and non-reactive tracers over a range of length scales. It comprised measurements of transport between various combinations of boreholes in a formation with overall dimensions of the order of 100 metres.

4.5.2 Description of the Site and Experimental Data

The location of WIPP is shown in Figure 4.5.1. The overall stratigraphy of the rocks in the region is shown in Figure 4.5.2.

The proposed WIPP repository location is in the Salado formation which is composed of thick beds of halite interbedded with anhydrite, polyhalite, dolomite and clay. The Salado formation is overlain by the Rustler formation which is divided into five members based on lithology.

Of the numerous investigations at the WIPP site, the INTRAVAL test case mainly used data on groundwater flow and transport in the Culebra Dolomite layer. The Culebra Dolomite layer of the Rustler Formation is considered to be the first laterally-continuous, transmissive radionuclide transport in the subsurface, should a breach of the repository occur. This layer is about 8 m thick.

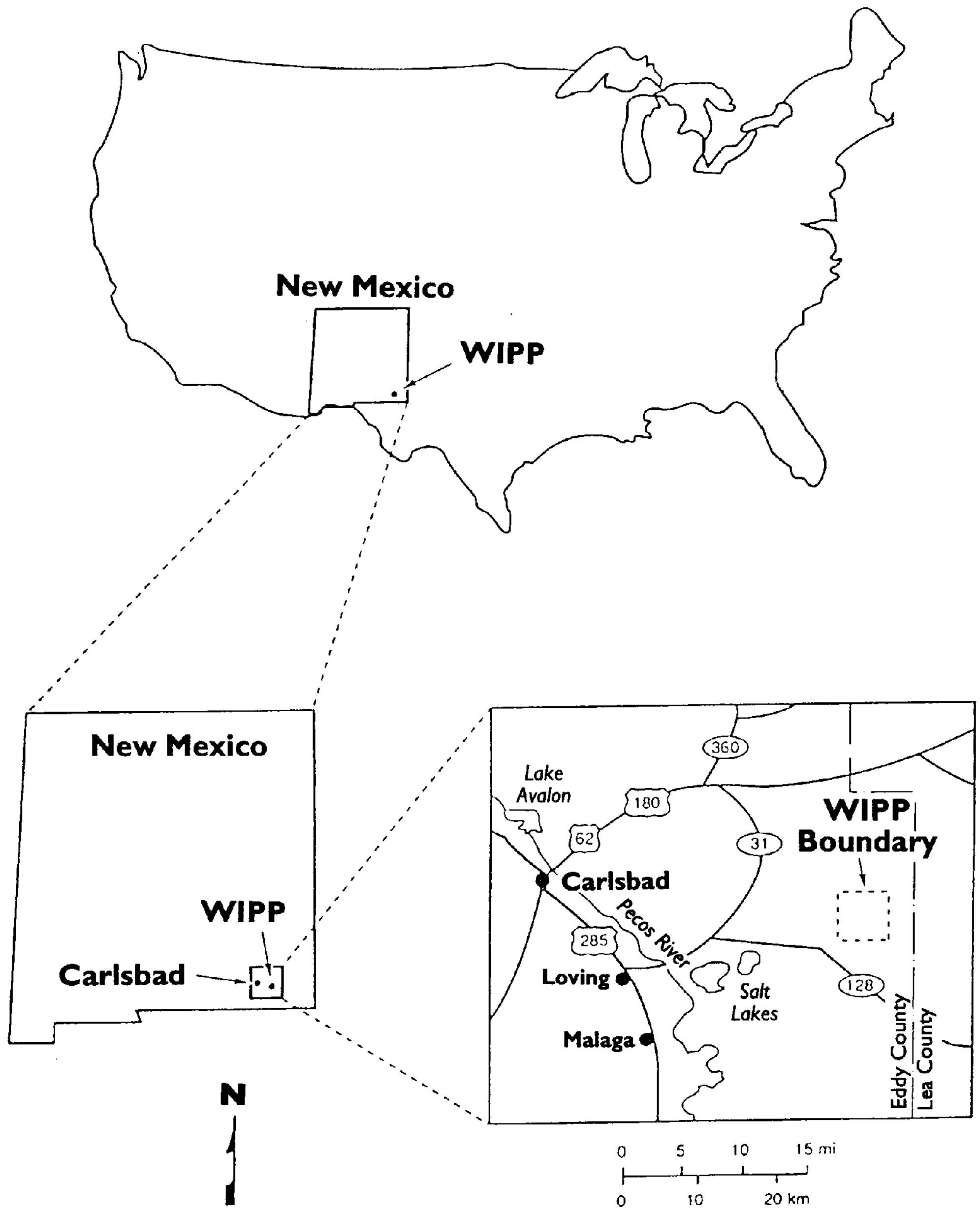


Figure 4.5.1. The location of the Waste Isolation Pilot Plant (WIPP).

Groundwater flow within the Culebra Dolomite is considered to occur mainly in fractures. The average spacing of all fractures is about 10 cm, and the average spacing of the fractures carrying flow is considered to be about 50 cm. It was assumed that a continuum porous-medium model would be a good approximation for modelling flow on the length scales of interest (many kilometres).

System	Series	Group	Formation	Member
Recent	Recent		Surficial deposits	
Quarternary	Pleistocene		Mescalero Caliche	
			Gatuña	
Triassic		Dockum	Undivided	
Permian	Ochoan		Dewey Lake Red Beds	
			Rustler	Forty-niner
				Magenta
				Tamarisk
				Culebra
				Unnamed
			Salado	Upper
				McNutt
				Lower
			Castile	
	Guadalupian	Delaware Mountain	Bell Canyon	
			Cherry Canyon	
			Brushy Canyon	

Figure 4.5.2. The stratigraphy of the rocks in the region of the WIPP site.

The transmissivity of the Culebra Dolomite has been measured at 41 different locations. The data exhibit considerable variability, covering a range of over seven orders of magnitude. On the large scale, the data appear to exhibit a pronounced trend with high values to the west and low values to the east. However, this trend appears to be reversed on the scale of the site. The matrix porosity of the Culebra Dolomite, which shows considerably less variability than the transmissivity, is about 0.16.

The general pattern of the groundwater head is that it is high to the north and decreases to the south, corresponding to a general water flow from north to south. The groundwater salinity measured at various locations and other data, such as results of transient cross-hole tests, were also available to the project teams.

4.5.3 Conceptual Models and Modelling Objectives

The studies undertaken by the different teams can be divided into three main groups:

- Issues included in the treatment of heterogeneity using stochastic models and a Monte Carlo approach were addressed by the AEA and UPV project teams.
- Issues related to the choice of conceptual model were investigated by the BGR and SNL project teams. They explored the importance of vertical flow between the Culebra and overlying formations as well as the importance of climate changes.
- The use of the test case to examine the merit of bounding calculations to highlight the most important processes and parameters was studied by the AECB project team.

The conceptual models and modelling objectives used by the five teams are summarised in Table 4.5.1.

Table 4.5.1. Conceptual models and modelling objectives.

Project Team	Conceptual model	Modelling objectives
AEA	Stochastic continuum porous medium model in two dimensions	Study of techniques for validating stochastic models. Framework of statistical hypothesis-testing techniques.
UPV	Stochastic continuum porous medium model in two dimensions	Extensive exploratory data analysis including attempt to correlate variability in transmissivity with geology. Evaluation of uncertainties in hydraulic head, travel time, boundary conditions, etc. Handling of transient data.
AECB	Continuum porous medium model in two dimensions	Demonstrating the use of bounding calculations and sensitivity studies to assess the importance of uncertainties in fluid density.
BGR	Continuum porous medium model in two dimensions	Addressing issues related to choice of conceptual model. Calculation of density distribution, tracking back pathlines, and groundwater inflow rates.
SNL	Continuum porous medium model in two and three dimensions	Exploration of the use of different conceptual models. Study of the importance of vertical flow and climate change.

4.5.4 Results

The AEA Team

The AEA project team used Monte-Carlo stochastic techniques to treat the uncertainty resulting from heterogeneity. The logarithm, Z, of the transmissivity of the Culebra Dolomite was treated as a random spatial process. A statistical model for Z was inferred from the available data. Many realisations of Z were generated using a suitable technique, and groundwater flow and transport were calculated numerically for each realisation. The uncertainty was then quantified from the range of behaviours shown by the realisations.

The project team used Gaussian statistical models, which are characterised by the first- and second-order moments, the mean, and the variogram. The investigators considered several different statistical models for Z, a model with an exponential covariance, a model with a power-law variogram (which leads to a field with fractal behaviour), a pure-nugget mode (i.e. a model in which Z is completely uncorrelated from point to point), and a model with a linear drift (or trend) and an exponential covariance. They compared different approaches for estimating the parameters for a statistical model of a chosen form (fitting by eye to the experimental variogram, least-squares fitting to the experimental variogram and maximum-likelihood parameter-estimation). They preferred automated methods for parameter estimation, once the form of the variogram had been chosen, which should take geological information into account. Such methods provide a quantitative estimate of the quality of the fit.

For the statistical model with an exponential covariance, the investigators also undertook a Monte-Carlo study of the bias in various automated parameter-estimation methods. They generated many (10 000) realisations of Z for known parameters of the statistical model, and for each realisation they used various methods to estimate the parameters of the statistical model from the values of Z, sampled at locations corresponding to the points at which the transmissivity of the Culebra had been measured. In this way, the distribution of the estimated parameters could be determined for the given parameter values and confidence intervals estimated. This was repeated for different selected values to build up a picture of the confidence intervals for the parameters of the underlying statistical model as functions of the estimated parameters.

The analysis showed that:

- all the methods were biased, i.e. the expected (or average) values of the estimated parameters, considered over the distribution of these parameters, were not equal to the underlying parameters, which were known in the circumstances of the study
- maximum-likelihood parameter estimation had tighter confidence intervals
- if the correlation length was comparable to the size of the domain, then it was not possible to estimate an upper limit to the correlation length. The project team commented that this might not be too significant in uncertainty analyses, provided that the realisations were conditioned on measured values of Z, since they would be strongly controlled by the data in this case.

The project team used the Monte-Carlo approach to quantify the uncertainties in quantities relevant to repository performance, such as the head at a point, the Darcy velocity at a point, the travel time along a pathline, and the position at which a pathline crosses a given boundary. They used the Turning Bands method to generate realisations. Constant-density groundwater flow for each realisation was calculated using the finite-element method, and then pathlines through the flow were calculated. The realisations were conditioned on the measured values of Z using a technique based on kriging. The project team studied the effect of conditioning the realisations on different numbers of transmissivity measurements. They found that the uncertainties were significantly reduced as the number of measurements used to condition the realisations was increased. For example, the uncertainties in travel time were five times larger if the realisations were not conditioned than if they were conditioned on the 39 transmissivity measurements in the domain modelled (Figure 4.5.3).

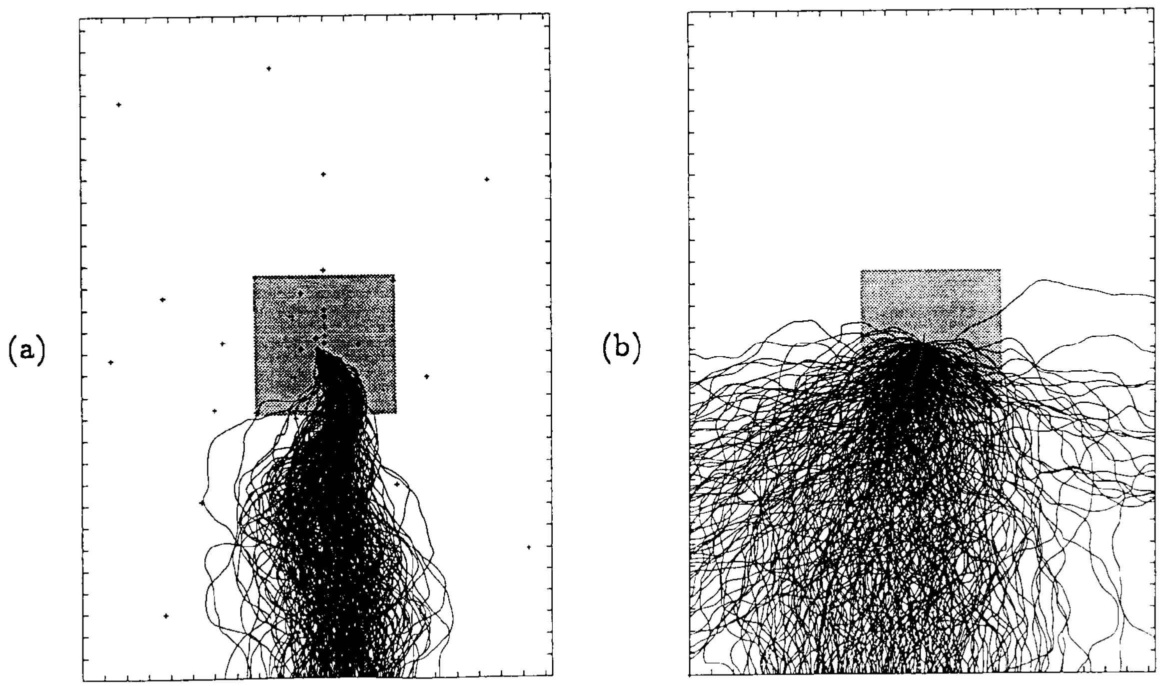


Figure 4.5.3. Pathlines obtained by the AEA project team for: a) realisations conditioned on all the measured values of Z, b) unconditioned realisations. (The ticks around the boundary are spaced at 1 km intervals, the central square is the WIPP site itself and (+) denotes a borehole.

The project team was particularly interested in studying techniques for validating stochastic models. They used the framework of statistical hypothesis testing. A suitable statistic was defined that would be expected to have a small value if the stochastic model was appropriate. The value of the statistic was calculated, and if this value was sufficiently large that it could not reasonably be expected to have arisen by chance, the model was rejected. For all models except the pure nugget model, it was necessary to take account of the correlations between the data.

The project team concluded that:

- the pure nugget model and the model with a trend and an exponential covariance were unlikely to be appropriate models for the Z data
- the model with an exponential covariance and the model with a power-law (fractal) covariance could be appropriate models for the Z data
- all models were unlikely to be appropriate models for the head data, noting that the calculations were for constant density flow and that inappropriate boundary conditions were used.

In most of their work, the realisations were conditioned on the measured values of Z only and the project team used the measured values of head to check the model. They noted that, although the uncertainties might be less, if all the data were used in the construction of the models, no data would then be left to check the model against. As it might be possible to condition an inappropriate statistical model to match all the measurements, careful statistical tests would have to be carried out to check models that had been conditioned on all the data. It would not be sufficient simply to point out that the model matched all of the data.

The project team also explored the use of a technique based on co-kriging for conditioning on measured heads.

The UPV Team

The UPV project team used the same basic Monte-Carlo approach to the treatment of heterogeneity as the AEA project team. They began by undertaking an extensive analysis of the data, including an attempt to correlate the variability in transmissivity with geology, and statistical testing whether a univariate Gaussian model for Z was acceptable. As the raw data were correlated, the project team declustered the data using declustering weights proportional to the kriging weights for the estimation of the average over the entire domain. First estimates of the experimental variograms were used. The Kolmogorov-Smirnov (KS) test was then applied to check for normality. They concluded that the data just passed the test.

As the data seemed to show anisotropy related to the geology (Figure 4.5.4), the project team used an anisotropic Gaussian model, but the project team stressed the need to consider also non-Gaussian models. In Gaussian models, extreme values are not connected over distances that are long compared to the correlation length. However, in performance assessment studies of a repository, it is important to consider models, in which high transmissivity regions are connected over long distances, as these regions might give rise to fast flow paths that may lead to major radiological consequences.

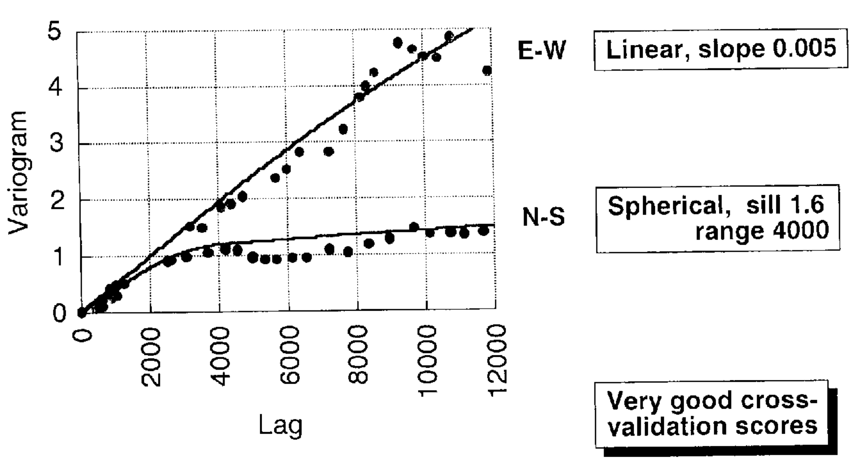


Figure 4.5.4. The directional variograms obtained by the UPV project team.

