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MASTER

A SURVEY OF NEAR-FIELD FLOW CALCULATIONS FOR NUCLEAR WASTE REPOSITORIES

NMA L21

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I

INTRODUCTION

The work statement of this purchase order calls for "a survey of methods and codes which describe the flow of groundwater and the migration of radioactive waste in and about underground nuclear repositories." Our method of conducting this survey has been to visit a number of laboratories engaged in studies of waste migration and groundwater flow, to discuss the general problem with those doing the research, and when possible, to obtain written reports of the work being performed.

In a word, our conclusion is that no one has yet formulated models nor performed calculations of the kind that we had originally envisaged and discussed with members of LLL. Some workers evinced an interest in the problem, and indicated an intent to address it in the future. Others were of the opinion that their codes could be adapted to solution of the repository flow problem, but saw no compelling reason to perform such detailed calculations, at least not at present. Still others have actually performed calculations on some aspect of the problem, but have not attacked the problem in its entirety.

In the following pages we shall describe our conclusions regarding the efforts of the various workers with whom we met. The modest level of effort funded under the purchase order precludes a detailed

analysis of any of these efforts or the machine codes they employ, so the discussion is necessarily qualitative and rather superficial. Nevertheless, we believe it is adequate to support our contention that the problem is one that should be studied as part of a repository design program, and has not been studied in the detail it deserves.

The facilities we visited and the personnel contacted therein are the following:

- 1) Rockwell Hanford Operations, Richland, WA, R.C. Arnett.
- 2) Battelle Pacific Northwest Laboratory, Richland, WA,
John Raymond et al.
- 3) Electric Power Research Institute, Palo Alto, CA, Robert F.
Williams.
- 4) Stanford University, Dept. of Geology, Palo Alto, CA,
Konrad B. Krauskopf.
- 5) Lawrence Berkeley Laboratory, Berkeley, CA, Chin-Fu Tsang.
- 6) Office of Nuclear Waste Isolation, Battelle Institute,
Columbus, OH, James O. Duguid.
- 7) Princeton University, Dept. of Civil Eng., Princeton, NJ,
George Pinder.
- 8) United States Geological Survey, Reston, VA, J. Robertson and
Peter Stevens.
- 9) Sandia Corp., Albuquerque, NM, James Campbell.

Summaries of our discussions at each of these facilities make up the body of this report. Without exception, the individuals contacted were friendly and obviously desirous of being helpful. It is a pleasure to thank them for their cooperation and their valuable time.

II

ROCKWELL HANFORD OPERATIONS (RHO)

CONTACT: R.C. ARNETT

Hanford Operations complex has a long history of involvement in virtually all areas of nuclear waste management. Currently Rockwell Hanford Operations (RHO) manages the Hanford nuclear waste activities for the U.S. Department of Energy (DOE). RHO is primarily applications oriented but works with Battelle Pacific Northwest Laboratories, which are more interested in research and development (see Ch. III). RHO with support from subcontractors is embarking on an intensive study of the near-field repository problem as part of the Basalt Waste Isolation Project (BWIP). Arnett believes that a good model of near-field effects is necessary as a part of the overall waste isolation modeling problem.

Arnett said that among the potentially important effects for the near-field problem are hydrologic, thermal, chemical reaction, stress-strain, and migration effects. Also, the definition of "near field" depends on which effect is under consideration. There are several approaches to the near-field problem. One good approach appears to be to model the near-field effects in such a way that the results of the model may be used as source terms for a far-field regional model. Arnett also favors analytic modeling of near-field effects where applicable as an aid to computer modeling and/or as a test of computer models.

The following remarks pertain to work in general at the RHO complex and do not necessarily pertain to the near-field repository problem.

In 1977 Rockwell International took over the Hanford waste management activities which were previously operated by the Atlantic Richfield Hanford Company for the DOE. The Hanford Department of Energy waste management contractor has historically been primarily involved with the problems associated with management of the nuclear waste shallow burial facility at the Hanford Reservation located in the Pasco Basin. The Pasco Basin is located in the southeastern part of Washington state, and the Columbia River passes through the basin.

Part of the RHO waste management program involves field experiments and computer code simulations of groundwater flow and nuclear waste transport. RHO has access to and/or runs a variety of computer models, making use of several computer facilities (e.g. The Boeing Computer Service UNIVAC, mini-computers, etc.) which they use in complementary modes.

