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FIELD, THEORETICAL AND NUMERICAL STUDIES OF DISPERSION

von

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- Gastwissenschaftler im Rahmen der DFG-Forschergruppe -

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Preface

This outline of a joint research concept is written as a result of numerous meetings, scientific seminars and individual efforts of the group of authors during the recent short sabbatical leave of Dr. G. Moltyaner from Chalk River Nuclear Laboratories, Ontario, Canada at the Institut für Wasserbau, Lehrstuhl für Hydraulik und Grundwasser, University of Stuttgart. It involves a cooperative effort between the University of Stuttgart that has developed an expertise in computational aspects of transport in geologic media and in the performance of large-scale laboratory tracer experiments and Chalk River Nuclear Laboratories, Ontario that has broad experience in the performance, analysis and interpretation of field tracer tests on a variety of scales. The proposed investigations respond to the current needs on resolving major scientific hypotheses required to advance the understanding and predictive modelling of contaminant transport in natural geologic environments. This concerns the migration of chemically inert tracers in geologic media, physical and numerical modelling of transport and theoretical aspects of migration. We propose to address two major problems.

(A) Validation of numerical models used for predicting the fate of contaminants in groundwaters and

(B) development of methods and techniques for analysing contaminant transport.

The first task in problem (A) is the compilation of a vast array of CRNL data collected in the 40- and 260-m tracer experiments in a computerized database. This unique database will serve not only as field support for remaining topics of problem (A) but will be used by the researchers of the Institut für Wasserbau for independent studies. Next we propose to address the important issues concerning the numerical modelling of contaminants in groundwater using supercomputers like the "CRAY-2". Furthermore we want to investigate the applicability of existing models which include finite element-, finite difference-, random-walk-, and method-of-characteristics-based 2D-computer codes. This in turn will feed information into the third task which involves the use of CRNL data in the context of a model validation study. This leads us naturally to the application of a model describing the best fit to the CRNL plumes for the subsequent three-dimensional simulation study. The manner in

which the proposed work will contribute to the Institute of Wasserbau's long-term goal of field experimentation at the Institute's tracer site, is self evident.

We shall address two major tasks and issues related to the problem (B). The first ist the adoption of sampling concepts recently developed at CRNL (7) to a highly heterogeneous geologic environment such as that encountered in the southern part of West Germany. These require consideration of the scale of the sampling device to be used for measurement of concentration distribution. The variabilities which appear due to phase heterogeneity and mineralogical features of an aquifer should be filtered out when using the sampling device. A series of laboratory experiments is planned to address this important issue. Next one should consider the important issues concerning the design of a monitoring network and sampling program within the context of the site and tracer plume characterization.

1. INTRODUCTION

Now that contaminant transport models have become widely available, many practioners are disappointed to find out that the ability of a model to explain phenomena observed in well defined laboratory experiments may be weakly correlated with its ability to make good predictions in a natural geologic environment. After all, if a contaminant transport model is fundamentally sound, if geometries and heterogeneities of a laboratory system are well known, system parameters may be adjusted to explain or reproduce an observed sequence of events. Making valid predictions about future events in a highly heterogeneous geologic environment is a different matter. One must use an appropriate conceptual model with the right parameters, initial and boundary conditions, and inputs. Since the results of models are used to assist in making decisions related to real world cases of contamination, model users seek answers to the following basic questions:

(1) How good are the model predictions in geologic media over the scales relevant to real cases of groundwater contamination?

(2) Which of the variety of available contaminant transport models leads to the "best" possible predictions?

Three large-scale field tests were conducted at CRNL in 1982, 1983 and 1987-1988 by introducing radioactive tracers into a shallow unconfined aquifer and monitoring their migration under the influence of the natural hydraulic gradient prevailing at the site. In 1982, radioactive ^{131}I was monitored as it migrated downstream from the source over a distance of 20 m in a near horizontal direction. In 1983, the same radioactive tracer and tritium were monitored as they travelled a distance of 40 m downstream. In 1987 to 1988, tritium alone was sampled along a migration path extending 260 m from the source. In all cases, the monitoring was done in boreholes drilled to the bottom of the aquifer and arranged in lines oriented more or less transverse to the mean direction of flow (see Figure 2 in the Appendix). The distance between boreholes in each transverse line was 0.5021 m, and the longitudinal distance between these lines for the first 40 m was 5 m: between 40 and 120 m from the source the lines were spaced at 5 to 20 m intervals. In each borehole, multilevel samplers were installed at vertical intervals of 1 m. During the 1983 test, gamma emission of ^{131}I was measured using a novel dry-access-

tube monitoring technique with a vertical resolution of 1 cm. This latter test has resulted in an unusually rich data base consisting of approximately 0.75 million recorded values. A comparison of ^{131}I and tritium migration has shown that at the test site, they behave similarly and therefore both can be treated as conservative tracers. In addition to this wealth of data about space-time distribution of tracer concentration, a large amount of site specific information has been accumulated over the past eight years in the form of hydrogeological, hydraulic, and stratigraphic records. These data provide a detailed picture of the environment within which tracer migration took place during each test. For additional details refer to the Appendix.