The project team used sequential simulation to generate realisations. Their initial simulations were for constant-density flow, and the realisations were only conditioned on measured values of Z. These simulations did not give a very good match to the measured heads, so the model was improved to take into account the effects of density variation, uncertainties in the boundary heads, and the measured heads. The project team found that, when heterogeneity was taken into account, the flow field calculated for variable-density flow in some parts of the domain differed significantly from the flow field calculated for constant-density flow.

The project team developed a method for conditioning on measured heads. The basic idea of the method was to compute a modification to the transmissivity field that would lead to an improved match to the measured heads. Figure 4.5.5 shows the improved match to the measured heads obtained for one realisation.

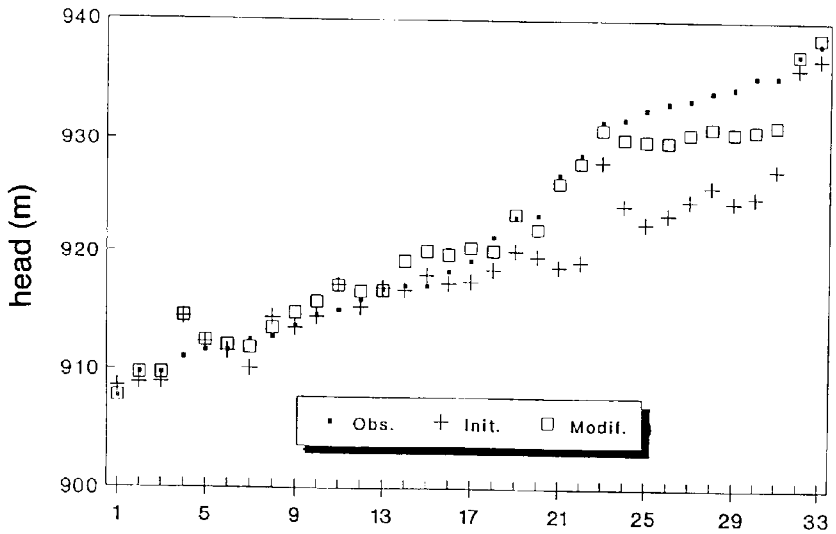


Figure 4.5.5. Illustration of the improved match to measured heads resulting from the use of the technique developed by the UPV project team. The figure presents the measured heads in order of size (shown by ▯ *), the corresponding heads computed for the realisation conditioned on measured values of Z only (shown by +), and the corresponding heads computed after the realisation was conditioned on measured heads as well (shown by* **9***).*

The BGR Team

The BGR project team addressed issues relating to the choice of conceptual model. The AEA, UPV and AECB project teams considered flow in two-dimensional areal models of the Culebra Dolomite, assuming that the permeabilities of the units above and below the Culebra were sufficiently small that vertical flow could be neglected. In contrast to this, the BGR project team applied an alternative model in which all the units above the Salado were represented. They modelled flow in a vertical cross section running parallel to the steepest surface gradients and normal to the margins of the halite beds in the Rustler formation, which represent a potential source of salinity. This choice of model was assumed to give a reasonable approximation to the three-dimensional flow.

Although all available relevant data were incorporated in the model, many parameters had to be estimated. The estimation was done in a manner consistent with the geological setting where possible. Average properties were used for the members of the Rustler formation other than the lower halite beds. Density-dependent groundwater flow was simulated, until an approximate steady-state was reached. The plausibility of the solution was checked by comparing the computed density distribution with experimental measurements.

The steep gradients in the Culebra west of the site were reproduced (Figure 4.5.6). The model predicted nearly freshwater in the Magenta at a position at which this was measured. Pathlines were also tracked back to provide estimates of groundwater age from the travel time along the pathlines. The estimated ages, which did not take account of dispersion, were tens of thousands of years. For comparison, an age of several thousand years was inferred from groundwater chemistry. The results showed that the model was reasonable. It should be noted that the model was not calibrated, but based on initial estimates of the parameters.

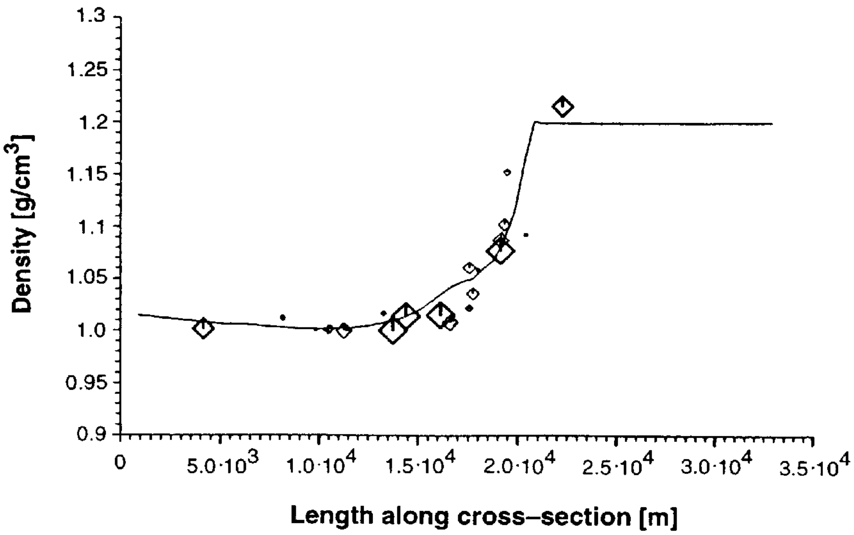


Figure 4.5.6. Comparison of computed and measured densities in the Culebra dolomite for the two-dimensional vertical cross-section model used by the BGR project team.

The SNL Team

The SNL project team explored the use of different conceptual models for the hydrogeology at the WIPP site. They used a three-dimensional regional model to study the importance of vertical flow between the Culebra Dolomite and the overlying units, and to examine the impact of climate change. The model represented all the rocks above the Salado and extended laterally to locations that were believed to correspond to groundwater divides for the entire simulated time. Each stratigraphic layer was considered to be homogeneous.

A period of 41 000 years was simulated. The initial condition was assumed to be steady-state corresponding to the water table at the surface. This was supposed to be representative of the conditions that prevailed in the region at the end of the Pleistocene. For the first 21 000 years simulated, infiltration was assumed to be zero, representing a dry period. The final 20 000 years simulated were taken to correspond to a somewhat wetter period with a maximum potential infiltration of 0.5 mm/year. This is less than 0.2% of current annual rainfall, representing the fact that most rainfall is lost due to surface runoff or evapotranspiration.

The project team noted that there were large uncertainties in many of the parameters used and, furthermore, various simplifying assumptions had to be made, so the results of their modelling should not be taken too literally. Rather the modelling should be considered as an aid to understanding the regional flow. Their calculations suggested that:

- C the flow of groundwater in confined units may be strongly influenced by the overlying water table
- C vertical flow through relatively low permeability layers may have an important effect on the flow in relatively permeable layers
- C climate changes may be important.

The AECB Team

The AECB project team performed bounding calculations to assess the importance of uncertainties in groundwater density in the performance assessment of the WIPP site. They compared the head and flow fields for a base-case distribution of salinity obtained by interpolating the available salinity data with head and flow fields computed for two different distributions of salinity: freshwater everywhere, and the salinity increased by 50% everywhere.

Based on the bounding calculations, the project team concluded that the uncertainties in the salinity (and hence groundwater density) did not significantly affect the flow paths in the Culebra dolomite from the centre of the WIPP site. All of the flow paths followed a high-transmissivity channel that is believed to exist based on hydraulic test results. This channel provides a preferred route for groundwater flow from the site towards the south, and for all of the modelled fluid density distributions, the flow field was able to adjust itself to cause the flow paths from the centre of the WIPP site to pass through the channel. The project team concluded that the flow paths were controlled by the transmissivity distribution, and they suggested that field studies to further characterise the high-transmissivity channel should be an important part of future site investigations.

4.5.5 Validation Issues

The test case provided a valuable opportunity to explore the issues involved in validation of field-scale models of groundwater flow and transport. The different project teams tackled different aspects of the test case. There was some overlap between the issues addressed by AEA and UPV and between the issues addressed by BGR and SNL, although the approaches used by the different project teams differed in detail. Taken together, the conclusions reached by the project teams were generally consistent and helped to build up the picture of flow and transport at the WIPP site.

4.5.6 Conclusions

The WIPP-2 test case proved to be very valuable for the development and study of stochastic models for the treatment of heterogeneity of hydrogeological properties. The different project teams showed that stochastic models could be used in performance assessments of nuclear waste repositories and helped to build confidence in their application. The modelling illustrated how uncertainties resulting from heterogeneity could be quantified and demonstrated the potential benefits of data in reducing the uncertainties.

During the course of INTRAVAL, the UPV project team developed a new technique for conditioning realisations on measured values of head and transmissivity. It was noted that, although the uncertainties might be reduced if all the data were used to construct the model, no data would then be left, against which the model could be checked.

The AEA team arrived at the conclusion that there is no single unique stochastic model. Several stochastic models might explain the data, and the resulting uncertainties are similar.

Since a repository performance assessment should be robust, a range of stochastic models consistent with the data should be looked at. The UPV team emphasised the need to include non-Gaussian models. These models may give fast flow paths which may be important for the performance of a repository but are unlikely to occur in Gaussian models.

The AEA team recommended the use of a statistical-hypothesis-testing framework for the validation of stochastic models. They proved that some models might be rejected using this approach.

The AEA team showed that estimates of the parameters of stochastic models are biased and that confidence intervals might be large. Indeed, it may not be possible to determine an upper limit of the correlation length, if the length is comparable to the size of the domain. However, this fact may not significantly affect the uncertainties computed from conditioned realisations, the reason being that the transmissivity will be strongly controlled by the data.

All project teams emphasised the need to take account of information on the geology in setting up the models. It is desirable to consider alternative conceptual models. In particular, vertical flow through low permeability formations may affect the flow in confined formations with higher permeability. Furthermore, the effects of climate changes may have to be considered.

4.6 Migration Experiment in Boom Clay Formation at the Mol Site, Belgium

4.6.1 Overview

This test case was based on experiments carried out at the Mol Underground Research Facility (URF). The site is located in the northern part of Belgium in a level area of the Belgian country with maximum height differences of a few metres only. An *in situ* migration experiment has been set up at the facility with the main objective of investigating, whether transport parameter values determined in laboratory experiments are also valid for larger temporal and spatial scales. The migration experiment, which is planned to last for fifteen years, was accepted as a test case for INTRAVAL Phase 2. Data from the operation of the facility during the last years were available for the test case.

The following six project teams participated in the INTRAVAL study:

- Studiecentrum voor Kernenergie, Belgium (SCK/CEN)
- National Institute of Public Health and Environmental Protection, The Netherlands (RIVM)
- Agence nationale pour la gestion des déchets radioactifs, France (ANDRA), Bureau de recherches géologique et minières, France (BRGM)
- Ecole nationale supérieure des mines de Paris (EdM)
- Commissariat à l'Energie Atomique, France (CEA/DMT)
- Sandia National Laboratories, USA (SNL), Department of Energy, USA (USDOE).

4.6.2 Description of the Site and Experimental Data

The research facility is constructed at a depth of 224 metres in the 110 m thick Boom clay formation underlying the nuclear research centre at Mol. The clay layer is the uppermost of an alternating sequence of clay and sand deposits and is about 30 million years old. In the facility a multiple-screen piezometer has been installed at the end of a horizontal drift. The multiple-screen piezometer consists of a pipe with a diameter of 4.6 cm that penetrates 10 m into the clay formation and contains nine equally spaced filters 8.5 m long (Figure 4.6.1). This installation is used for the large scale *in situ* tritiated water (HTO) injection experiment.

About 2.5 years after the installation of the piezometers, the clay formation had settled and HTO was injected into the fifth filter at a flow rate of 5.61 ml/day for fifty days. The system was then left alone and the HTO migrated in three dimensions. The tracer arriving at the other filters was monitored by sampling at regular time intervals. The sampling frequency and the amount of liquid was kept as low as possible to avoid disturbance of the HTO concentration in the clay due to the sampling. A vertical experimental shaft lined with concrete bricks that had been built near the end of the URF imposed an enhanced hydraulic pressure gradient in the vicinity of the piezometer.

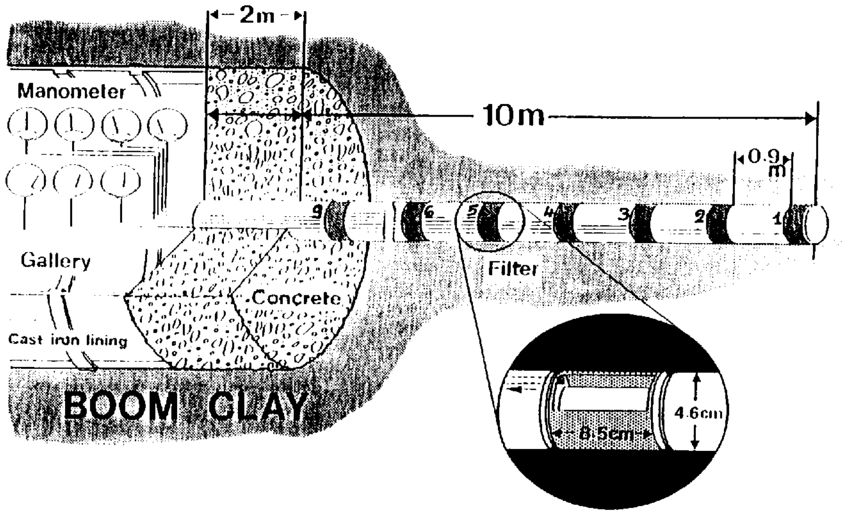


Figure 4.6.1. Experimental set-up at URF, Mol

Different types of migration experiments were performed on clay samples taken from the underground deposit. Reshaped and reconsolidated clay plugs were used for flow-through diffusion experiments. Clay cores drilled parallel with, and perpendicular to, the stratification of the formation were employed for percolation experiments. The values of the migration parameters obtained from the small scale-laboratory experiments were used for long-term safety assessment calculations.

Despite precautions taken during sample collection and preparation of the diffusion experiments, parameters determined in the laboratory were subject to uncertainty. One of the objectives of the large-scale *in situ* experiment was to improve confidence in the laboratory data.

The following data were available to the modellers:

- steady-state pressure distribution in the clay
- HTO concentration as a function of time for each filter
- tracer injection data.

4.6.3 Conceptual Models

The following models were used:

- SCK/CEN as pilot group employed the semi-analytical code MICOF, which incorporates a three-dimensional analytical solution of the transport equation.
- The RIVM team used an analytical solution of the transport equation and the finite–element code METROPOL.
- The EdM team used the finite–element code METIS.

- The CEA/DMT team used an analytical solution of the transport equation and the finite–element code TRIO-EF.
- The ANDRA/BRGM team studied the case by means of an analytical solution of the transport equation.
- The SNL team used the finite–difference code SWIFT.

The six project teams analysed the test case with basically the same conceptual models. The transport equation was solved either analytically or numerically.

4.6.4 Results

The SCK/CEN Team

The main effort on this test case was made by the SCK/CEN project team. Figure 4.6.2 shows the measured concentration in the filters 3 to 7 as a function of the time since injection of the tracer and the simulation results as calculated with the MICOF code.

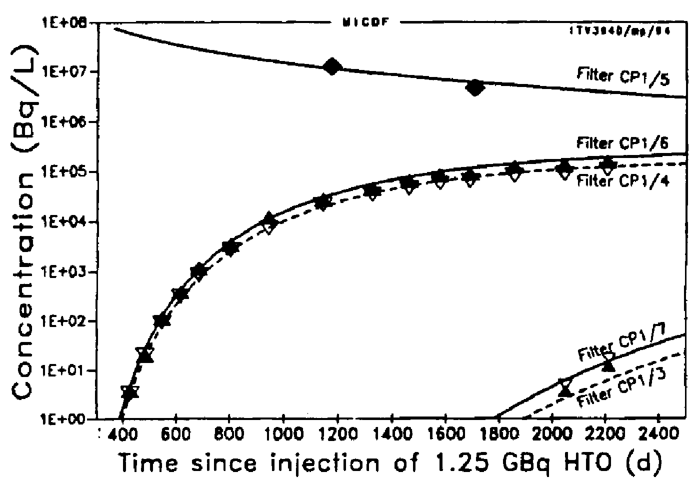


Figure 4.6.2 Measured concentration of HTO in filters CP1/4, CP1/5 and CP1/6 as a function of time since injection of tracer and simulation results as calculated by SCK/CEN with the MICOF code.

The team obtained a very good agreement between calculated results and experimental data. An analytical approximation for the experimental conditions was used to study the sensitivity of the model output to the parameters. As initial condition, a bar-shaped source was considered. The horizontal diffusion coefficient was the most sensitive parameter and the best estimate, $4.05 \cdot 10^{-10}$ m^2/s, was in agreement with the value obtained from laboratory experiments. The horizontal water flow was small, $1.7 \cdot 10^{-10}$ m/s. The vertical diffusion coefficient was estimated to be 1.88 times larger than the horizontal one as a result of the anisotropy of the clay. The parameter values obtained from the *in situ* experiment were in good agreement with the values obtained from migration experiments on clay cores.

The team considered the model and the values of the parameters as validated for the experimental time span.