Rockwell is conducting the Basalt Waste Isolation Project (BWIP) for the DOE. Part of this project involves studying the feasibility of a deep geologic repository in basalt. Some of the activities of the BWIP are in the following areas:

- 1) Groundwater flow and nuclear waste transport
- 2) Repository design engineering
- 3) Multiple barriers
- 4) Near-field effects.

REFERENCES

- 2-1. S.W. Ahlstrom et al., Multicomponent Transport Model: Theory and Numerical Implementation (Discrete-Parcel Random-Walk Version), BNWL-2127, Battelle Pacific Northwest Laboratories, Richland, WA, May, 1977.
- 2-2. R.C. Arnett et al., Conceptual and Mathematical Modeling of the Hanford Groundwater Flow Regime, ARH-ST-140, Atlantic Richfield Hanford Co., Richland, WA, Oct., 1976.

Both of these reports are available from RHO. In addition, a new review report is forthcoming early in 1980.

III

BATTELLE PACIFIC NORTHWEST LABORATORIES (BNW)

CONTACTS: J.R. RAYMOND, A. BRANDSTETTER, C.R. COLE, AND
A.E. REISENAUER

Battelle Pacific Northwest Laboratories have currently about 2,700 personnel working in many different areas. The hydrology and waste migration group is a very competent team with fifteen years experience in the field. This group (hereafter referred to as BNW) works closely with RHO, which stresses applications, while BNW is more intimately concerned with development.

The BNW effort is part of the Assessment of Effectiveness of Geologic Isolation Systems (AEGIS) Program, which is funded by DOE through the Office of Nuclear Waste Isolation (ONWI) of the Battelle Project Management Division, Columbus, OH. AEGIS is a successor of part of the previous Waste Isolation Safety Assessment Program (WISAP) which was terminated at the end of FY-1979 (30 September 1979). The scope of WISAP was generally restricted to the development and demonstration of methodology for the assessment of far-field effects of nuclear waste isolation following repository closure. Exceptions were waste form leach studies and methodology demonstrations requiring near-field assumptions. The scope of AEGIS is being expanded to gradually incorporate near-field assessment methodology.

The formulation of overall repository safety assessment methodology is being coordinated by ONWI under its new (in FY-1980) Waste Isolation Performance Assessment Program (WIPAP). A contractor is currently being selected by ONWI to assemble available near-field assessment methodology. This methodology will eventually be transferred to AEGIS, and similarly, AEGIS methodology will be transferred to this new contractor. Eventually then, ONWI will have two contractors with equal capabilities for comprehensive post-closure performance assessments of waste repositories.

AEGIS (and previously WISAP) has improved existing and developed new models for the mathematical simulation of groundwater flow, radionuclide transport in geologic media, and radiological doses to humans. Models of different levels of complexity are available to meet differing requirements for initial coarse site screening and later, more detailed site assessments for licensing. Both analytical and numerical solution techniques are being used; some of the models are coupled by common output-input interfaces. Most models are isothermal; a new version of the 3-dimensional finite-element groundwater flow model also simulates the transport of heat and total dissolved salts, and their effects on the flow regime. Table 1 gives a summary of the principal codes.

One of the more attractive features of the AEGIS codes is the ease of operator interaction. The user can easily upgrade the experimental

Table 1 - AEGIS Code Summary

GROUNDWATER FLOW MODELS

- PATHS - TWO-DIMENSIONAL, ANALYTICAL/NUMERICAL FINITE DIFFERENCE METHOD, HOMOGENEOUS GEOLOGY, SATURATED FLOW
- VTT - TWO-DIMENSIONAL, NUMERICAL FINITE DIFFERENCE METHOD, HETEROGENEOUS GEOLOGY, SATURATED FLOW
- FE - THREE-DIMENSIONAL, NUMERICAL FINITE ELEMENT METHOD, HETEROGENEOUS GEOLOGY, SATURATED FLOW

GROUNDWATER CONTAMINANT TRANSPORT MODELS

- GETOUT - ONE-DIMENSIONAL, ANALYTICAL METHOD, CHAIN DECAY, SINGLE SPECIATION, EQUILIBRIUM SORPTION, CONSTANT LEACH RATE, DISPERSION
- MMT - THREE-DIMENSIONAL, NUMERICAL FINITE DIFFERENCE/RANDOM WALK METHOD, CHAIN DECAY, SINGLE SPECIATION, EQUILIBRIUM SORPTION, TIME VARIANT LEACH RATE, DISPERSION

RADIOLOGICAL DOSE MODELS

WATER DOSE

- ARRG - DRINKING WATER, IMMERSION, EXTERNAL SHORELINE, AND AQUATIC FOOD DOSES
- FOOD - TERRESTRIAL FOOD DOSE

AIR DOSE

- KRONIC - CHRONIC EXTERNAL DOSE
- SUBDOSA - ACUTE EXTERNAL DOSE
- DACRIN - CHRONIC OR ACUTE INHALATION DOSE

data which are input to the system. The system is also replete with CRT and plot package displays of the system output; thus the system is well adapted to the efficient incorporation of the user's intuition. Another feature of this system is its ability to deal with data of varying degrees of quality; given the input data, a subsystem of AEGIS codes can be picked whose running time and output are consistent with the quality of the input data.