A number of preliminary analyses of the available data have been performed. The analysis of the tracer plumes has suggested that conventional advection-dispersion concepts explain many important aspects of their behaviour /1 - 13/. In particular, the 1983 tracer test data were reproduced with considerable success by means of computer code based on the Galerkin finite element method /4, 12/. An important lesson learned from this modelling study was that Eulerian grid techniques, such as conventional finite difference and finite element methods, are inappropriate unless the space-time grid is made fine enough to eliminate major errors due to numerical dispersion. Unfortunately, such grid refinement requires large amounts of computer time and storage. The final assessment of the computational efficiency of conventional finite-element and finite difference methods may be made using the computer facilities available at the University of Stuttgart. We believe that numerical methods such as random walk and method of characteristics offer some advantages as compared with the conventional numerical methods. However, for a very fine space grid which is required to reproduce the velocity field with vertical spacing of 1 cm, the random walk method may be uneconomical. The difficulty may be overcome by means of mixed Eulerian-Lagrangian method in which advection is handled by the method of characteristics. Although the method is virtually free of numerical dispersion, it suffers from instability when the time step size exceeds a certain limit. In an effort to find an answer to the question of which of the methods is most appropriate for the simulation of the essentially three dimensional movement of contaminant, we attempt several simulations of Chalk River plumes along the mean direction of flow first using the two-dimensional computer models which include finite-element-, finite

difference-, random-walk-, and method-of characteristics-based computer codes and then to apply the most efficient and economical model to simulate the three-dimensional movement of these plumes.

A limited financial support obtained through the University of Stuttgart from the German Science Foundation has allowed us to initiate a study on the validation of two-dimensional model of contaminant transport. The joint University of Stuttgart - CRNL team has just obtained the first results of the numerical analysis of an extremely extensive CRNL data set. Experience gained in analyzing Chalk River experiments performed in sandy environments will be used to address all the problems associated with task (B) in a precise manner.

2. TASKS, ISSUES AND APPROACHES

The particular tasks and issues we wish to tackle within the proposed investigations are listed below:

2.1 Preparation of Computerized CRNL Data Base

The extensive data base established at CRNL to date will be compiled for easy access and retrieval by means of a user-friendly, commercially available computer software package. The data base will include geological and hydrogeological data collected at the tracer test site. The data base will include the results of laboratory experiments conducted at CRNL using tracer test sediments. It will be supported and made accessible by the Mathematics and Computation branch at CRNL. The task is a prerequisite for all subsequent steps in model application.

2.2 Intercomparison of 2-D Numerical Models

We propose to evaluate the relatively neglected issue of the required accuracy of reproduction of the velocity field for predictive modelling. The quantitative impact of the spatial variability of the flow velocity on the contaminant transport may be evaluated with the accuracy of 1 cm using the flow velocities obtained from the CRNL tracer test.

2.3 Validation of Transport Models

The availability of results from several tracer tests conducted on different space-time scales, with more than one tracer at a single CRNL site, provides an unique opportunity to validate conceptual and computational models of subsurface contaminant transport. As a simple illustration of this concept, one can ask the question "how well do dispersion experiments determined on the basis of the 1983 tracer test reproduce the longer and more extensive 1987-1988 test?" If the reproduction produced by one of the models named in the introduction is poor, why is it, and what must be done to improve it? This

issue is closely related to the predictive capability of transport models and the development of a state-of-the-art methodology for validating numerical models of contaminant transport.

2.4 3-D Simulation of CRNL Plumes

We stated earlier that, at CRNL, concentration data are available for small scale samples recorded at vertical distances of 1 cm and 1 m, and horizontal distances of 0,5 and 5 m. In practical studies of subsurface contamination sampling is usually done on a much coarser spatial scale. Such extensive information available from the CRNL test may be used for testing the "best" 3-D model of contaminant transport which can be identified after completing the topic three of this study. This in turn will feed information in the important issue of the sampling of contaminant plumes as related to the scale of sampling device and the spacing of the monitoring network to be considered in task (B). The proposed effort will contribute significantly to the advancement of scientific unterstanding of the three-dimensional contaminant behaviour in the subsurface environment.