The RIVM Team

The RIVM project team used two models, an analytic solution of the transport equation and the numerical code METROPOL. The analytical solution was based on the assumption that the clay was isotropic in all horizontal directions. The numerical code METROPOL was based on a finite–element method in space and the Euler implicit method in time. The METROPOL code solves the equations of water flow and solute transport in porous media.

As a result of the fitting the project team concluded that the analytical solution accurately described the migration experiment and that the parameters obtained by the laboratory experiments seemed to be reliable. Furthermore, the team considered that the code METROPOL could be used to solve the advective–diffusive transport equation, but that discretisation errors were important. With a fine mesh, the METROPOL solution approximated both the experiment and the analytical solution quite well. However, the analytical solution was closer to the experimental values than the METROPOL simulation. The accuracy of METROPOL could be increased by using a finer mesh size, but this would lead to an excessively long computation time.

The BRGM/ANDRA Team

The project team from BRGM/ANDRA used an analytical solution to the advective–diffusion transport equation including radioactive decay. The experimental results were fitted for a number of assumptions concerning diffusivity coefficient, injection cell volume, porosity and water flow velocity. A sensitivity analysis showed that the horizontal diffusivity coefficient was the most robust parameter, confirming that diffusion was the predominant transport process. The value of the horizontal diffusivity coefficient was around $4 \cdot 10^{-10}$ m^2/s, which is in agreement with the data obtained from laboratory experiments. The best fit was obtained if the diffusivity coefficients in all horizontal directions were equal. As initial condition, it was assumed that all the injected mass uniformly filled a rectangular volume. The best fit was obtained for a cubic volume. The uncertainty in the value of the porosity was rather large, between 0.20 and 0.30. The assumption that the solute transport was determined only by diffusion is valid only if the porosity is low, less than 0.20. The water flow was estimated to between $2 \cdot 10^{-10}$ m/s and $5 \cdot 10^{-10}$ m/s.

The project team concluded the conceptual model to be validated for transport distances up to 1 m and for a time extrapolation of 1100 days, once the behaviour during the first 700 days was known.

The EdM Team

The EdM project team used a numerical code METIS to solve the advection–diffusion transport equation. The clay was assumed to be horizontally isotropic. A non-horizontal flow field was allowed in the model. As initial condition, the team assumed injection during a period of 50 days. The solution was then fitted according to a generalised reduced-gradient algorithm. It was concluded that the angle of the flow was of no importance. A sensitivity analysis was performed showing the effect of the horizontal and vertical diffusion coefficients as well as of the water flow velocity. The quality of the fit was mainly influenced by the horizontal diffusion coefficient. Depending on the error interval, this parameter may vary between $4.05 \cdot 10^{-10}$ and $4.51 \cdot 10^{-10}$ m^2/s, giving a value of the Peclet number close to 1, which means that dispersion could be neglected. The vertical diffusion coefficient was poorly defined in the experiment and varied between $2.9 \cdot 10^{-10}$ and $8.7 \cdot 10^{-10}$ m^2/s. The third parameter, the horizontal water flow velocity along the experimental set up, had low influence on the quality of the fit. Its value was estimated at $3.5 \cdot 10^{-11}$ m/s. More measurements over a longer time would be necessary to get a better estimation of this parameter.

The team concluded that the experimental data were well simulated by an advective (convective)–diffusive model, characterised by the predominant role of diffusion and a nearly isotropic diffusion coefficient. It was also noted that only limited data were available for calibration of the model.

The CEA Team

The CEA project team used an analytical solution of the transport equation. The equation was solved assuming an isotropic clay. As initial condition, they considered a constant flux injection of tritiated water during 50 days. The influence of the volume of the piezometer screen was neglected and a simplified injection process was assumed. To estimate the influence of these simplifications, the equation was also solved with the finite–element code TRIO-EF. The numerical solution showed a higher solute concentration than the analytical solution, but the difference between the two solutions diminished with time. The difference could not be neglected for times less than 1500 days and the project team claimed that the difference was due to the extension of the injection source. The dimension of the piezometer could not be neglected and was thus taken into account in all the calculations.

The fitting of parameters was done as a two-step process. First, the diffusion–dispersion coefficients were fitted and the mean concentration from filters at opposite positions from the injection cell were estimated. Because the dispersion was much smaller than the molecular diffusion, the mean was a solution of pure diffusive transport. In a second step, the solution of transport equation was fitted with the diffusion coefficients obtained from the first step. A well defined value for the horizontal diffusion coefficient between $3.5 \cdot 10^{-10}$ and $4.6 \cdot 10^{-10}$ m^2/s was obtained.

The values for the vertical diffusion coefficient and the flow velocity were more difficult to define. In parameter space, the fitting error function showed a valley parallel to the vertical diffusion coefficient without any pronounced minimum for the pore velocity. The lack of sensitivity of the fitting error for these parameters was caused by the absence of long time information, as the experiment was still in an early phase, in which molecular diffusion was the dominant mechanism. To make good estimates of anisotropy of the diffusion and the pore velocity, the experiment would have to be monitored for a much longer time period.

The SNL Team

The project team from SNL presented an initial analysis of the effect of anion exclusion on transport in the Boom clay at one of the INTRAVAL workshops. At the time, they could not apply their anion exclusion model to the Mol data, due to lack of information concerning ionic strengths, z potential and pore-size distribution.

4.6.5 Conclusions

The Mol test case treated migration through a clay formation. All project teams could describe the results of the *in situ* experiments with a conceptual model based on advection–diffusion in porous media. The transport equation could be solved either analytically or numerically.

It was confirmed that advective flow may be neglected in such a medium and that molecular diffusion was the predominant transport process during the time period considered. The diffusion coefficient was the most sensitive parameter to estimate accurately. All teams obtained approximately the same value of this parameter, which confirmed its robustness. The values obtained were all in very good agreement with values estimated from laboratory experiments.

The other transport parameters, vertical diffusion coefficient and water flow velocity, were difficult to determine from the experimental data presently available. Measurements over a much longer time period would be needed, as well as data on the concentrations in the plane perpendicular to the horizontal flow direction.

4.7 Saline Groundwater Movements in the Vicinity of the Gorleben Salt Dome, Germany

4.7.1 Overview

The test case was based on the hydrogeological investigation programme carried out for characterisation of the potential German site for a HLW repository at a salt dome in Gorleben. As a result of density variations, salt leaching out from the salt dome influences the flow field. These processes were studied in the Gorleben test case.

The test case was divided into two parts, a pumping test *Weisses Moor* and a regional model of the *Gorleben erosion channel*. Both locations are characterised by a highly heterogeneous geology with large permeability contrasts and a salinity that varies from freshwater near the surface to saturated brine at depth.

The test case was carried over from INTRAVAL Phase 1.

4.7.2 Site Description and Experimental Data

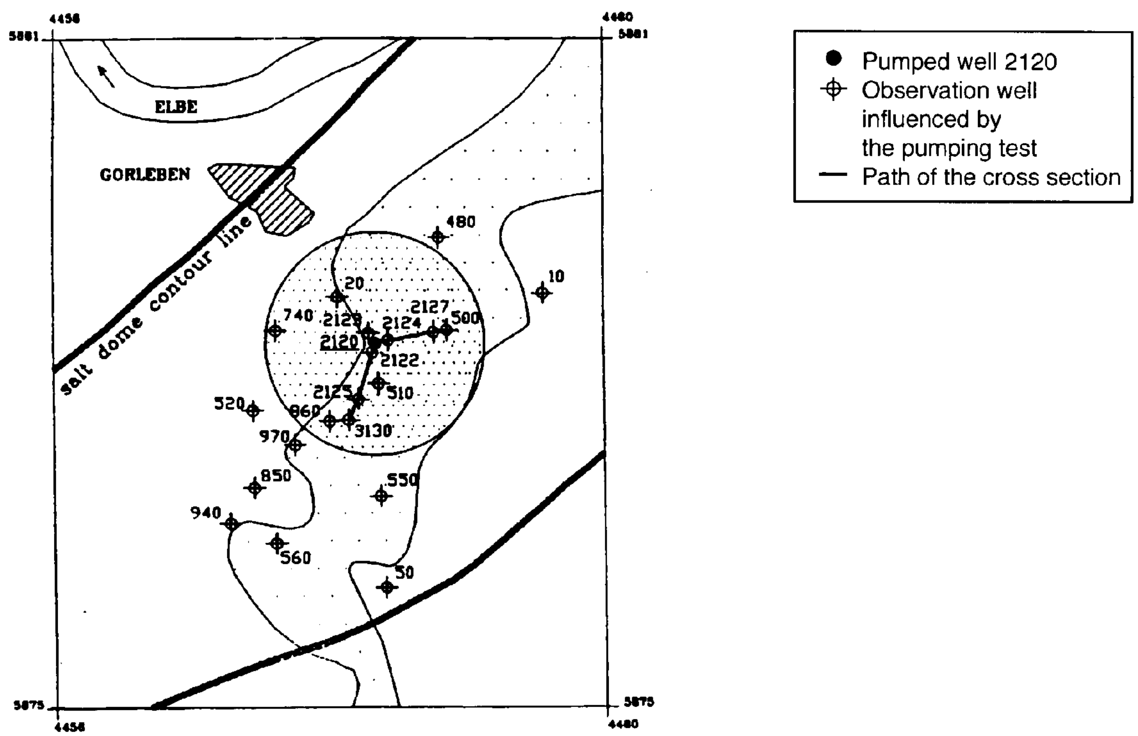
The Gorleben site is located in the northeastern part of Lower Saxony, Germany. The salt dome, which is proposed as a host rock for a HLW repository, is approximately 14 km long and 4 km wide and its base is more than 3000 m below the land surface. As a result of erosion during the Elsterian glaciation, channels were cut into the land surface by melting waters. One of these channels is the Gorleben erosion channel, which crosses the salt dome in an approximately south-north direction. The channel is roughly 10 km long, 2 km wide and 300 m deep. Tertiary and Quaternary sandy and gravelly sediments form a system of two aquifers which are separated by the Lauenburg clay complex. In some places, the lower aquifer is in direct contact with the salt dome. Thus, the deep groundwater is highly saline in this region due to salt dissolution. The groundwater infiltrates almost down to the top of the salt dome at 200 to 250 m depth, where saline water is found. The interface between fresh and saline water is at a depth between 150 m and 50 m.

The ground surface is quite flat with elevation differences of 5 to 15 m. In the regions of higher elevations, the groundwater table is about 8 m higher than the level of the discharge areas. The recharge is about 180 mm/yr south of the salt dome. The regional groundwater flow is predominantly from the southeast to the northwest with a hydraulic gradient in the uppermost aquifer of $1.5 \cdot 10^{-3}$ m/m. Darcy velocities range from 5 to 250 m/yr.

During the site investigation programme, 145 boreholes were drilled to carry out field experiments, such as core sampling and geophysical logging, water sampling, velocity measurements and pumping tests, thus acquiring data on the hydrogeological structure, hydraulic parameters, and groundwater movement and salinity distribution.

Two data sets were selected for validation purposes within the INTRAVAL project. The first concerned a pumping test *Weisses Moor* and the second the groundwater flow field and the salinity distribution in the *Gorleben erosion channel*. The spatial scale of the pumping test was a few hundreds of metres and the duration was three weeks. The main motive for this type of test was to obtain information on boundaries, hydrogeological structure, aquifer connections, etc, as well as hydraulic parameters (permeability, storage, leakage coefficients) and their distribution in the pumped area. During the geological and hydrogeological investigation programme, large quantities of data were acquired that were used as a data base for the modelling of the regional groundwater flow, salt dissolution and their interaction in the erosion channel. An overview of the site is found in Figure 4.7.1.

Figure 4.7.1 Ground plan of the pumping test "Weisses Moor".



4.7.3 Validation Issues

Usually groundwater near salt formations contains dissolved salt with concentrations varying with depth, from saturated brine in the immediate vicinity of the salt formation to freshwater near the surface. The dependency of the fluid density on the salt concentration influences the movement of the groundwater due to buoyancy effects. If this results in slowing down the groundwater velocity in the vertical direction, as is commonly assumed, it will have a large impact on the migration of radionuclides. Therefore, this phenomenon has to be properly accounted for in safety assessments, since simulations must be based on a good knowledge of the groundwater flow field.

To address these issues, the Gorleben test case studied the groundwater movement in an erosion channel crossing the Gorleben salt dome. The aim was to compare simulation results with the measured salinity distribution on a spatial scale, ranging from a few hundred metres in the case of the pumping test Weisses Moor to ten kilometres in the regional flow study.

4.7.4 Modelling Strategies

Six project teams carried out simulations on this test case.

On the pumping test Weisses Moor:
- Bundesamt für Strahlenschutz (BfS), Germany, using an analytical Theis solution and the finite–element codes SUTRA and ROCKFLOW
- Sandia National Laboratories (SNL), USA, with the computer code INTERPRET/2, which employs a Theis solution
- Rijksinstituut voor Volksgezondheid en Milieuhygiene (RIVM), The Netherlands, using the analytical computer code AQ-AT and the finite–element code METROPOL.

On the regional flow system of the Gorleben erosion channel:
- Bundesanstalt für Geowissenschaften und Rohstoffe (BGR), Germany, as the pilot group, using the finite–element code SUTRA
- Gesellschaft für Anlagen- und Reaktorsicherheit (GRS), Germany, using the finite–element code NAMMU.

A geostatistical study of the hydrogeologic system was carried out by
- AEA Technology, United Kingdom.

Table 4.7.1 gives an overview of applied conceptual models and modelling objectives.

Table 4.7.1. Gorleben, conceptual models and modelling objectives.

Project Team	Conceptual model	Modelling objectives
Weisses Moor pumping test		
BfS	Analytical solution for radial geometry (Theis solution) complemented with 2D vertical cross section including also variable density (numerical code)	Demonstrate the influence of density stratification on groundwater flow.
SNL	Analytical solution for radial geometry (Theis solution)	Determine the applicability of analysis techniques based on the Theis solution.
RIVM	Analytical solution for radial geometry (Theis solution). 2D areal numerical model without varying density	Integrated approach. Use pump test to obtain hydraulic properties to construct model to simulate observed pressure distribution and salt concentration.
Regional Erosional Channel		
BGR		Demonstrate whether steady-state conditions exist in the observed salt-water system and check the sensitivity of the model by changing hydrogeological and hydraulic parameters.
GRS		
Geostatistics		
AEA		Qualitative data from boreholes logs were used in a statistical framework to estimate the distribution and variability of the clay formation at the site.

4.7.5 Results

Geostatistical Analysis

The geostatistical approach applied by AEA was based on an indicator methodology, a technique that is often used in oil or mining exploration**.** Similar information as for oil exploration is needed at Gorleben, where an important issue for the safety studies is, whether the Lauenburg Clay complex covers the lower aquifer completely, or whether connections exist between the lower and the upper aquifers near the discharge region.

The geological cross section that was selected to test the methodology was the regional flow system along the channel axis. The borehole logs given in the Gorleben data set were analysed in terms of a binary indicator function, which depended on whether, at a particular depth of the borehole, the log consisted of clay, for which a value of 1 was assigned to the indicator function, or of more permeable material, e.g. sands or silts, for which a value of 0 was assigned. Using this information, a variogram analysis of the indicator function was carried out. The best defined results were obtained, when the co-ordinates were transformed in a way that certain stratigraphic horizons were mapped to a horizontal line. These variograms were used to perform indicator kriging that provided an estimate of the probability, that a particular type of material is present at a certain location. Assuming the 0.5 probability contour to be the interface between clay and non-clay, the results were then compared to the cross section provided by the hydrogeologists. Some discrepancies were observed, which pointed to particular problems in the interpretation of the borehole logs. In one place, it was obvious that the original log, as it was supplied in the test case data set, did not contain any clay. However, for the preparation of the hydrogeological cross section the data had been reassessed. The reinterpretation of this particular borehole log identified a certain section as clay rather than silt, but this information had not been supplied with the data set. This accounts for the discrepancy between the hydrogeologists' interpretation and the cross sections obtained by kriging.

The aim of the work was to use indicator simulation methods to scope the uncertainty in the results of groundwater flow calculations arising from the uncertainty in the geological model. Although this was not possible within the frame of the INTRAVAL project, the analysis carried out was a valuable test of the methodology.

Pumping Test Weisses Moor

The pumping test Weisses Moor was evaluated using both analytical solutions and numerical simulations. The analyses carried out by the RIVM and SNL teams employing a Theis solution demonstrated that the analytical solution was only appropriate, if it was modified to account for lateral anisotropy in the aquifer system and for boundary effects. Another problem in the interpretation of the test arose from partially-penetrating wells. However, this affects mainly the monitoring boreholes in the immediate vicinity of the pumped well, that is at distances of a few tens of metres. Those boreholes should not be included in a Theis-type analysis. Figure 4.7.2 shows the result of the SNL team for one observation borehole. It was not possible to fit the complete time history of the test. If the drawdown part was fitted, the recovery was slower than measured, whereas if the recovery was fitted, the initial pressure was calculated to be lower than the measured one. Both observations indicated a rising water level during the experiment.