BNW has a model of waste migration (developed by personnel at BNW and RHO) called Discrete Particle Random Walk (DPRW), which is well adapted to dealing with nuclear chain decay problems and in addition purports to avoid some of the numerical diffusion problems connected with numerical solutions of the advective diffusion equation. The BNW system has also been applied to several real engineering problems (e.g. dry dock construction, oil field applications) with great success.

The BNW group feels that the proliferation of analytic/numeric systems throughout the community which is involved in the waste isolation program indicates a need for evaluation of the various systems by a disinterested agency, i.e., an organization which is not in the business of developing waste migration models.

The two reports referred to in Chapter II are also available from

BNW. New BNW reports are due to be published in late 1979 and early 1980 documenting the current state of the AEGIS models.

REFERENCES

- PNL-2652 C.R. Cole and S.K. Gupta, A Brief Description of the Three Dimensional Finite Element Ground-Water Flow Model Adapted for the Waste Isolation Safety Assessment Program, Pacific Northwest Laboratory, August 1973.
- *PNL-2892 J.A. Stottlemire, G.M. Petrie and G.L. Benson, A Conceptual Simulation Model for Release Scenario Analysis of a Hypothetical Site in Columbia Plateau Basalts, Pacific Northwest Laboratory.
- *PNL-2939 S.K. Gupta, C.R. Cole, and F.W. Bond, Methodology for Release Consequence Analysis - Part III, A Three-Dimensional Finite Element Groundwater Flow Model, Pacific Northwest Laboratory.
- *PNL-3160 A.E. Reisenauer, Methodology for Release Consequence Analysis - Part II. Variable Thickness Transient Groundwater Flow Model, Pacific Northwest Laboratory.
- *PNL-3161 D.R. Friedrichs and R.S. Argo, Methodology for Release Consequence Analysis - Part VI. Data System, Pacific Northwest Laboratory.

* The starred reports are unpublished and in various stages of preparation. The titles may change upon final publication.

- *PNL-3162 R.W. Nelson and J.A. Schur, Methodology for Release Consequence Analysis - Part I. PATES Groundwater Flow Hydrologic Model, Pacific Northwest Laboratory.
- *PNL-3179 J.F. Washburn, Methodology for Release Consequence Analysis - Part IV. MultiComponent Mass Transport Model, Pacific Northwest Laboratory.
- *PNL-3180 J.K. Soldat, Methodology for Release Consequence Analysis - Part V. Radiological Dose Models, Pacific Northwest Laboratory.

IV

ELECTRIC POWER RESEARCH INSTITUTE (EPRI)

CONTACT: ROBERT F. WILLIAMS

EPRI has a rather modest program consisting of about a five-man level of effort to study nuclear waste disposal. In addition to the work performed in house at EPRI, they are also funding work by Science Applications, Inc. (SAI) and The Analytic Sciences Corp. (TASC). Some of the TASC work involves modeling of nuclide migration from a simplified repository which is essentially a backfilled cavity in a deep geologic barrier layer. This is related to the question of repository flow, but does not represent an attack on the problem of calculating details of the flow in and about a real repository of very complex geometry.

EPRI does not view its role as attempting to compete with larger government agencies (e.g. NRC, DOE, EPA) in mounting a large effort whose eventual goal is the production of the very complex machine codes used in the analysis of waste management options and risk assessment for storage in deep geologic media. Rather, in the words of Williams (Ref. 4-1) "The EPRI projects are intended to provide an illustration of feasible waste disposal technology, an example of prospective criteria, and a comprehensive perspective to the public on the U.S. program, drawing upon the much larger efforts of the DOE, the NRC, and the EPA."

To illustrate the desired approach and a model for the form the results might take, Williams cites the first volume and reference

documents of the Swedish KBS Study (Ref. 4-2). A similar report with supporting documents covering the U.S. program would be a constructive input to reviews of energy and waste disposal policy expected to be made in the 1980-81 time frame.