2.5 Development of Sampling Techniques and Methods for a Highly Heterogeneous Environment

One of the major problems related to the performance and analysis of large-scale field tracer tests in a highly heterogeneous environment such as that encountered in the southern part of West Germany is the development of appropriate techniques and methods for collecting groundwater samples. We propose to adopt the concepts developed at CRNL for this purpose during three natural-gradient dispersion experiments.

Conceptually, analysis of concentration data collected from tracer tests is based on the advection-dispersion equation. The equation contains variables and parameters that are averaged over some representative volume but are associated with a mathematical point. In the field experiments the size of the averaging volume depends upon the methods and scales of averaging associated with sampling devices used for measurement of concentration distribution /7/.

Examination of scales of averaging related to the measurement devices is critically important to the application of the advection-dispersion equation.

At CRNL the volume of aquifer over which the tracer concentration was integrated during the field measurements was examined in laboratory conditions and was found representative for characterizing the variability of the interstitial velocities important for risk assessment in groundwater contamination studies. The field measurement process itself represents a natural device for filtering out the phase heterogeneity associated with the presence of solids and liquids in the system and establishes the size of the volume over which process variable, concentration, and parameters of the process are integrated. With the aid of a novel dry-access-tube monitoring technique the next level in the succession of various scales of variability encountered in the aquifer which is commonly referred to as layered heterogeneity was identified with a high degree of resolution. This type of variability appears due to the alternation of strata. For this case, a theoretical approach was suggested in /7/ for analyzing the concentration distributions. The novel measurement techniques and advances in theoretical analysis and interpretation of a great amount of experimental data, provide the necessary background for extending accumulated expertise into the performance and analysis of tracer tests in a highly heterogeneous environment. The above described procedure for filtering phase heterogeneities offers significant advantages as compared with the conventionally used ones. The second type of variability which appears due to the layered nature of a sedimentary geologic environment should be analysed in the context of the homogenization procedure. First, experimental results from the large-scale laboratory setups available at the University of Stuttgart can be used for this purpose. The experience which will be accumulated from laboratory experiments coupled with the results of analysing Chalk River plumes offer an opportunity to develop methods and techniques suitable for a highly variable geologic environment. We propose to verify subsequently the laboratory techniques in field experiments.

2.6 Design of the Monitoring Network and Sampling Program

In addition to laboratory tests with nonreactive tracers, we propose to address

an important issue of space-time tradeoff in the sampling of tracer solution as related to the scale of the sampling device and the optimum design of the monitoring network. Dispersion coefficients are measures of the spread of a tracer or contaminant plume about its center of mass. To measure this spread and thus evaluate the dispersion coefficient directly from field concentration data, a large number of sampling points is required that provide a dense coverage of the plume in space-time. The smaller the scale of sampling network, the more accurately can the plume be delineated and its spread established. The dispersive properties of the geologic medium can then be evaluated directly by calculating the first and second spatial moments.

In practical studies of subsurface contamination, sampling is usually done on a much coarser spatial scales: the samples represent mixtures of waters over aquifer depths spanned by the screened intervals of wells, and the number of such screened intervals is relatively small. Such information may not be amenable to analysis by the existing mathematical methods. It may, however, be possible to sample each screened interval with sufficient frequency in time to obtain a good description of the rate at which the tracer or contaminant breaks through. The fact that it is generally easier to monitor concentration variations with time at a few spatial locations than to observe the actual spread of a plume at given instances in time gives rise to the very important question of space-time tradeoff: to what extent and in what way can the dispersive properties of a heterogeneous geologic medium be determined on the basis of relatively frequent sampling at selected points, rather than on the basis of equally or less frequent sampling at more numerous points? And how is the answer to this question related to the scale of the sampling plume? Answers to these questions will be sought in the context of our recent analysis of numerous breakthrough curves collected at CRNL. Based on such answers, we will attempt to come up with suggestions for improved design of field tracer tests. We will pay special attention to the effect of different tracer injection procedures on the determination of dispersion coefficients by comparing the results from 1982 and 1983 tracer tests with that from 1987-1988, as the modes of injection in these tests were different. The same type of comparison will be performed in a series of laboratory-scale experiments.