The lateral anisotropy and heterogeneity of the system was further studied by RIVM by means of a horizontal two-dimensional numerical model. The hydrogeological data used were based on the available geological information, including estimates of the aquifer thickness. They assumed that the main axis of the permeability tensor coincides with the channel axis. The hydrology of the system was characterised by six parameters, namely the storativity, the anisotropic permeabilities, and multiplication factors to account for the heterogeneous permeability in three different regions. It was then possible to obtain a reasonable fit for the pumping period of the test.

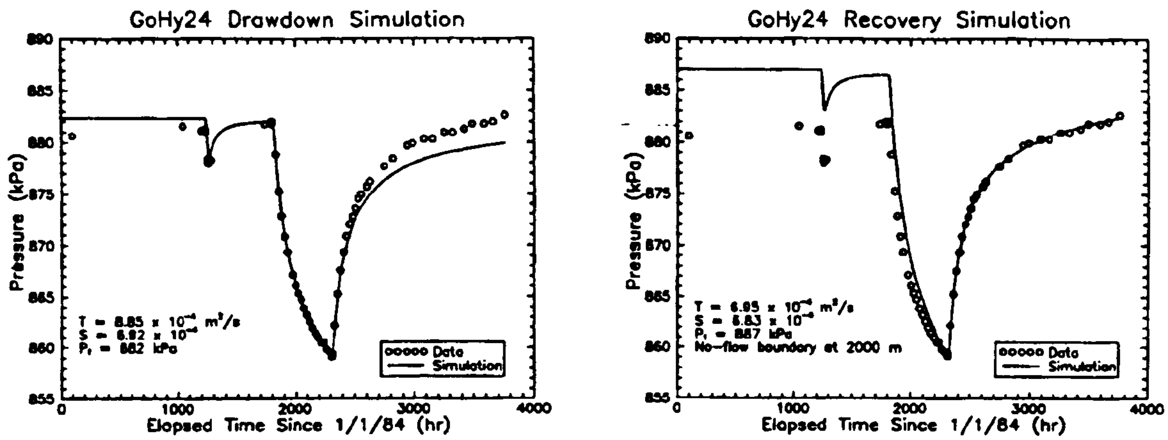


Figure 4.7.2. Weisses Moor. Drawdown at observation borehole GoHy24.

Despite the limitations mentioned above, the Theis solution provided a reasonable estimate for the average values of aquifer transmissivity and storativity for use in numerical simulations, even if anisotropy and heterogeneity were not taken into account. This was demonstrated by the BfS team. Based on those values, they constructed a two-dimensional vertical model to study the impact of density variations on the flow field during the pumping test. They used two different codes. Both gave nearly identical results in the drawdown curves, if a constant density approach was used. The drawdown curves agreed very well with the Theis solution except for the immediate vicinity of the pumped well. This can be attributed to two-dimensional effects. However, no significant differences were observed between results obtained from constant- and from varying-density models.

The Gorleben Erosion Channel

It was first intended to study of the regional flow model of the Gorleben erosion channel with a three-dimensional model. Freshwater studies were carried out by GRS within this framework. However, in view of the very large amount of resources needed in computer memory and computing time, this idea was abandoned. Instead, a two-dimensional cross section along the channel axis was selected and modified to account for connections between the lower and upper aquifers not present at the exact location of this particular cross section (Figure 4.7.3).

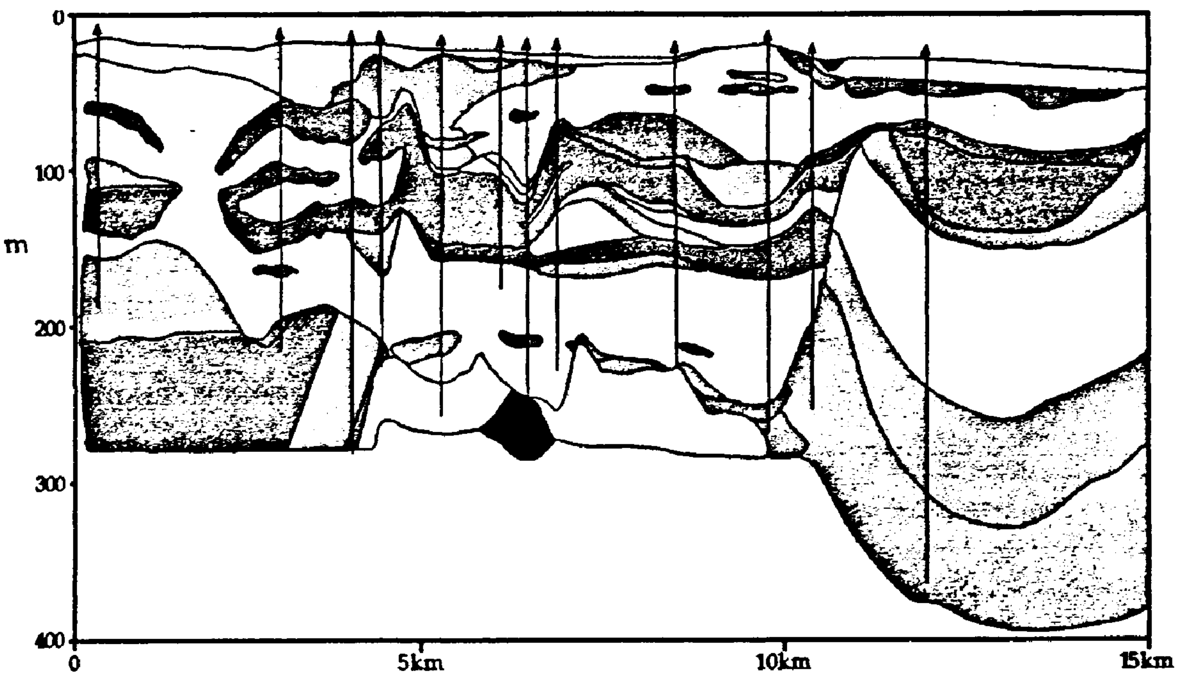


Figure 4.7.3. Gorleben erosion channel, geological cross section.

As initial studies had shown that it was not possible to obtain the current measured salinity distribution with a steady-state approach, transient salt transport simulations were performed by the BGR and the GRS teams. The teams used different discretisations for their models and different approaches for the initial conditions of the system.

The BGR team defined an initial salinity distribution with a 20 m thick transition zone at a depth of approximately 180 m. Based on assumptions about the salinity distribution under permafrost conditions during the last ice age, the fluid in the transition zone was varied from saturated brine to nearly freshwater. A sensitivity study was carried out on the depth of the transition zone. Only one of the variations resulted in a salinity distribution after 10 000 years simulation time that showed similarity to the measured distribution (Figure 4.7.4).

A second sensitivity study was performed on potential connections between the upper and lower aquifers in the discharge region. This analysis showed significant influence on the calculated salinity distribution. Finally, the importance of the transverse dispersivity was demonstrated. The use of a high value resulted in a larger spreading of the transition zone than observed in the field investigation.

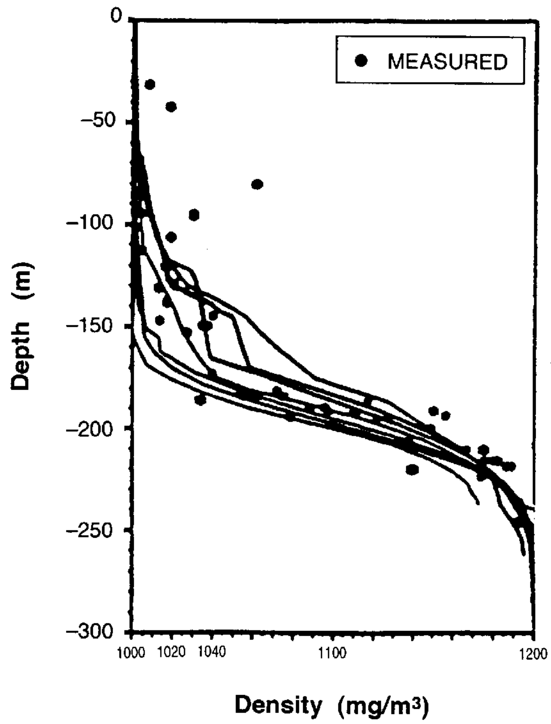


Figure 4.7.4. Gorleben, salinity versus depth at 1000 years.

In their model, the GRS team used a very fine discretisation to overcome limitations on the size of the dispersion length due to numerical stability criteria. It was assumed that no salt was present in the system at the beginning of the simulation. Saturated brine was allowed to enter the system at the contact area between the lower aquifer and the salt dome. During the simulation, the lower parts of the aquifer system, filled with brine, slowed down the vertical groundwater velocities. Figure 4.7.5 shows the state of the system after 1700 years simulation time, when salt has already entered the right hand side of the model.

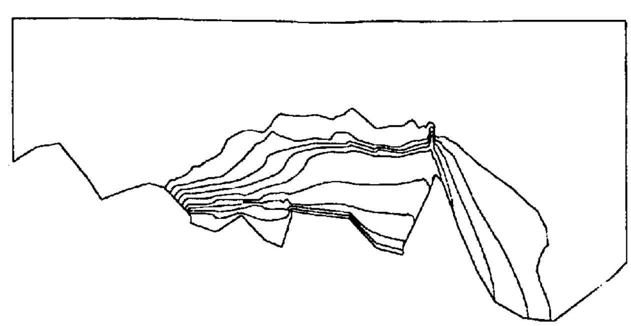


Figure 4.7.5. Gorleben, salinity distribution after 1700 years simulation time.

In order to get a good understanding of the current state of the system, it would be useful to have better founded assumptions on the initial salinity distributions using information from different scientific disciplines, like paleohydrogelogy. Specially-designed experiments would also be needed to validate variable-density flow models.

4.7.6 Conclusions

Data from site characterisation were used in the Gorleben test case to test models on variable density flow. Analysis of the pumping test *Weisses Moor* did not reveal any effects of density variations on the flow field. However, to obtain a realistic interpretation of the flow field, it is important to take account of the heterogeneities and anisotropies of the aquifer system. The study of the regional flow system of the Gorleben erosion channel demonstrated that fully three-dimensional simulations of salt transport are currently not feasible due to the demands on computer resources. Improvements are needed in the understanding of the past evolution of the system to cope with the long time periods involved in the development of the salinity distribution observed today. Specially designed field experiments would be useful for future efforts in validating variable-density flow and salt-transport models.

4.8 Brine Inflow through Bedded Evaporities at the Waste Isolation Pilot Plant (WIPP) in Carlsbad, New Mexico

4.8.1 Overview

This case was based on experiments carried out at the Waste Isolation Pilot Plant in New Mexico, USA (Figure 4.8.1). WIPP is an underground research and development facility lying 655 m below ground surface within bedded evaporites, primarily halite of the Permian Salado Formation (Figure 4.8.2). The aim of the experiments was to study the flow of brine from a bedded salt formation into open excavations under pressure gradients. A number of *in situ* experiments were carried out, their scale ranging from small boreholes to large excavated rooms. The focus of the WIPP 1 test case was to define an appropriate model for long-term simulation of brine flow.

The test case was analysed by three project teams:

- Sandia National Laboratory (SNL), USA
- The National Institute of Public Health and Environmental Protection (RIVM), The Netherlands
- Ecole nationale supérieure de Mines de Paris (EdM), France.

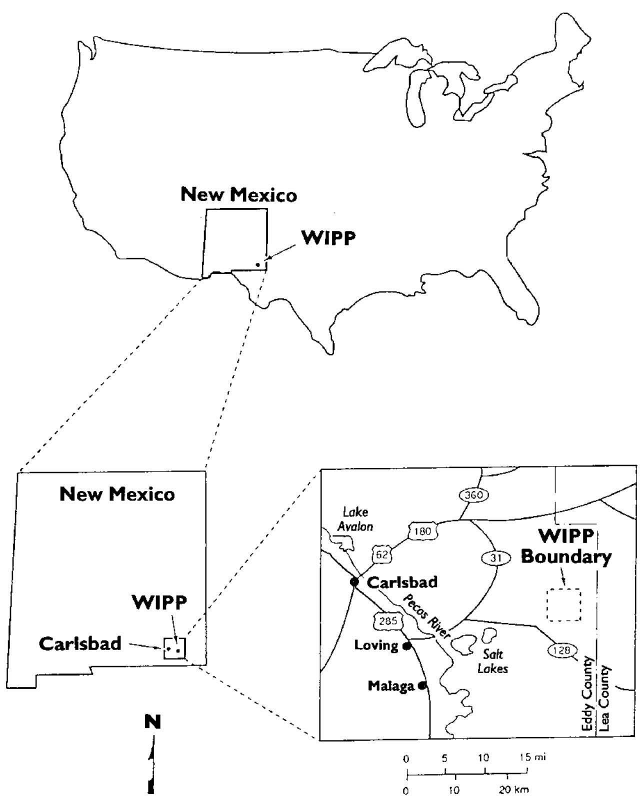


Figure 4.8.1. The WIPP site at Carlsbad in New Mexico, USA.

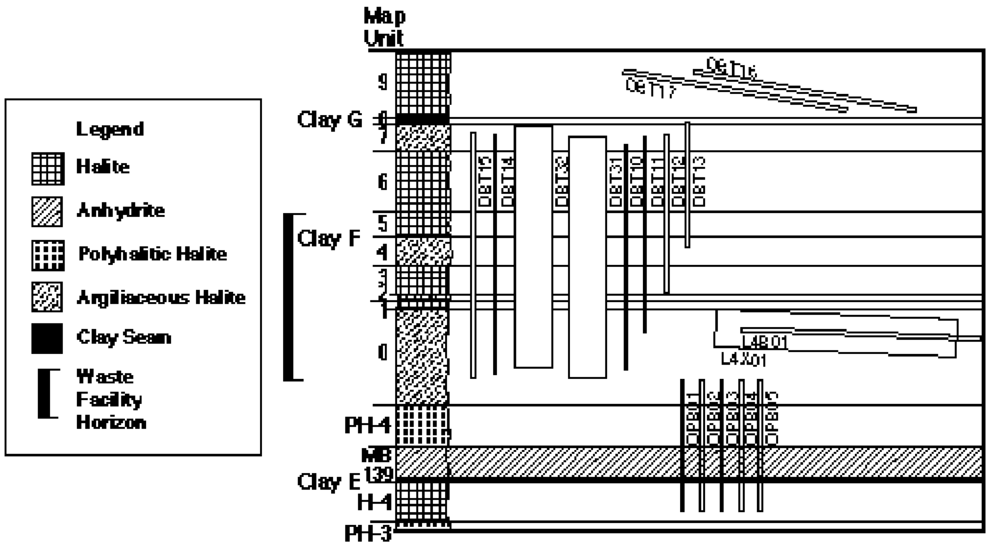


Figure 4.8.2. WIPP 1. Brine inflow boreholes.

4.8.2 Site Description and Experimental Design

The WIPP site is located in the northern region of the Delaware Basin in southeastern New Mexico, USA. The underground facility lies in the lower part of the Salado Formation, which is of Permian age, at an approximate depth of 655 m below ground surface. At the WIPP site, the Salado Formation is approximately 600 m thick and composed largely of halite with minor amounts of interspersed clay and polyhalite. It also contains interbeds of anhydrite, polyhalite, clay, and siltstone.

The WIPP 1 experiments provided data on the hydraulic behaviour of the Salado Formation under a variety of conditions. The objective was to define an appropriate model for the long-term simulation of brine flow and to determine whether brine flow through evaporites under different *in situ* test conditions could be accurately simulated with a Darcy-type flow model. Such a model might then be reliably used in safety assessments to predict rates and volumes of brine inflow to the WIPP repository.

Tests were made to evaluate formation responses under different conditions. Data from the following three types of experiments at three different scales formed the basis of the test case:

- small-scale brine-inflow experiments to measure the long-term flow of brine from the formation to boreholes maintained at atmospheric pressure
- pore-pressure and permeability tests to provide information on pore pressures, permeabilities, and other hydraulic properties at different positions around the repository
- large-scale brine-inflow experiments (Room Q) to provide data on inflow to a room-sized opening in the halite, with supporting data provided by pore-pressure and permeability measurements in the surrounding rock.

The data from the tests were given to the project teams, who used different subsets of the data as the basis for their individual models.

Small-Scale Brine-Inflow Experiments

For the small-scale brine-inflow experiments, boreholes with diameters of 10 cm and 1 m were drilled from the repository into the formation, oriented either vertically downward or horizontally at lengths from 3 to 6 m. The accumulation of brine seeping into each borehole was measured as a function of time. The boreholes were open over their entire span, but each borehole opening was sealed to prevent moisture loss through evaporation and air circulation. Humidity measurements were made to aid in quantifying the total moisture entering a borehole.

The WIPP 1 test case data set includes data from four 10 cm boreholes drilled vertically downward (DBT boreholes) intersecting a sequence of pure halite and argillaceous halite. Brine-inflow measurements generally showed rapidly declining flow rates for the first few months, followed by steady or slowly declining flow rates for periods as long as two years. Initial flow rates ranged from about 5 to 25 g/day, while steady flow rates ranged from about 2 to 10 g/day. Inflow rates into some boreholes began to increase two to three years after the holes were drilled. In addition, data from two 10 cm and 36 cm horizontal boreholes drilled into the argillaceous halite in test room L4 were used. One of these boreholes produced as much as 25 g/day during the first few months after it was drilled, but the flow rate then declined to near zero. The other yielded only about 2 g/day of brine. The humidity in these holes appeared to be in equilibrium with free-standing brine.