As part of their technical effort, EPRI has performed a probabilistic analysis to assess risks associated with various portions of the fuel cycle. They concluded that the radiological risk to society of the entire fuel cycle, including transportation, enrichment, fabrication, reprocessing and waste disposal, is only about one percent of that involved in plant operation. Waste disposal was found to be the least hazardous step by many orders of magnitude. Both plant and fuel cycle risk were found to be small in comparison with the hazard of natural background radiation.

According to EPRI, many reviewers of the Interagency Review Group (IRG) report on nuclear waste management felt that the report did not reflect the large variations in the risks associated with waste disposal that were implied by previous studies. Since these studies were based on a considerable range of significant parameters and environmental scenarios, EPRI "normalized" seven different analyses by applying them to the same repository design, at the same location and storing the same contents. Results for peak individual doses fall into two groups:

- (1) A "conservative" class of calculations where the objective was to determine a reasonable upper bound to the potential hazard. These results were centered at about one percent of the dose

from background radiation.

- (2) A "best estimate" class that led to calculated doses about 10^{-5} of the natural background.

EPRI believes their results are useful because they portray the states of waste migration risk assessments more clearly than available program documents.

In summary, EPRI believes that discussions of uncertainties in waste management risks and of the numerous alternative methods of mitigating these uncertainties are buried and diffuse in the technical literature. They propose to ameliorate this situation by detailed studies of the literature supplemented by trade-off studies of their own, with the goal of providing a coherent picture of the complex, multi-agency U.S. research and development effort that has been devoted to waste management and disposal. EPRI envisages a report similar to the Swedish KBS report as a means of presenting the results of their studies. Williams also stated the belief that in many cases large R and D efforts may be avoided by seeking engineering solutions to problems rather than insisting on detailed mathematical studies over wide parameter ranges. A case in point is the plethora of problems arising when large thermal gradients are considered. It may be possible to avoid the need to consider these problems in detail if proper engineering procedures are adopted. This question is discussed in more detail in Chapter V.

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- 4-1. Robert F. Williams, Utility Programs and Approaches for Acceptable Radioactive Waste Management, EPRI, Palo Alto, CA, Sept. 1979.
- 4-2. Nuclear Fuel Safety Project KBS (Kärnbränslesäkerhet), Handling of Spent Nuclear Fuel and Final Storage of Vitrified High Level Reprocessing Waste, 5 Vols., Sweden, Nov., 1977.

DEPT. OF GEOLOGY, STANFORD UNIVERSITY

CONTACT: KONRAD B. KRAUSKOPF

Krauskopf is a geologist, and has not been concerned with groundwater flow as such; nevertheless, he believes that transport of waste to the biosphere by virtue of groundwater contamination is the greatest risk associated with storage in deep geologic repositories. This belief stems from his conviction that geology, although an admittedly imprecise science, is still capable of providing guarantees of admissibly low risk levels for volcanic and earthquake activity or meteoric impact in selected geologic sites.

The uncertainties in groundwater transport calculations, Krauskopf believes, are greater than the uncertainties in purely geologic predictions. Two of the major uncertainties are:

- 1) Long-term chemical interactions between groundwater, canister metal, and solid waste
- 2) The rate of groundwater movement through heterogeneous rock material intersected by cracks and zones of shear.

Both classes of uncertainties are aggravated by the fact both rocks and water are heated by the energy released in radioactive decay of the waste. The increased temperature changes the rates of dissolution, chemical reactions, and sorption, and also shifts equilibrium concentration ratios. The temperature gradients established also tend to cause brine migration toward the canisters in salt repositories, thus increasing the canister dissolution rate. The

thermal gradients also lead to density gradients in groundwater, so that convection must be taken into account, and this complicates the flow calculations. The thermal gradients also give rise to stresses in the rock formation, which may cause additional fracturing of the rock, thus complicating the fracture flow problem still farther.

All of these effects are coupled to some extent; if the couplings are strong enough to be important, the problem stands to become very complex indeed. The difficulties associated with thermal effects can be ameliorated by decreasing the thermal loading of the repository. The thermal loading of the repository can be decreased by a combination of increasing the period of aging the waste before its final emplacement in the repository, decreasing the amount of waste stored in each canister, and increasing the canister spacing in the repository. For example, Sweden is presently planning to allow the waste to age forty years before final emplacement, and then to dispose the waste in such a way that the maximum temperature reached in their granite repositories is 80°C . Such a plan may greatly reduce not only the thermal effects themselves, but also reduce the huge research and development effort that would be required to solve the problem over a temperature range that extended up to several hundred degrees.