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APPENDIX

GROUNDWATER CONTAMINANT TRANSPORT STUDIES AT CRNL

The Chalk River Nuclear Laboratories (CRNL) are located 200 km northwest of Ottawa in the Valley of the Ottawa River. The 37 km^2 property lies on the Canadian shield, with a Precambrian bedrock consisting primarily of granitic gneiss. Bedrock is exposed or is buried beneath less than 1 m of overburden over about 10 % of the site. The remainder of the CRNL property is covered by unconsolidated sediments of late Wisconsin age to modern. For the most part, overburden consists of bouldary sandy till, fluvial sands laid down during high stages in the Ottawa River, aeolian sands reworked from the fluvial deposits, and organic soils currently accumulating in wetlands. Apart from the organic deposits, all sediments have a granitic mineralogy. Climate is temperate-humid, with an annual average precipitation of 73 cm, of which 22 cm is available for infiltration or runoff. Most of the site is forested with a mixed coniferous-deciduous cover.

The Environmental Research Branch is studying contaminant behaviour in water, sediments and biota at the CRNL site. Small land areas are devoted to disposal and storage of radioactive materials. In a number of these areas, radionuclides have reached the underlying aquifers forming plumes of contaminated groundwater. Although they present no health or environmental hazard, these plumes have proved useful for experimental work and have been intensively studied in the past 40 years. The majority of the research are remains as a controlled - access outdoor laboratory in which a variety of large-scale field experiments are being conducted in support of radioactive waste management program. Field experiments include: (1) The glass block experiment, a 27-year test of waste disposal technology; (2) the rock-site experiments, a field-scale experiment used for study of rock properties relevant to the technology and safety assessment of a future spent-fuel repository (including field tracer studies in fractured rock); and (3) 20-, 40- and 270-m natural-gradient tracers experiments in unconsolidated materials.

The expertise in physical, chemical, and biological science and technology acquired in this work provides the breadth of knowledge needed to handle

concerns with other toxic chemicals. A highly qualified staff has experience in the field of hydrogeology, geochemistry, computer modelling and remote sensing technology. They draw on skills and knowledge of more than 400 scientists and engineers in related fields, such as computational mathematics, waste management, and chemical engineering. The Environmental Research Branch provides solutions to the broad range of contamination problems. Results are presented in such a way that clients can understand technical issues and make informed decisions.

Figure 1 shows the CRNL property, surface drainage, and locations of waste management facilities. Low and intermediate level wastes have been managed in a variety of shallow land burial facilities since 1947; all of these facilities are situated above the water table in sands on local topographic highs, the only locations where there is substantial thickness of unsaturated sediments. A number of these facilities have released radionuclides to the underlying aquifers over the past 40 years. These contaminant plumes have provided much of the impetus for past studies of subsurface contaminant migration and provide a data base of current interest in the development and testing of improved simulation models. CRNL has long recognized the importance of field testing and validation of conceptual and mathematical models, and a great deal of aquifer testing, ranging from in situ column studies to large scale controlled tracer migration studies have been and are being performed. This Appendix is intended to provide a brief summary of some of the key features of the site, groundwater contamination and tracer related data, and study facilities. The largest groundwater experimental program is currently under way at the Twin lake tracer test site.

The Twin lake site was selected in 1982 after preliminary drilling in three areas on the CRNL property. The site was chosen for stratigraphic simplicity, the apparent uniformity of the sands comprising the aquifer, and high natural groundwater flow velocities. The water table in this unconfined aquifer lies 6 to 20 m below grade; the saturated thickness of the aquifer ranges from 6 to 9 m. Total groundwater flowpath length from the injection well to the groundwater discharge area is 270 m, and at present there are 170 monitoring installations in the aquifer around and downgradient of the injection well. Each installation consists of 0.64 cm ID polyethylene piezometers with short screens

located at 1 m depth increments through the zone of saturation and a 3.2 cm ID PVC pipe that fully penetrates the aquifer and is used for gamma scanning. Figure 2 shows the current layout of monitors out to distance of 120 m from the injection well. At present, there are only a couple of monitors between 120 m and 260 m, where the groundwater flow path traverses beneath a steep sand dune. The groundwater discharge area, a wetland at the toe of the dune ridge, currently contains 36 of the monitoring installations, mostly at the base of the hill where there is a line of springs and seepage areas.