Pore-Pressure and Permeability Tests

The WIPP 1 test case included results of permeability and pore-pressure experiments from argillaceous halite layers, anhydrite layers, as well as sequences of halite, polyhalitic halite, and clay. Pore-pressure and permeability tests were conducted in 10 cm boreholes drilled in a variety of orientations through different layers at locations of older and younger excavations in the underground facility. The testing sequence in the test zone consisted mostly of an initial buildup period followed by pulse-withdrawal tests.

Pressures were measured in intervals of the boreholes isolated by packers. They ranged from 0.3 MPa (measured within 2 m of a repository room) to 12.5 MPa (measured at locations farther than 22 m from a repository room).The lithostatic pressure at the WIPP repository level was 14.8 MPa. This shows that a depressurised zone exists around the repository. Stratigraphic heterogeneity and stress relief around the excavation may also have significant effects on the pressures observed in the test boreholes.

Permeability experiments in the boreholes involved pressure-pulse, constant-pressure flow, and pressure-buildup tests. Pressures, temperatures, and flow rates were measured as well as packer pressure, radial borehole deformation, and borehole elongation.

Integrated Large-Scale Experiments in Room Q

A large-scale experiment was conducted in test Room Q, a cylindrical room, 110 m long and 2.9 m in diameter, bored parallel to bedding in the upper host rock strata of the planned waste disposal stratigraphic interval. Its location represented an isolated, undisturbed area, where pre-mining values for pore pressure and fluid flow could be established in a far-field location. Boreholes were drilled and instrumented to allow for assessment of pre- and post-mining hydrologic conditions. Data from four of these boreholes were included in the test case.

4.8.3 Validation Issues

The goal of the test case was to establish the applicability of Darcy's equation, or alternative models, to describe brine flow through evaporites under a pressure gradient. In the test case, the flow mechanisms were examined at various scales, from 10 cm diameter boreholes to 3 m diameter rooms. The applicability of a Darcy-flow model to evaporites was investigated with suggested possible refinements dealing with two-phase flow and the inclusion of rock-creep effects and coupling of fluid pressures to the stress field in the rock mass. The need for alternative models, such as one in which porosity becomes interconnected and brine is squeezed from the salt as a result of creep, was also considered.

Investigation of the appropriateness of a flow model includes identification of all relevant phenomena and quantification of all necessary parameters that fit into the model. The modelling efforts were expected to identify additional experiments, if any, needed to validate Darcy-flow or alternative models.

4.8.4 Conceptual Models

The tests were analysed by three international teams using several modelling strategies. The pilot group at SNL used a variety of numerical models and analytical solutions. The RIVM team used the METROPOL-2 code. The EdM team used a two-stage mathematical modelling technique employing the HYDREF code.

All three teams modelled the brine-inflow experiments in the DBT boreholes. Data from the L4 boreholes were only studied by the SNL team. However, since brine flow in the L4 holes was scattered and erratic, modelling based on these data was restricted. The RIVM group did limited modelling of one permeability test. The SNL group performed extensive modelling of all three permeability tests. Only the SNL team modelled the Room Q experiment.

4.8.5 Results

When comparing the parameters estimated by the three teams in their interpretation of the small-scale brine-inflow experiments, allowances must be made for slight differences in the input parameters, i.e. initial formation pore-pressure, brine density, and brine viscosity, used by the three teams and the effects of those differences on the interpreted parameter values. All results discussed here were appropriately compensated for these differences.

The RIVM and EdM teams distinguished between pure and impure halite in estimating values for permeability. They assumed that pure halite would have a lower permeability than impure halite and sought single values for each that, when combined with the different thicknesses of pure and impure halite in the different test holes, would allow replication of the entire set of experimental results. The SNL team treated the strata penetrated by each hole as homogeneous and sought values for hydraulic properties, different at each hole that would best match the observed data. Thus, the RIVM and EdM teams determined values for the permeability of pure and impure halite that provided the most satisfactory overall match to the brine-inflow data in the aggregate but not to the brine-inflow data from any individual hole, whereas the SNL team determined average permeability values for each borehole.

To compare the RIVM and EdM results to the SNL results, the pure and impure halite permeabilities were weighted according to the stratigraphy of each individual borehole to determine an average permeability for that borehole. These average permeabilities are shown in Table 4.8.1, along with the average permeabilities calculated by the SNL team using different parts of the data. The teams agreed on the average permeability of each of the boreholes within a factor of five. The total range of inferred permeability values spans only an order of magnitude, from $2.3 \cdot 10^{-22}$ to $2.6 \cdot 10^{-21}$ m^2. These values were slightly lower than the range of 10^{-21} to 10^{-20} m^2 normally used to predict brine inflows to WIPP disposal rooms. Interpretations by the RIVM and EdM teams were constrained by their determination of reasonable values for specific capacitance, while the interpretations by the SNL team treated specific capacitance as a free parameter to be fitted.

Table 4.8.1. Comparison of permeabilities calculated by different teams.

Borehole	Calculated permeabilities[1)], m^2				
	RIVM Entire data set	EdM Entire data set	SNL Full flux	SNL Cumulative volume	SNL Late-time data
DBT10	$1.8 \cdot 10^{-21}$	$9.9 \cdot 10^{-22}$	$3.7 \cdot 10^{-22}$	$6.6 \cdot 10^{-22}$	$8.2 \cdot 10^{-22}$
DBT11	$2.1 \cdot 10^{-21}$	$1.2 \cdot 10^{-21}$	$1.5 \cdot 10^{-21}$	$1.6 \cdot 10^{-21}$	$2.0 \cdot 10^{-21}$
DBT12	$1.5 \cdot 10^{-21}$		$8.3 \cdot 10^{-22}$	$8.4 \cdot 10^{-22}$	$2.6 \cdot 10^{-21}$
DBT13	$8.5 \cdot 10^{-22}$	$3.0 \cdot 10^{-22}$	$2.3 \cdot 10^{-22}$	$3.0 \cdot 10^{-22}$	$4.3 \cdot 10^{-22}$

1) assuming initial formation pore pressure = $1.0 \cdot 10^7$ Pa
viscosity = $2.1 \cdot 10^{-3}$ Pa·s
brine density = 1220 kg/m^3

Figure 4.8.3 shows a comparison of the measured data from borehole DBT 10 with the results of the SNL calculation.

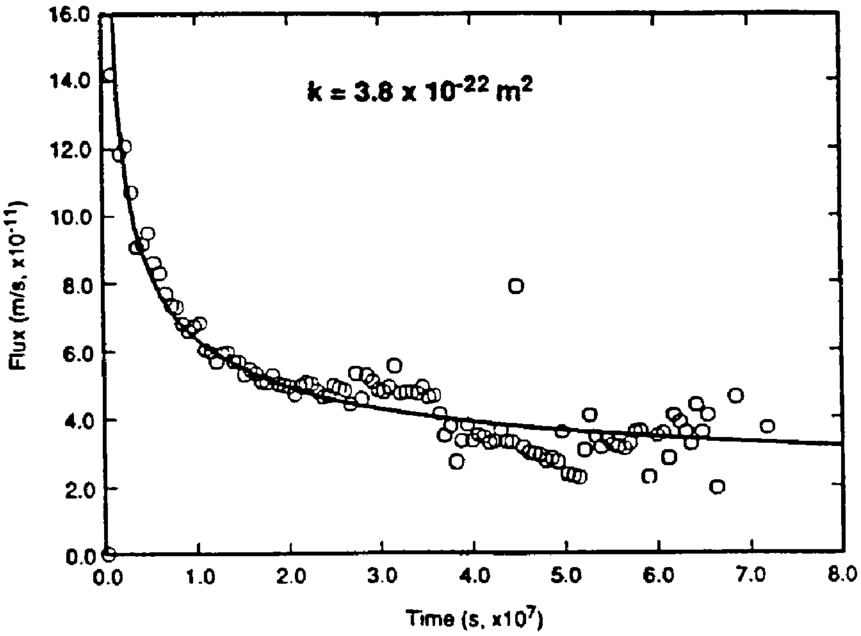


Figure 4.8.3. WIPP 1. Borehole DBT10, measured and calculated brine inflow rate.

In the first part of the experiment the curve agreed quite well with the rapidly decreasing inflow rates and the simulation also gave a reasonable average fit for the later part, when the inflow rates stayed almost constant. None of the teams attempted to model the late-time data from the brine-inflow experiments that showed increasing rates of brine flow. To make brine-inflow rates to increase with time, the permeability around the borehole, or the driving pressure differential, or both, must increase. Increased permeability is the most likely explanation for the increased inflow. Permeability could increase as halite creeps towards the overlying room. Existing fractures may dilate, new fractures may form, and bedding planes may separate as the salt creeps. Increased permeability in any of these cases would, in effect, allow a borehole to draw brine from a larger volume of rock. However, simulation of changes in creep-induced permeability and the resulting changes in brine-inflow rates would require coupling between a geomechanical model and a hydrological flow code.

All test teams interpreting the brine-inflow experiments concluded that the average permeabilities of the halite strata penetrated by the holes were between approximately 10^{-22} and 10^{-21} m^2. The teams interpreting the permeability experiments, which in addition to halite included a distinct clay seam, found the average permeability to be between 10^{-21} and 10^{-20} m^2. Specific capacitances from the brine-inflow and permeability experiments ranged from 10^{-11} to 10^{-9} Pa^{-1}. Values in the order of 10^{-10} and 10^{9} Pa^{-1} are inconsistent with the known constitutive properties of halite and are attributed to deformation, possibly ongoing, of the halite around the WIPP excavations.

Results of one of the permeability tests and the comparison with the simulation performed by SNL are shown in Figure 4.8.4.

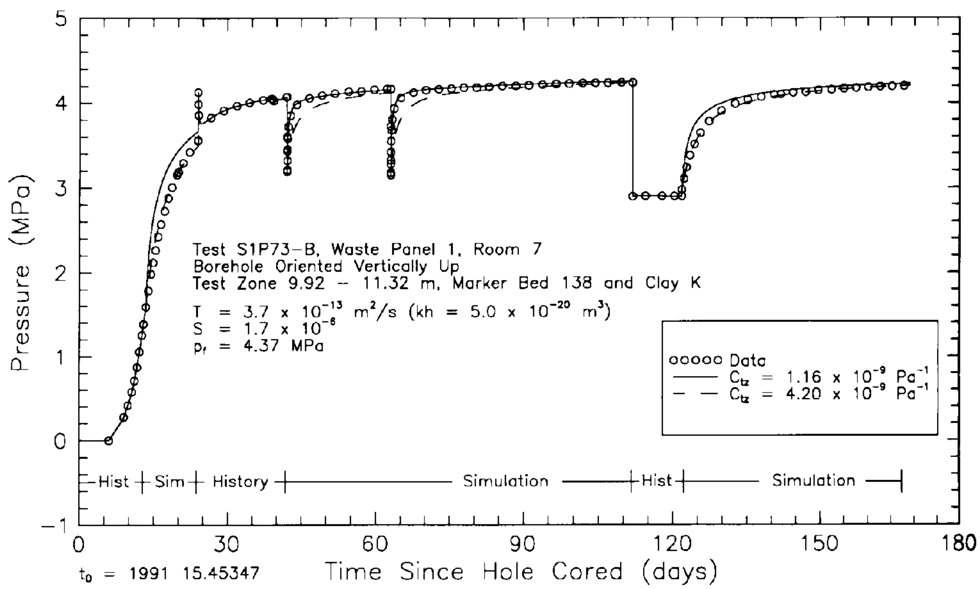


Figure 4.8.4. WIPP 1. Calculated and measured pressures during S1P73-B testing (SAND92-0533).

This test included an anhydrite (MB138) and a clay seam (Clay K). A value of $5 \cdot 10^{-20}$ m^2 provided the best fit for the permeability averaged over the total length of the test zone. Assuming that the fluid produced originated only from the anhydrite and the clay, the permeability of anhydrite was found to be $2.9 \cdot 10^{-19}$ m^2, that is roughly two orders of magnitude higher than the permeability of halite. This difference was attributed to the presence of fractures in the anhydrite. The SNL team concluded from their simulations that both the numerical and analytical radial-flow models based on Darcy's law provided good fits to the pressure-transient and the flow-transient tests with consistent parameter values.

4.8.6 Conclusions

The general approach to the evaluation of the applicability of Darcy's law was to try to obtain values of permeability and specific capacitance that would be consistent with other available data and to provide reasonable simulations of the performed hydrology experiments. Even if it was not to be expected that single values of permeability and specific capacitance would lead to exact replication of all of the experiments, the results would be consistent with a Darcian flow model, if the values of the experiments could be matched to the simulated values within an order of magnitude.

While Darcy's law cannot be said to have been validated by the experiments, the interpretations performed by the different teams demonstrated that models based on Darcy's law were able to replicate the experimental results within reasonable and acceptable bounds. Although the interpretations presented could not be considered unique in terms of representing the only possible model that could fit the data, this conclusion did not provide any motivation to look for alternative models that might better fit the data. To the extent that the simulations differ from the experimental results, refinement of the basic Darcy-flow model was suggested rather than replacing the Darcy-flow model with a model that is fundamentally different.

WIPP 1 tested the applicability of Darcy's law to the movement of brine under pressure gradients in salt formations. In principle, fluid flow in anhydrite and clay layers may be described by a Darcian flow model. However, it cannot be stated that this holds also for pure halite. Coupled hydrological and geomechanical models may provide a better understanding of the system. No evidence has been found that brine movement alone may cause significant releases of radionuclides from a repository in bedded salt. However, brine movement combined with other processes, such as gas generation, may lead to different conclusions.

4.9 Natural Analogue Studies at the Koongarra Site in the Alligator Rivers Area of the Northern Territory

4.9.1 Overview

The Alligator Rivers test case was based on work conducted at the Koongarra uranium deposit in the Alligator Rivers Region of the Northern Territory about 200 km east of Darwin, Australia. The uranium deposit at Koongarra is one of the best studied natural analogues in the world and extensive field studies have been carried out there since 1981. The site was initially investigated with the intention of developing a uranium mine, but these plans were later abandoned. The site was then used as a research facility aimed at obtaining an understanding of processes that have acted upon the original uranium deposit over time and which resulted in the present uranium ore. The Alligator Rivers Analogue Project (ARAP) was set up in 1987 under the auspices of OECD Nuclear Energy Agency and was completed in 1992. The modelling work within ARAP was mainly focused on hydrology, geochemistry, and geochemical processes. The ARAP study was included as a test case in both Phase 1 and 2 of INTRAVAL.

The modelling work on the Alligator Rivers test case in INTRAVAL Phase 1 was a joint venture between ARAP and INTRAVAL. The primary objective of the test case in INTRAVAL Phase 2 was directed towards obtaining a consistent picture of the processes that have controlled the transport of nuclides in the weathered zone and the time scale over which these processes have operated. Another objective was to test and evaluate models and concepts that are used in performance assessment of radioactive waste repositories.

The main contributors to the test case in INTRAVAL Phase 2 were the National Institute of Public Health and Environmental Protection (RIVM) in the Netherlands and Kemakta Konsult in Sweden.

4.9.2 Site Description and Data Examination

Site Description

The uranium mineralisation comprises two distinct, but related, ore bodies, separated by 100 m of barren schists that strike and dip broadly parallel to the Koongarra Reverse Fault. The main ore body, which was the subject of the study, persists to 100 m depth. It has a strike length of 450 m and a width averaging 30 m at the top of the unweathered schists (Figure 4.9.1).

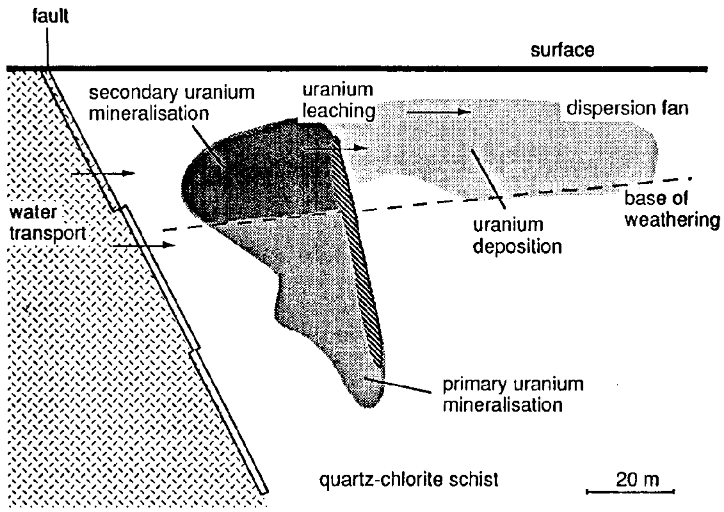


Figure 4.9.1. Cross-section of the main ore body at Koongarra.