Lowering the temperature by a combination of procedures is an example of mitigating problems by engineering solutions rather than

meeting the problems head-on with an expensive, and expansive research program. This is the approach recommended by Williams, of EPRI (see Chapter IV), Krauskopf believes it may work in this instance, but even so, a great deal of work remains to be done on fracture flow. This should comprise a combination of theory and in situ measurements.

REFERENCES

- 5-1. Konrad Krauskopf, Current Perspectives in Geologic Disposal of Radioactive Waste, in Proceedings of the Symposium on Waste Management, Tucson, Univ. of Arizona, Feb. 1979.
- 5-2. KBS Report (see Ref. 4-2).

VI

LAWRENCE BERKELEY LABORATORY (LBL)

CONTACT: CHIN-FU TSANG

A group at LBL headed by Paul A. Witherspoon works in the area of nuclear waste isolation, and Chin-Fu Tsang contributes to the analytic/numeric modeling effort of this group.

LBL's position on the repository problem appears to be that many models have been developed which cover some, but not all of the pertinent phenomena. Much work remains to be done on models for thermal-hydrologic-mechanical behavior of fractured crystalline and argillaceous rocks as well as sorption and chemical effects. LBL has a program to review and evaluate work on fracture hydrology modeling. They have compiled a list of about 600 recent articles on existing models and have picked ten numerical models for detailed evaluation. Tsang believes that analytic/numeric tools exist which could be applied to the far-field repository problem, but the computation times could be very long. On the other hand, there are great uncertainties regarding fracture flow, sorption, and chemical effects in the near-field region. He believes that major work has to be done to study near-field effects until these uncertainties are cleared up.

LBL is the lead U.S. research group in a joint U.S./Sweden project at the Stripa mine, Sweden. This project is concerned with the feasibility of placing a repository in crystalline rock.

Experimental and theoretical investigations are being carried out to determine thermal-mechanical effects, fracture effects, etc. LBL is also participating with LLL in the Climax Stock experiment. In this experiment a large array of heaters and canisters is to be placed within underground excavations in a granitic rock mass at the Nevada Test Site (NTS) for a period of 3 to 4 years. The LBL group is planning to use an array of acoustical sensors to monitor the fracturing of the rock. By processing this information, they hope to construct a three-dimensional representation of the fracture network and to learn how the bulk permeability of the rock changes due to thermal stresses.

REFERENCES

- 6-1. J.S.Y. Wang et al., A Study of Regional Temperature and Thermohydrological Effects of an Underground Repository for Nuclear Wastes in Hard Rock, LBL-9271, Oct. 1979.
- 6-2. Tin Chan et al., Theoretical Temperature Fields for the Stripa Heater Project, LBL-7092, Sept. 1978.
- 6-3. Geotechnical Assessment and Instrumentation Needs for Nuclear Waste Isolation in Crystalline and Argillaceous Rocks, LBL-7096, July, 1979.

VII

OFFICE OF NUCLEAR WASTE ISOLATION (ONWI) BATTELLE-COLUMBUS

CONTACT: JAMES O. DUGUID

Battelle-Columbus operates ONWI for the Department of Energy (DOE). ONWI shoulders all of the responsibility which was previously assumed by the Office of Waste Isolation (OWI) located at Oak Ridge National Laboratory (ORNL). In addition, ONWI is assuming a larger overview role for the National Waste Terminal Storage (NWTS) program.

Duguid thinks that the near-field repository problem is very important and that there presently exist no codes and/or programs which address this problem in a systematic way consistent with its importance. However, many of the individual components of such a system already exist. ONWI is in the process of negotiating a substantial contract in this area (contractor unspecified). Duguid believes that analytic as well as numeric modeling is required for an appropriate treatment of the near-field problem.