Three locally-non-reactive radiotracer injections have been performed at the Twin lake site in 1982, 1983, and 1987; mapping of the tracer distribution downgradient of the injection well extended for 20 m, 40 m, and 270 m, respectively. In the 1982 and 1983 experiments, ^{131}I was used, so that tracer distrubution could be mapped by gamma scanning. In the 1983 experiment, a small amount of tritiated water was also added and groundwater samples collected downgradient to verify that no retardation of the radioiodine took place. Tritiated water was used in last year's injection; as yet, we have been unable to select or synthesize a suitable non-reactive gamma emitter with a half life of between several weeks and a few months. Work toward the development of such a tracer is continuing.

Results from the 1982 and 1983 experiments are presented and discussed in several papers and reports listed under "References". Briefly, the results showed the presence of a number of sub-horizontal strata with seemingly uniform intralayer hydraulic properties but with up to a two-fold difference in hydraulic conductivities between layers. Local longitudinal and transverse dispersivities within these strata were found to be similar to laboratory measured values, with no apparent trend toward increasing dispersivity with transport distance. Aquifer-averaged dispersivity appeared to vary erratically in response to a partial separation of the input slug as it encountered stratigraphic variations along the flow system. A detailed finite element model in vertical section along the tracer flow path has provided good agreement between simulated and observed tracer distributions /12/.

The 1987 tritium injection experiment was undertaken to allow extension of the monitoring grid from 40 m to the groundwater discharge area downstream (with

boreholes placed in appropriate positions), and to obtain some preliminary data on dispersive behaviour over the longer flowpath. Tracer was injected over a 3-day period, beginning on July 14, and the progress of the injection slug was mapped by sampling the multilevel piezometers. First arrival of the tritiated water in the groundwater discharge area occured in the first week of March of this year, and the last of the labelled water discharge to the surface in mid-May. Analysis of the results is under way. The experiment confirmed the long-term stability of groundwater flow patterns at the tracer site, and strata-controlled distribution of the tracer was still very evident at 270 m downstream from the source.