The primary ore consists of pitchblende or uraninite–uranium dioxide veins and veinlets which either follow or cross-cut the layering in the schist. Minor amounts of scattered sulphide minerals, primarily galena (PbS), chalcopyrite ($CuFeS_2$), and pyrite (FeS_2), are associated with the high-grade ore. Uranium in this primary ore zone has been mobilised through oxidation and subsequently immobilised through formation of a uranyl silicate zone. The schist is weathered from a level near the surface down to a depth of 25–30 m. In this weathered zone, another secondary uranium mineralisation, consisting of uranyl phosphates, forms a tongue-like fan. Away from the tail of the fan, uranium is dispersed in the weathered schists and adsorbed onto clays and iron oxides. The dispersion fan of ore-grade materials extends down-slope for about 80 m. The transformation of the original primary mineralisation zones into the present secondary minerals is perceived to have taken place during a period of well over one million years.

Interpretation of the present hydrology at the site suggests that recharge of groundwater to the weathered Cahill schists occurs via downflow parallel to and in close proximity to the reverse fault in the underlying Kombolgie sandstone and schists. Although the fault zone breccia was found to be practically impermeable, it has been discovered that some water flows from the Kombolgie sandstone into the schists via cross fractures that offset the fault. Once in the schist, the groundwater flow is directed towards the south and south-east, away from the sandstone cliffs behind the deposit. Like much of northern Australia, the studied region has a monsoonal climate with almost all rainfall occurring in the wet season between November and March. This causes fluctuations in the water table in the order of 5 to 10 m between the wet and dry seasons.

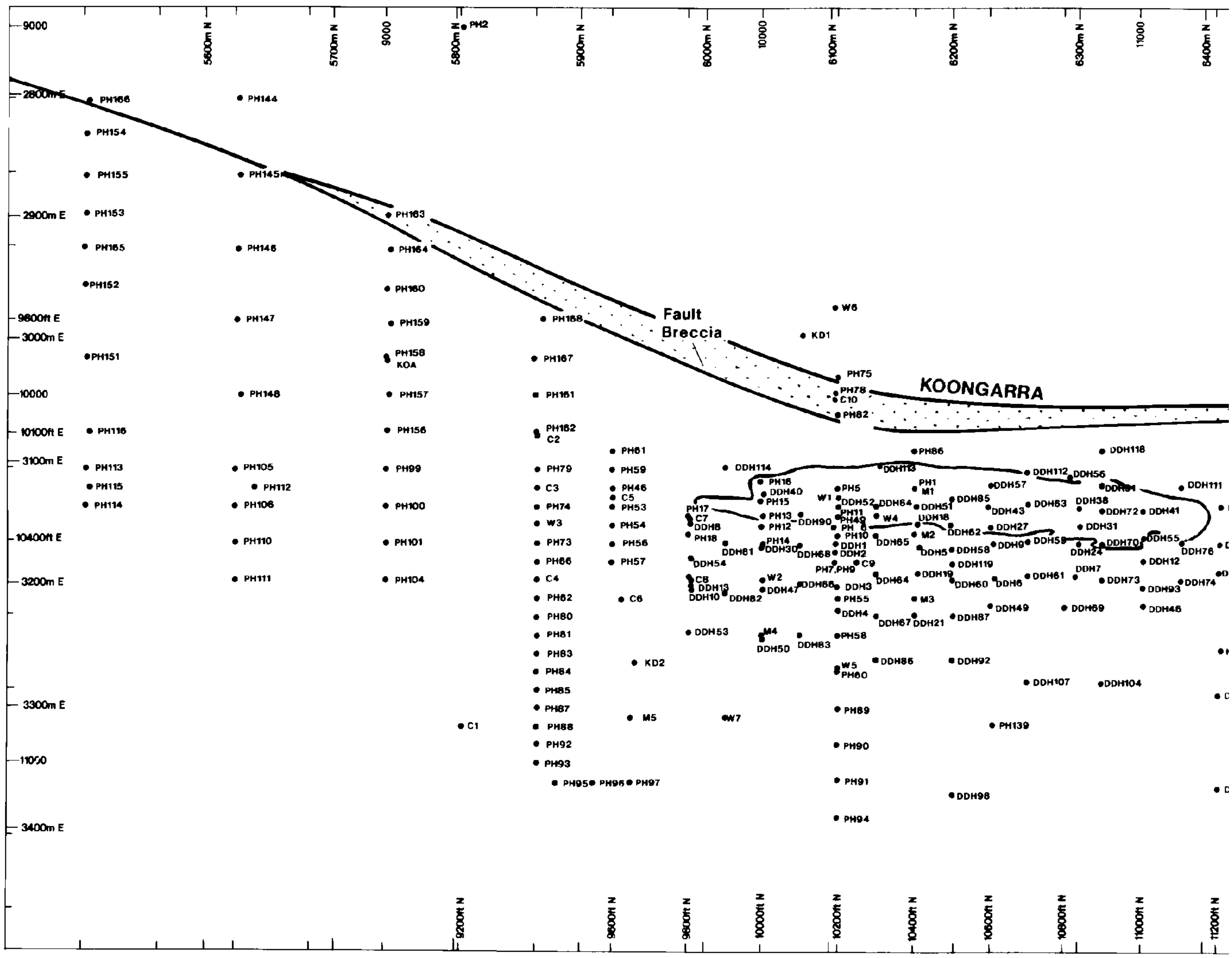


Figure 4.9.2. Location of boreholes at Koongarra to collect site characterisation data.

Data Examination

An extensive experimental programme including both field and laboratory investigations has resulted in a large amount of data characterising the site. For the test case, the hydrogeological data were taken from drawdown and recovery tests and from water pressure tests. The geological data were based on mineralogic and uranium assay logs from 140 percussion holes and 107 drill cores in the immediate vicinity of the uranium deposit. The groundwater chemical data were compiled from more than 70 boreholes which give a general understanding of the groundwater chemistry. Distributions of uranium, thorium and radium isotopes were determined for the different mineralisation zones. The distribution of uranium and thorium between different mineral phases in the weathered zone was also studied. Laboratory sorption experiments were performed using samples from drill cores retrieved at the site. In addition, distribution coefficients were measured on natural particles in Koongarra groundwaters. The large number of boreholes that were used to collect site characterisation data are shown in Figures 4.9.2 and 4.9.3.

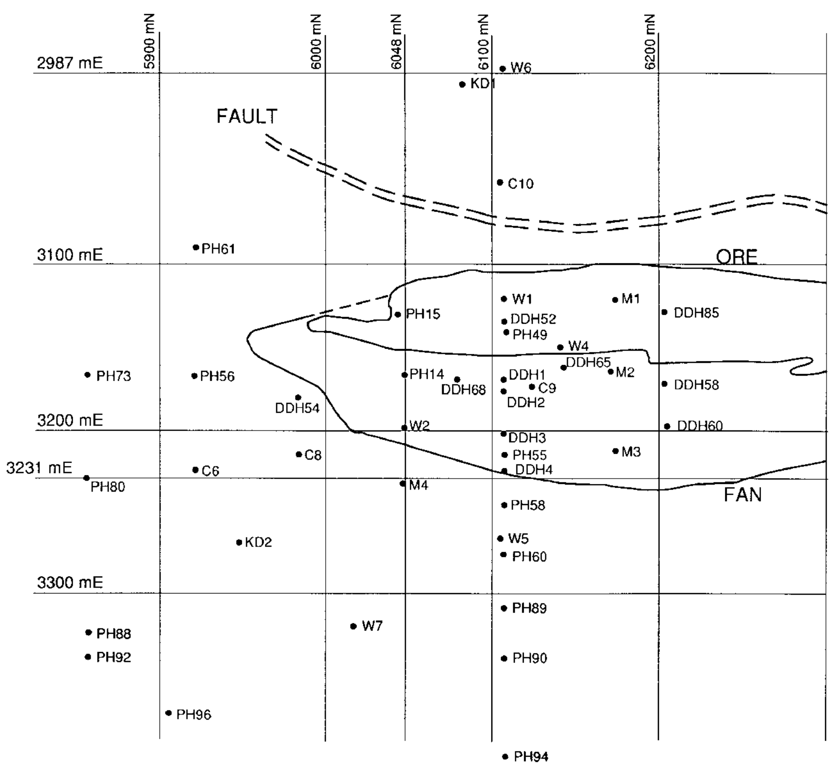


Figure 4.9.3. Area of transect 6110 m N.

In contrast to laboratory and field experiments, which are normally well-defined experiments designed and carried out to study one or several processes, natural analogues, based on naturally occurring processes, are generally much more complicated to evaluate, since the conditions and time scales are usually not well known. Both Kemakta and RIVM devoted a lot of effort to data examination in order to obtain a conceptual platform for the subsequent migration modelling.

Kemakta primarily focused their interest on the data required for the modelling of the selected system, such as the distribution of uranium in the bulk rock and its individual mineral phases. Radiochemical data were used to study alternative processes of radionuclide migration. RIVM used solid phase uranium concentrations that were analysed and reported within ARAP to examine the migration distance and the main direction of dispersion at various depths.

The review of the available solid uranium concentrations showed that the extension of the dispersed fan in the south direction from the fault was around 350 metres, whereas the extension in the south-east direction was around 100 metres. Information from different depths indicated that the pattern of the dispersion was similar at all depths in the weathered zone. This supports the hypothesis that groundwater movement and dispersion of uranium have taken place mainly in the transition zone. If significant transport had occurred in the fully weathered top layer, the dispersion distance from the ore body would have decreased with depth. Moreover, the concentration distribution pattern suggested that neither the direction nor the magnitude of the average groundwater flow had changed significantly during the past few million years.

However, the hypothesis that groundwater movement and dispersion of uranium have taken place mainly in the transition zone is not supported by the observed activity ratio $^{230}Th/^{234}U$. The similarity in the activity-ratio profile at different depths in the weathered zone, with values below 1 at the uranium dispersion front, indicates that uranium migration has taken place at all depths in the weathered zone during the last 200 000 years. The similarity in both uranium concentration distribution pattern and $^{230}Th/^{234}U$ activity-ratio profile at different depths may be explained by assuming an initially very fast movement of the weathering front down to the present base of weathering, which initiated uranium migration at all depths in the weathered zone.

There appeared to be a linear relationship between accessible uranium in the solid phase of the weathered rock and the uranium concentration in the groundwater. This suggests that the sorption process can be described by a linear adsorption isotherm with a distribution coefficient calculated from the measured concentration of accessible uranium in the solid phase and the uranium concentration in solution.

The activity ratios of $^{234}U/^{238}U$ and $^{230}Th/^{234}U$ in the accessible phase were generally lower than in the inaccessible phase, which indicated a more recent deposition of uranium in the accessible phase and/or a preferential transfer of ^{234}U and ^{230}Th from the accessible to the inaccessible phase. The preferential transfer may have been a result of "-recoil.

4.9.3 Migration Calculations

Kemakta and RIVM simulated the migration distance of uranium for a number of parameter combinations and model concepts to test, whether the observed migration distances could be predicted. Both teams based their calculations on data that had been determined and reported within the ARAP project, such as porosity, K_d and rock densities, and also on the extensive hydrological work performed within ARAP and INTRAVAL Phase 1.

The model concepts applied in the migration modelling were founded on rather simple performance assessment models, accounting for advection, dispersion and linear sorption in one or two dimensions. One of the 1-D models was extended to include "-recoil and transfer between solid phases. The vertical movement of the weathering front was part of the 2-D model.

The Kemakta Team

The Kemakta team concentrated its work on calculations of the dispersion of uranium and daughter nuclides in the weathered zone. The aim was to test the applicability of the rather simple models that generally are used in performance assessment of radioactive waste repositories.

The modelling work was carried out in several iterations with increasing level of complexity. Each iteration included a review of available laboratory and field data, determining the system to be modelled, selecting a suitable model and finally making a comparison of modelling results with field observations.

Three iterations were performed and the following model concepts were applied:

C advection–dispersion model with linear sorption
C advection–dispersion model with linear sorption and chain-decay
C advection–dispersion model with linear sorption, chain-decay, "-recoil, and phase transfer.

In the first modelling attempt, a simple 1-D advection–dispersion model, including linear sorption according to the K_d-concept, was used to simulate the dispersion of uranium in the weathered zone. This model may be considered as a simple performance assessment model.

In the second iteration, the system was extended to include the transport of the daughter nuclides ^{234}U and ^{230}Th. In addition, an attempt was made to consider also "-recoil. Furthermore, the sensitivity of the results to different combinations of groundwater flux and migration time was studied as well as the effects of alternating periods of flow and no-flow.

In the third and final iteration, the model was further extended by involving transfer of radionuclides between different phases of the rock and by using a more detailed model of "-recoil. This model was based on the assumption that radionuclides in the groundwater were sorbed to accessible phases of the weathered rock (amorphous iron oxides and clays) and that sorbed radionuclides were further included in inaccessible crystalline phases of the rock due to recoil effects and recrystallisation of amorphous iron oxides and clays.

Advection–Dispersion Model with Linear Sorption

The calculated solid concentration of uranium at different distances from the source together with available small-sample data from the depth interval 10–30 m in holes located along the transect 6110 m N (Figure 4.9.3) are shown in Figure 4.9.4. The simulations were based on a migration time of 2 million years. A K_d-value of 10 would overpredict the solid uranium concentration, if the concentration of dissolved uranium at the source is 1000 mg/m^3, but would give a prediction that would agree fairly well with observed values, if the source concentration is 100 mg/m^3. The combination of a K_d-value of 10 and a Darcy flux of 1 m/yr apparently predicted the migration distance fairly well, whereas a higher water flux overpredicted and a lower water flux underpredicted the migration distance.

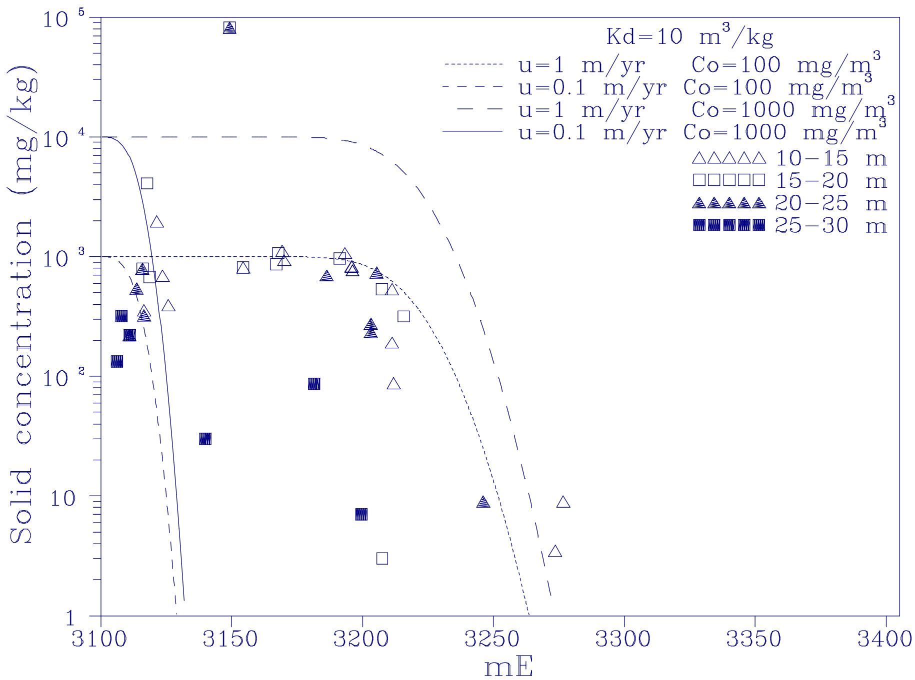


Figure 4.9.4. Kemakta results. Predicted and observed uranium concentrations along the transect 6110 m N.

With this model, the migration distance is dependent on the ratio of the Darcy flux to the distribution coefficient, and the maximum solid concentration level is dependent on the product of the liquid source concentration and the distribution coefficient. This means that there are an infinite number of combinations of parameter values that would give good predictions. However, the results also showed that it is possible to simulate the observed migration distance and concentration levels with a few parameters having values consistent with what has been recommended in independent interpretations.

Advection–Dispersion Model with Linear Sorption and Chain Decay

In the second iteration, the system was extended to include transport of the ^{238}U daughter nuclides ^{234}U and ^{230}Th. The observed activity ratios between ^{234}U and ^{238}U indicated a retention of ^{234}U relative to ^{238}U. This could be due to "-recoil of the short-lived ^{234}Th into the solid phase, making

^{234}U, the daughter nuclide of ^{234}Th, more attracted to the solid phase than ^{238}U, the parent nuclide of ^{234}Th. This effect was simulated in a simple manner by assigning a higher K_d-value to ^{234}U than to ^{238}U.

As was found in the first modelling iteration, it was possible to obtain almost identical simulations of the uranium concentration versus distance with different combinations of the values of the distribution coefficient, source concentration, water flux, and migration time. However, the activity ratio $^{230}Th/^{234}U$ versus distance from the source is dependent on the migration time, irrespective of the other parameter values. A set of calculations with different combinations of water flux and migration time was carried out, all matching the observed uranium concentration profile. A comparison between predicted activity ratios and observed data indicated that a migration time of 0.2 million years was too short, and that a migration time in the order of millions of years gave a better match to the observed data (Figure 4.9.5).

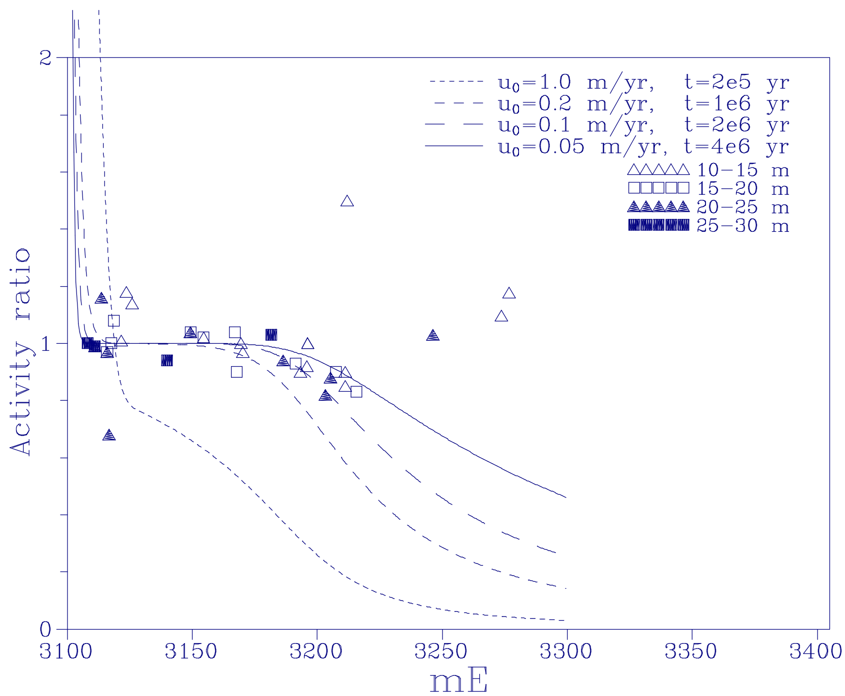


Figure 4.9.5. Kemakta results. Predicted and observed $^{230}Th/^{234}U$ activity ratios. Effect of different combinations of water flux and migration time.

Simulation of variable climatic conditions by assuming alternating periods of flow and no flow showed that the flow conditions during the last 200 000 years were important to the results, assuming that an average flow rate could be used for times prior to 200 000 years ago.

Advection–Dispersion Model with Linear Sorption, Chain Decay,"-recoil, and Phase Transfer

In the third iteration, the advection–dispersion model was extended in order to investigate the influence of phase transfer and "-recoil on the activity ratios. However, a comparison between calculated and observed data suggested that the results were not significantly improved by including phase transfer and "-recoil in the model, at least not with the combination of the phase-transfer rates and K_d-values used in the calculations. Including only the process of "-recoil gave similar results to the simple advection–dispersion–reversible sorption model, while the introduction of phase transfer gave results that were less in agreement with observed data.

The RIVM Team

The contours of solid phase uranium concentrations at different depths suggested that the migration of radionuclides in the fully weathered zone and in the unweathered zone were negligible. RIVM therefore concentrated its attention on the transition zone between the highly weathered and the unweathered rock when developing the conceptual transport model. The transition zone was modelled as a two-dimensional region. The main parameters and processes considered were velocity distribution, downward movement of the transition zone and a few geochemical processes.

The governing equations incorporated the movement of the weathering zone and hence the loss of uranium at the top of the zone and the entering of clean schist at the bottom of the zone (Figure 4.9.6). Diffusion of uranium from the highly weathered zone into the transition zone was also included.

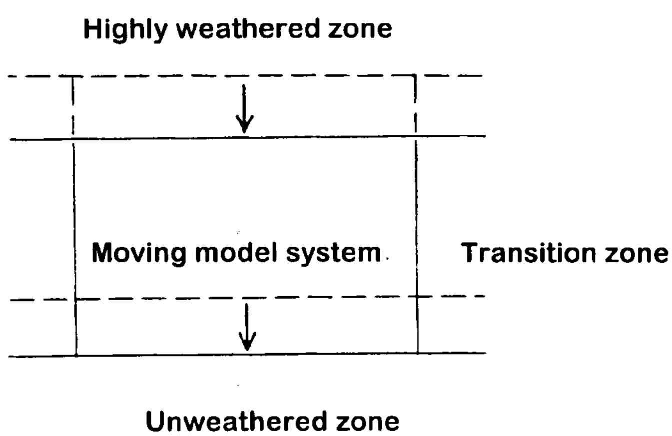


Figure 4.9.6. RIVM results. Schematic illustration of the moving transition zone.

As the number of measured values of uranium concentrations in the liquid phase were scarce and in order to be able to compare the modelling results with the present situation, the calculated values of liquid-phase uranium concentrations were converted into solid phase concentrations using the K_d value.

Rate of Downward Movement of the Transition Zone of Weathering

Uranium-series disequilibria data on the secondary dispersion fan mineralisation indicated that the weathering front reached the top of the ore body sometime in the interval 1–3 million years ago. The lowering of the sea level from 1.8 million years age onwards should have increased stream gradients, resulting in increased erosion rates.

If it is assumed that the transition zone has moved about 20 m downward over a time period of 1.8 million years, then a mean velocity of $1.1 \cdot 10^{-5}$ m/y is obtained for the transition zone. However, it cannot be reasonable to assume a constant downward velocity of the transition zone during the past 1.8 million years, since this time period involves cycles of alternative cold and warm climates in combination with advancing and retreating ice sheets, and falling and rising sea levels. Nevertheless, it was considered acceptable to work with an average value of the velocity of the transition zone, since data on dry and wet periods and sea level fluctuations were not available or were too uncertain to provide any reasonably good estimate of the variations in the weathering front velocity. The thickness of the transition zone was assumed to be 5 m, based on available field data.

Modelling of Uranium Transport in the Present Transition Zone—Effect of Variations in the Velocity Field

To assess the effect of the groundwater velocity field, three simulations were carried out, neglecting the movement of the transition zone. The groundwater velocities were constant over time in the simulations. Both spatially-homogeneous and spatially variable velocity fields were applied. A qualitatively fairly good agreement between the calculated and measured uranium concentration in the solid phase was obtained for the constant-velocity-field case and for one of the variable-velocity-field cases. These simulations showed that the uranium concentration distribution pattern was highly dependent on the velocity field. The use of a spatially variable velocity field could not be justified because of the large uncertainties in the boundary conditions.

Modelling Uranium Transport with a Moving Transition Zone

The boundary conditions used for the calculation of the velocity field are very uncertain. They may be valid for the present transition zone, but are unknown for the past. This being the case, the calculations that included the downward movement of the transition zone were performed with a velocity field that was constant in time and space. The results from one of the simulations is illustrated in Figure 4.9.7 at four different depths. A K_d-value of 0.7 m^3/kg, an effective velocity of 1.3 m/y, and a downward velocity of the transition zone of $1.1 \cdot 10^{-5}$ m/y were applied in this specific simulation. A concentration distribution pattern that was almost constant with depth was observed in these simulations, which is in agreement with the observations at Koongarra.

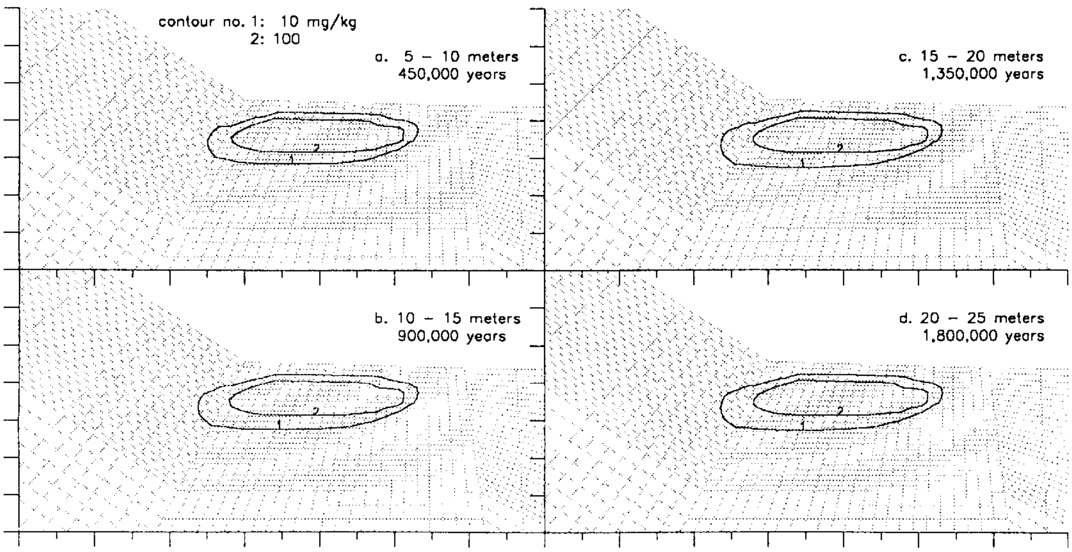


Figure 4.9.7. RIVM results. Simulation with a velocity constant in time and space and a downward moving transition zone.

One conclusion that could be drawn from these simulations was that the present situation in Koongarra can be simulated by including a moving transition zone. However, the calculated dispersion distance from the ore body was shorter than observed at Koongarra. It is believed that a better "fit" with the measured solid-phase uranium concentration distribution could be obtained by changing some of the model parameters like the groundwater velocity, the downward velocity of the transition zone, the adsorption distribution coefficient, or the dissolution source-term parameters.

4.9.4 Results from the ARAP

Modelling of the uranium migration was also carried out in the ARAP by the Australian Nuclear Science and Technology Organisation (ANSTO) and other organisations. The migration modelling in the ARAP was performed using models ranging from rather simple advection–dispersion–linear sorption models to complex multi-phase models considering recoil and chemical transfer. The advection–dispersion–linear sorption models were found to simulate the observed extension of the uranium migration fairly well. The more complex multi-phase models, considering recoil and chemical transfer, gave a good description of observed uranium concentrations and activity ratios in the different mineral phases of the rock. The migration modelling carried out in the ARAP as well as by RIVM and Kemakta in INTRAVAL indicated that the uranium migration has continued for a time period of half a million up to a few million years. This result is in agreement with results from geomorphological investigations.

4.9.5 Summary of Results

The dispersion distance and solid uranium concentrations calculated with the simplified one-dimensional advection–dispersion model, including sorption, were in fair agreement with the observed migration distance and the solid uranium concentrations in the dispersion fan. The model involved extensive simplifications of the system, but the results showed that it was possible to simulate the observed migration distance and concentration levels with a few parameters having values consistent with what has been recommended in independent interpretations.

Extending the model to include chain-decay made it possible to get an independent estimation of the migration time by studying the $^{230}Th/^{234}U$ ratio. This ratio indicated that the migration has continued for a time period in the order of millions of years.

The introduction of "-recoil and phase transfer allowed simulation of some observed effects, e.g. a decrease in activity ratios in the bulk rock with distance and a general trend that most of the observed thorium/uranium activity ratios fall below 1 in the accessible phase and above 1 in the inaccessible phase. However, the extended model did not improve the match between the calculated and observed uranium concentrations in the bulk rock. This model gave a description of the system that was more consistent with what is observed but the number of free parameters was larger. In addition, more data on the system were required, compared to the simpler advection–dispersion–reversible sorption model. This may possibly explain the difficulty in improving the simulation results using the extended model.

Two-dimensional calculations of uranium transport in the present transition zone, not considering the moving transition zone, resulted in contour lines of the uranium concentration in the solid phase that were qualitatively in agreement with the contour lines from the observed concentrations. Taking into account the movement of the transition zone, a dispersion pattern that was stationary with depth was obtained in the weathered zone, in agreement with the observations at Koongarra. However, the calculated dispersion length was shorter than the measured length. By calibration a better estimate of the dispersion length could be obtained, e.g. by increasing the effective velocity and/or the dissolution rate of uranium. Thus, the 2-D study showed that it is possible to simulate the present situation in Koongarra using the concept of a moving transition zone.

4.9.6 Validation Aspects

The overall aim of the case was to test and, if possible, validate simple models used in performance assessment of radioactive waste repositories. Although the results from this INTRAVAL study do not suffice to validate performance assessment models in a strict sense, it has been shown that even simple models, based on established transport processes and reasonably selected parameter values, are able to describe the present day distribution of uranium in the weathered zone at Koongarra.

4.9.7. Conclusions

Studies of the Alligator Rivers Natural Analogue have demonstrated that the structure of the uranium deposit at Koongarra is very complex. The interaction of many geochemical and geohydrological processes, which have continued over long times, makes it difficult to create a quantitative model of the history of groundwater flow and nuclide transport. The study within INTRAVAL has shown the importance of a joint interpretation of different types of data and the need for an iterative procedure for data collection, data interpretation and modelling in order to get a consistent picture of the evolution of the site. It was shown that sorption is a major retardation mechanism at the site, that uranium fixation in crystalline phases is a potentially important retardation mechanism in geologic media, where significant alteration of the rock is expected, and that "-recoil may have an impact on the distribution of uranium isotopes in the groundwater. Modelling simulations indicated migration times in fair agreement with independent geomorphological information.

A general conclusion from the INTRAVAL study is that rather simple and robust concepts and models seem to be able to adequately describe the long-range migration processes that have occurred at Koongarra. On the other hand, for more detailed modelling and to attain comprehensive understanding, geochemical processes have to be addressed more carefully.

5 Discussion of Results Obtained

5.1 General

When INTRACOIN, the first of the series of international cooperation projects on modelling the transport of radionuclides from nuclear waste repositories started in 1981, interest was focused on validation of transport models. Very soon it became obvious that the road toward validation required several successive steps. In INTRACOIN, most of the work was then devoted to model calibration, while keeping the validation aspects in mind. The next cooperation study, HYDROCOIN, should be seen as a necessary complement to INTRACOIN. That project comprised a study of the capabilities of different models to describe field and laboratory experiments and the impact on the groundwater flow calculations of incorporating various physical phenomena.

Although INTRACOIN was aimed at validation, as was also HYDROCOIN to some extent, it was only within INTRAVAL that the validation issues could be studied more thoroughly. In particular, INTRAVAL Part 2 has been almost entirely devoted to validation.

It should be born in mind that the objective of INTRAVAL and its forerunners was not to validate any specific model, but rather to explore the possibilities and limitations of models dealing with nuclide transport phenomena in natural rocks. Such studies are, of course, closely coupled to the validation process.

Performance assessment is a process of paramount importance in licensing repositories for nuclear waste. It is in that framework the need for computer models of transport of radionuclides should be viewed.

Of primary concern to INTRAVAL was the study of the application of models to different rock types. The four types investigated in INTRAVAL Phase 2 were saturated fractured rock (Stripa and Finnsjön in Sweden), unsaturated rock (Las Cruces and Apache Leap in the USA), clay (Mol in Belgium) and salt (WIPP in USA and Gorleben in Germany). Two additional sites were studied to some extent, namely Yucca Mountain in USA and Twin Lake in Canada, but these studies did not result in final reports and are not included here.

Although the INTRAVAL parties embraced all major states having nuclear power programmes except the former Soviet Union and the east-European states, it was very difficult to find new suitable sites to study within the INTRAVAL Phase 2. That is one of the reasons why most field sites selected for INTRAVAL Phase 2 were included already in Phase 1.

5.2 The INTRAVAL Subcommittee for Integration (ISI)

A special subcommittee for integration was formed at the start of INTRAVAL Phase 2. The committee was asked to carefully follow the progress of the work and to give guidance to the managers of the work. Its support was extremely valuable during the realisation of the project. The committee was also asked to issue a report on its findings after conclusion of the project. The committee's report, published in 1996 *[25],* covers the whole INTRAVAL study, both Phase 1 and 2. It concentrates on general observations and findings. The report also contains recommendations for site characterisation and performance assessment of radioactive waste repositories based on the results of the studies.

Of particular importance is the statement in the report that validation primarily is a confidence building feature and that there is no such thing as a "validated model". The validity of a model or set of models tends to be "application specific" for a certain site or for special geological conditions.

5.3 Conclusions from the Test Cases of INTRAVAL Phase 2

The detailed conclusions from the test cases have been treated previously. Under this heading only some more general remarks will be made.

Blind Predictions

The understanding how models can predict the transport of radionuclides from a disposal site over time is of major concern to the performance assessment of radioactive waste repositories. All project teams used their models to make predictions and evaluated their findings against results that were already known. Obviously, it was possible during their work to make changes in the modelling to improve the fit. Only in one case was it possible for the investigators to make predictions before results were known to the project teams, namely at Las Cruces Trench site. Experiences from that site pointed at the necessity of making "blind predictions" of real cases in order to evaluate the predictive force of a model for nuclide transport and also at the importance of field experiments being designed for validation purposes.

Scale Effects

The possibility of making predictions from small-scale investigations to larger scales was investigated in several of the studies. In the Apache Leap experiments, it was found that permeability tests at different scales in a 30 m deep borehole indicated some dependency of the mean permeability on measurement support (length of test interval). Although the observed variability of air permeabilities was over 3.5 orders of magnitude, the data were amenable to classical geostatistical analysis and yielded well-defined semivariograms. The investigators proposed that hydrologic data should be collected on a spectrum of scales relevant to performance assessment.