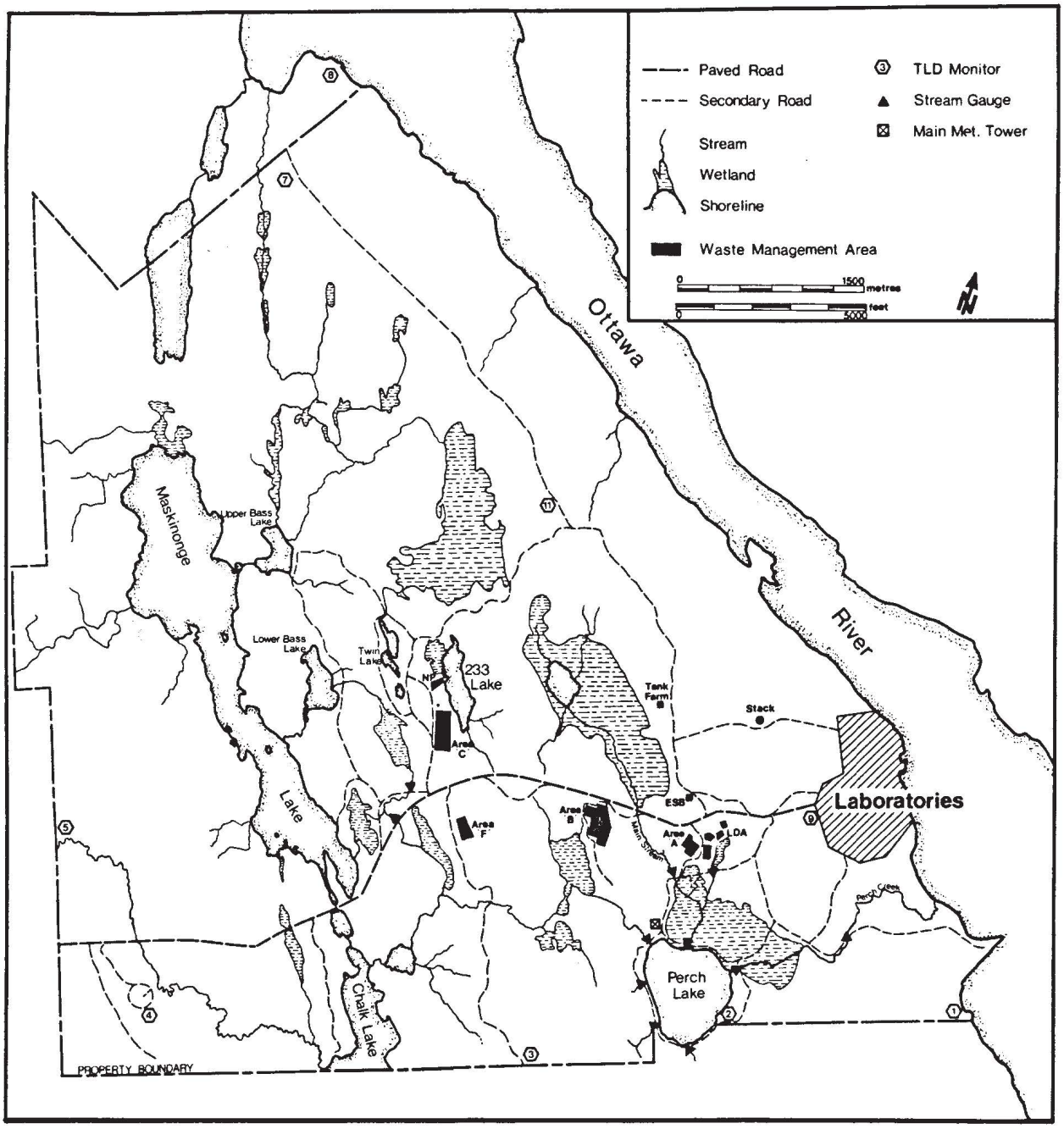

Figure 1: Location of Chalk River Nuclear Laboratories and Waste Management Areas

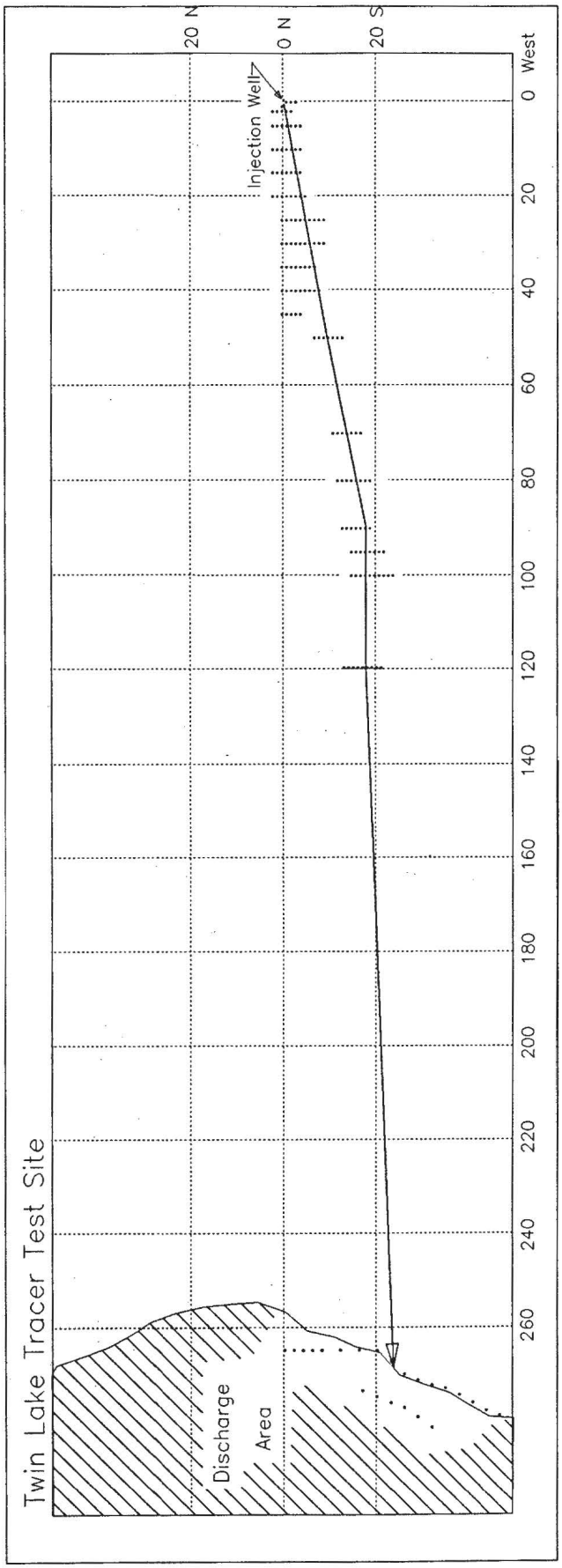

Figure 2: A schematic illustration of the monitoring network at Twin Lake tracer test site

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