From the Finnsjön test case, the conclusion from a stochastic approach was that a model calibrated on an experimental scale would not be validated on a larger far-field scale, the reason being that local-scale conditioning data do not suffice to also describe far-field scale heterogeneity.

A comparative study of a "synthetic case" based on Finnsjön data, aimed at quantifying the predictive uncertainty when extrapolating the calibrated models to larger transport scales, demonstrated that four out of five applied models provided results which were fairly similar on the two transport scales considered. However, the fifth model which incorporated a mixing zone and matrix diffusion gave different results. This illustrates the importance of identifying all relevant processes when extrapolating small-scale experiments to large-scale modelling.

One team investigating the WIPP 2 test case pointed out that it is important to consider models in which high transmissivity regions are connected over long distances, as these regions might give rise to fast flow paths that may lead to major radiological consequences.

Source Term

The time-varying injection flow rates in the Stripa test case made interpretation of arrival data difficult. One team showed that deconvolution techniques appeared to be an interesting tool to treat such disturbed data, although the physical interpretation of the deconvoluted results should be made with great care.

Discrimination between Models

Several teams looked into the possibility of using the Finnsjön test case to discriminate between different models of advection. The conclusion arrived at was the same as in INTRAVAL Phase 1—that the data from the test site were not sufficient to make such discrimination between models or active processes and that different approaches could be used to successfully model the experiments.

In the Stripa test case, the assumptions used by the project teams were in some cases very different. Nevertheless, the various channel models were able to reproduce most of the trends observed in the experiment. This indicates that the experimental data could not be used to discriminate between the channel models. The same conclusion was drawn from the WIPP 2 case, where it seemed that several stochastic models might explain the data, resulting in similar uncertainties.

In many of the cases studied, it was found that no one model could be said to be consistently superior to the others, in spite of the models and modellers sometimes taking very different approaches in their conceptualisation of the particular site and their choice of model. Thus it was found in the Stripa case that the use of sophisticated numerical transport models with a large number of parameters for the fitting of the experimental breakthrough curves did not improve on the fits obtained by the use of simple analytical models. Similarly, in handling the Alligator Rivers data, extended models did not improve the match between the calculated and observed uranium concentrations in the bulk rock, probably due to the increased number of free parameters and the need for additional data.

Dimensionality

In principle, increased detail in model structure should increase the accuracy of the predictions. However, in many cases this is counterbalanced by the fact that the effects of characterisation uncertainty can have a greater impact on model predictions than the differences in the way the models conceptualise the rock. Examples from Las Cruces confirm this conclusion. This might be one reason why 1-D models often can perform as well as, or sometimes even better than, 2-D or 3-D models. In the Finnsjön case, the dimensionality of the models did not seem to be decisive for the ability to accurately reproduce the field responses.

Stochastic Models

Four teams used geostatistical methods in the Finnsjön test case. It was demonstrated that stochastic approaches may be used within the context of a validation process, although the question remains how to formally validate a stochastic continuum model.

Monte-Carlo stochastic techniques was used in the WIPP 2 test case to treat the uncertainty resulting from heterogeneity. One interesting conclusion was that, although the uncertainties might be less if all the data were used in the construction of the models, no data would then be left to check the model against. Furthermore, it might be possible to condition an inappropriate statistical model to match all the measurements and therefore careful statistical tests would have to be carried out to check models that are conditioned on all the data.

Matrix Diffusion

The effect of matrix diffusion was studied primarily in the Finnsjön test case and also to some degree in the Stripa test case. The results from Finnsjön were somewhat ambiguous. Some teams found that the role of matrix diffusion was not negligible at Finnsjön, but one team, using basically the same data, arrived at the opposite conclusion and did not consider matrix diffusion in their analysis. However, most teams finally agreed that matrix diffusion had no, or only a very small effect in the experiments, given the high induced velocities and the corresponding short travel times.

One project team studying the Stripa test case came to the result that experimental breakthrough data could be explained by hydrodynamic dispersion and that matrix diffusion did not seem to play an important role in the Stripa 3-D experiments.

Validation Issues

The term validation is not well defined in the context of models of transport of radionuclides. The issue is discussed in detail in the ISI report *[25]*. The "site specificity" of validation might be one of the reasons why validation is treated so differently between the test cases and the project teams in INTRAVAL Phase 2. The teams agreed that the possibility to fit predictive models to experimental data with sufficient accuracy is not in itself a proof that the applied model is validated.

However, it is part of a validation process that can be more or less complete.

The results from the Las Cruces Trench test case 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 criteria.

In the Finnsjön case, it was shown that the multiple conceptual model approach provided valuable insights into the validation of prediction models.

The project teams assessing the Stripa case demonstrated that the experiment could be described with highly-channelled flow-path models, and an independent demonstration of the one-dimensional flow-path approach was provided by one team. However, the low recovery rates, and sometimes complete loss, of tracer could not be explained. Possible explanations were proposed, but the data to verify the hypotheses were lacking. Although the applied models were able to reproduce some of the field observations, it can hardly be seen how they could have predicted them.

The project teams which treated the WIPP 2 case tackled different aspects of the test case with some overlap between the teams. Taken together, the conclusions reached by the project teams were generally consistent and helped to build up the picture of flow and transport at the WIPP site.

In the WIPP 1 test case it was concluded that, although Darcy's law could not be said to have been validated by the experiments, the interpretations performed by the different teams demonstrated that models based on Darcy's law were able to replicate the experimental results within reasonable and acceptable bounds.

The general conclusion from the Alligator Rivers test case was that, although the results from the study did not suffice to validate simple performance assessment models in a strict sense, it was shown that even simple models, based on established transport processes and reasonably selected parameter values, were able to describe the present day distribution of uranium in the weathered zone at Koongarra.

6 Final Remarks

At the time when the Swedish Nuclear Power Inspectorate initiated the INTRACOIN study in 1981, it was difficult to foresee that the study was the beginning of an international cooperation between a number of devoted specialists that would last up to the end of 1993, and including report writing until 1997. The three studies, INTRACOIN, HYDROCOIN and INTRAVAL has given the SKI ample opportunity to follow the ongoing development and application of models for the transport of radionuclides from a radioactive waste repository. The projects have significantly increased the necessary scientific competence of SKI in its licensing work regarding radioactive waste.

The fairly loose organisation of the administration of the projects proved to be very valuable. However, the good results that were obtained entirely depended on the engagement and abilities of the project teams who devoted many long hours to the projects.

The publication of this summary report completes the INTRAVAL project. It remains for the Swedish Nuclear Power Inspectorate to thank all the involved parties, the project teams and the observers. The SKI expresses its gratitude to the OECD/NEA organisation that has taken part in the secretariat and printed all INTRAVAL reports. The SKI is very grateful to Her Majesty's Inspectorate of Pollution, UK, which made possible a British participation in the secretariat. Finally, special thanks are due to Kemakta Consultants who served as principal investigator within the project secretariat and whose help has been invaluable during this long period since 1981.

References

1. INTRACOIN, Final Report Level 1 (1984): Code verification, SKI 84:3, Swedish Nuclear Power Inspectorate.

2. INTRACOIN, Final Report, Level 2 and 3 (1986): Model validation and uncertainty analysis, SKI 86:2, Swedish Nuclear Power Inspectorate.

3. The International HYDROCOIN Project (1987): Background and results, Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

4. The International HYDROCOIN Project, Level 1 (1988): Code verification, Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

5. The International HYDROCOIN Project, Level 2 (1990): Model validation, Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

6. The International HYDROCOIN Project, Level 3 (1991): Uncertainty and sensitivity analysis, Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

7. The International HYDROCOIN Project (1992): Summary Report, Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

8. Swedish Nuclear Power Inspectorate (1987): Geosphere transport model validation — a status report, SKI 87:4, Stockholm.

9. Swedish Nuclear Power Inspectorate (1987): INTRAVAL project proposal, SKI 87:3, Stockholm.

10. The International INTRAVAL Project (1990): Background and results, Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

11. The International INTRAVAL Project, Phase 1 (1992):Test Cases, Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

12. The International INTRAVAL Project, Phase 1 (1992): Case la, Mass transfer through clay by diffusion and advection, editor: Jackson C.P., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

13. The International INTRAVAL Project, Phase 1 (1992): Case lb, Uranium migration in crystalline rock; borecore pressure infiltration experiments, editor: Hadermann J., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

14. The International INTRAVAL Project, Phase 1 (1992): Case 2, Radionuclide migration in single natural fractures in granite, editor: Skagius K., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

15. The International INTRAVAL Project, Phase 1 (1992): Case 4, Flow and tracer experiment in crystalline rock based on the Stripa 3-D experiment, editors: Hodgkinson D. and Grindrod P., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

16. The International INTRAVAL Project, Phase 1 (1992): Case 5, Studies of tracer experiments in a fracture zone at the Finnsjön research area, editors: Tsang C.-F. and Neuman S., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

17. The International INTRAVAL Project, Phase 1 (1992): Case 6, Synthetic migration experiment, editor: Codell R., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

18. The International INTRAVAL Project, Phase 1 (1992): Case 7, The Poços de Caldas natural analogue: studies of redox front movement, editor: Chapman N., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

19. The International INTRAVAL Project, Phase 1 (1992): Case 8, The Alligator Rivers natural analogue, editor: Duerden P., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

20. The International INTRAVAL Project, Phase 1 (1992): Case 9, Radionuclide migration in a block of crystalline rock, editor: Jackson C.P., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

21. The International INTRAVAL Project, Phase 1 (1993): Cases 10, 11, 12, Flow and tracer experiments in unsaturated tuff and soil, editors: Voss C.F. and Nicholson T.J., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

22. The International INTRAVAL Project, Phase 1 (1993): Test Cases 10, 11 and 12, Flow and tracer experiments in unsaturated tuff and soil, Appendices, Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Stockholm.

23. The International INTRAVAL Project, Phase 1 (1992): Case 13, Experimental study of brine transport in porous media, editor: Glasbergen P., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

24. The International INTRAVAL Project (1994), Summary Report, Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

25. The International INTRAVAL Project (1996): Developing groundwater flow and transport models for radioactive waste disposal, Six years of experience from the INTRAVAL project, Final results, Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

26. The International INTRAVAL Project, Phase 2, Working group 1 report (1996): Flow and tracer experiments in unsaturated tuff and soil, Las Cruces Trench and Apache Leap Tuff studies, Nicholson, T.J., Guzman-Guzman, A., Hills R., Rasmussen T.C., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

27. The International INTRAVAL Project, Phase 2, Working group 2 report (1996): Finnsjön, Stripa and WIPP 2, Andersson P., Billaux D., Guérin F., Jackson C.P., Neuman S.P., Tsang C.-F., Winberg A., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

28. The International INTRAVAL Project, Phase 2, Working group 4 report (1996): The analyses of the Alligator Rivers natural analogue, Birgersson L. , Larsson A. , Skagius K., Swedish Nuclear Power Inspectorate and OECD/Nuclear Energy Agency, Paris.

29. Bogorinsky P., Conclusions from INTRAVAL Working Group 3, Salt- and clay-related cases, Proceedings from Geoval '94, OECD Documents, Paris 1995.

30. Hills, R.G. and Wierenga, G.W, INTRAVAL Phase II Model Testing at the Las Cruces Trench Site, NUREG/CR-6063, U.S. Nuclear Regulatory Commission, Washington, D.C. 1994.

31. Rockhold, M.L., Rossi, R.E. and Hills, R.G., Application of similar media scaling and conditional simulation for modeling water flow and tritium transport at the Las Cruces Trench Site, Water Resources Research, Volume 32, pp. 595-609, 1996.

32. Basset, R.L., Neuman, S.P., Rasmussen, T.C., Guzman, A., Davidson, G.R. and Lohrsdorfer, C.F., Validation studies for assessing unsaturated flow and transport through fractured rock, NUREG/CR-6203, U.S. Nuclear Regulatoy Commission, Washington, D.C., August 1994.

33. Guzman-Guzman, A. And Neuman, S.P., Field air injection experiments, Chapter 6 in Rasmussen, T.C., Rhodes, A., Guzman, A. and Neuman, S.P., Apache Leap Tuff INTRAVAL Experiments: Results and Lessons Learned, NUREG/CR-6096, U.S. Nuclear Regulatory Commission, Washington, D.C., March 1996.

34. Rasmussen, t.c., Rhodes, S.C., Guzman, A. And Neuman, S.P. Apache Leap Tuff INTRAVAL experiments: Results and lessons learned, NUREG/CR-6096, U.S. Nuclear Regulatory Commission, Washington, D.C., March 1996.

35. Andersson P., Winberg A., Conclusions from WG-2: The analysis of the Finnsjön experiments, Proceedings from Geoval '94, OECD Documents, Paris 1995.

Appendix

List of INTRAVAL Phase 2 Participants

Party		Project Team	
Agence Nationale pour la Gestion des Déchets Radioactifs, France	(ANDRA)	Commissariat à l'Energie Atomique	CEA/DMT)
		Bureau de Recherches Géologiques et Minières	(BRGM/STO)
Atomic Energy of Canada Ltd., Canada	(AECL)	Atomic Energy of Canada Ltd.	(AECL)
Atomic Energy Control Board, Canada	(AECB)	Atomic Energy Control Board	(AECB)
Australian Nuclear Science and Technology Organisation, Australia	(ANSTO)	Australian Nuclear Science and Technology Organisation	(ANSTO)
Bundesanstalt für Geowissenschaften und Rohstoffe/Bundesamt für Strahlenschutz, Germany	(BGR/BfS)	Bundesanstalt für Geowissenschaften und Rohstoffe	(BGR)
		Bundesamt für Strahlenschutz	(BfS)
Commissariat à l'Energie Atomique/Institut de Protection et de Sûreté Nucléaire, France	(CEA/IPSN)	Ecole Nationale Supérieure des Mines de Paris	(EdM)
Empresa Nacional de Residuos Radioactivos S.A., Spain	(ENRESA)	Universidad Politécnica de Valencia	(UPV)
Gesellschaft für Reaktorsicherheit mbH, Germany	(GRS)	Gesellschaft für Reaktorsicherheit mbH	(GRS)
Forschungszentrum für Umwelt und Gesundheit, Germany	(GSF)	Forschungszentrum für Umwelt und Gesundheit	(GSF)
Her Majesty's Inspectorate of Pollution, United Kingdom	(HMIP/DoE)	Atkins Engineering Sciences	(AES)
		Intera Information Technologies Ltd.	(INTERA)
Industrial Power Company Ltd., Finland	(TVO)	Technical Research Centre of Finland	(VTT)

List of INTRAVAL Phase 2 Participants (Cont.)

Party		Project Team	
Japan Atomic Energy Research Institute, Japan	(JAERI)	Japan Atomic Energy Research Institute	(JAERI)
		Central Research Institute for the Electric Power Industry	(CRIEPI)
		Hazama-gumi	(HAZAMA)
Nationale Genossenschaft für die Lagerung Radioaktiver Abfälle, Switzerland	(NAGRA)	Paul Scherrer Institute	(PSI)
National Institute of Public Health and Environmental Protection, The Netherlands	(RIVM)	National Institute of Public Health and Environmental Protection	(RIVM)
Power Reactor and Nuclear Fuel Development Corporation, Japan	(PNC)	Power Reactor and Nuclear Fuel Development Corporation	(PNC)
Studiecentrum voor Kernenergie, Belgium	(SCK/CEN)	Studiecentrum voor Kernenergie	(SCK/CEN)
Swedish Nuclear Fuel and Waste Management Co., Sweden	(SKB)	The Royal Institute of Technology	(SKB/KTH)
Swedish Nuclear Power Inspectorate, Sweden	(SKI)	The Royal Institute of Technology	(SKI/KTH)
		Kemakta Consultants	(KEMAKTA)
UK Nirex Ltd., United Kingdom	(NIREX)	AEA Technology	(AEA)
		Intera Information Technologies Ltd.	(INTERA)
U.S. Department of Energy/ OCRWM, United States of America	(USDOE)	Pacific Northwest Laboratories	(PNL)
		U.S. Geological Survey	(USGS)
		Lawrence Livermore National Laboratory	(LLNL)
		Golder Associates Inc.	(GOLDER)

List of INTRAVAL Phase 2 Participants (Cont.)

Party		Project Team	
U.S. Department of Energy/ WIPP, United States of America	(USDOE)	Sandia National Laboratories	(SNL)
U.S. Environmental Protection Agency, United States of America	(USEPA)	U.S. Environmental Protection Agency	(USEPA)
U.S. Nuclear Regulatory Commission, United States of America	(USNRC)	U.S. Nuclear Regulatory Commission	(USNRC)
		Center for Nuclear Waste Regulatory Analyses	(CNWRA)
		Massachusetts Institute of Technology	(MIT)
		Pacific Northwest Laboratories	(PNL)
		Sandia National Laboratories	(SNL)
		University of Arizona	(UAZ)
Organisation for Economic Cooperation and Development/Nuclear Energy Agency (member of secretariat)	(OECD/NEA)		
Her Majesty's Inspectorate of Pollution, United Kingdom (member of secretariat)			
International Atomic Energy Agency (observer)	(IAEA)		
Environmental Evaluation Group, United States of America (observer)	(EEG)		
State of Nevada (observer)			