Duguid supplied us with a variety of information regarding ONWI's technical interests and the methods by means of which they fund contract efforts. Some points of possible interest are as follows:

(1) Near-Field Problems

- (a) Thermal-mechanical models coupled to hydrological models are needed

- (b) Bentonite as a backfill material is not well modeled
  - (c) RE/SPEC, Rapid City, South Dakota is good at rock mechanics modeling.
- (2) ONWI is issuing new RFP's on a number of subjects.
  - (3) ONWI thinks that the Intera Corporation is among the best in the areas of hydrologic flow and waste migration modeling.
  - (4) Some natural phenomena of possible experimental interest to the waste isolation problem are:
    - (a) Thorium deposits in Brazil-large rainfall area
    - (b) Study of old water, of order 5×10^4 years old
    - (c) Helium accumulation from alpha decay
    - (d) Oklo
  - (5) Some ongoing and planned experiments which may yield useful information are:
    - (a) Climax experiment-NTS
    - (b) Stripa experiment-Sweden
    - (c) A Lawrence Livermore experiment involving the development and placement of an electromagnetic transceiver in a 3 inch diameter borehole. By pulsing the transmitter and sensing the reflected signal, one hopes to obtain information about anomalies in the surrounding formation.
  - (6) ONWI is continually reviewing Nuclear Regulatory Commission (NRC) specifications and is beginning to have a dialog with NRC.
  - (7) The BNW WISAP system and an Intera Corp. code (similar to

SWIFT) have been exercised on the Waste Isolation Pilot Project (WIPP) site problem and agree reasonably well with each other.

- (8) ONWI and the United States Geological Survey (USGS) are preparing a technical plan report on geologic disposal of nuclear waste. The Working Group Leader on this effort is Duguid and a draft report has been produced.

REFERENCES

- 7-1. ONWI and USGS, Earth Sciences Technical Plan for Mined Geologic Disposal of Radioactive Waste, TID-29018 (Draft), Jan. 1979.
- 7-2. J.O. Duguid and P.C.Y. Lee, Flow in Fractured Media, Water Sources Research 13, 558 (1977).

VIII

DEPT. OF CIVIL ENG., PRINCETON UNIVERSITY

CONTACT: GEORGE F. PINDER

Pinder said that, in a sense, one may consider the near- and far-field problems to be solved. The authors' impression of Pinder's position is that he believes that the numerical models available are sufficiently general to solve the repository problem as well as it can be solved in view of the uncertainties in the site data. The key here is data uncertainty; the data base will break down before the non-generalizability of the numerical models becomes crucial.

The Princeton group is now actively working on the nuclear waste isolation problem. They are doing some work for Sandia on methods of solving partial differential equations when the parameters in the equations are stochastic. The group does not use the Monte Carlo method, but instead has developed new techniques based on Keller's method. This method makes use of perturbation theory; one perturbs the solution about that corresponding to the mean values of the randomly varying parameters. Pinder and Tang developed this method because of their concern about modeling efforts in general; there are too many unknowns in the data base and one must therefore incorporate stochastic parameters in the models.

The Princeton group has a variety of numerical models among which are the following:

- (1) Three-dimensional triangular-prism finite elements code with mass transport. Since mass and heat transport are governed by the same equations, the code can be used for thermal calculations. The code allows discontinuities of 3 to 4 orders of magnitude in the hydraulic conductivity.
- (2) Three-dimensional fractured flow plus porous-medium flow with mass (or heat) transport.
- (3) Geothermal multiphase steam code. This code allows water to flash to steam; it allows a six-order-of-magnitude change in the density in one time step.
- (4) A nonlinear finite element equation solving package. The user must supply his own front end for this code.

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- 8-1. D.H. Tang and G.F. Pinder, Simulation of Ground Water Flow and Mass Transport Under Uncertainty, Advances in Water Resources 1, 25 (1977).
- 8-2. D.H. Tang and G. F. Pinder, Analysis of Mass Transport with Uncertain Physical Parameters, Dept. of Civil Engineering, Princeton Univ., Sept. 1978.

IX

UNITED STATES GEOLOGICAL SURVEY (USGS)

CONTACTS: JOHN B. ROBERTSON AND PETER STEVENS

USGS has several numeric hydrologic codes, which they have used in calculations of regional flow fields in their studies of the waste isolation problem. Their arsenal includes both finite difference and finite element codes. Robertson believes that some one of these codes, or perhaps several used in conjunction, could be employed in near-field repository flow calculations. No such calculations have been undertaken up to the present time, however, nor does it appear that USGS plans to attack the near-field problem in the immediate future.

USGS has expended considerable effort on modeling geothermal flow systems in igneous rock and in fractured sedimentary rock overlying thermally fractured igneous rock. The knowledge gained from these investigations may be useful in attacking fracture flow in the neighborhood of waste repositories where substantial thermal gradients have been produced by the energy released in radioactive decay.

One approach to flow in fractured media is simply to treat the fractures as pores, and use Darcy's law for flow through porous media. If this procedure has any merit at all, it can only be when the representative elementary volume contains many fractures. We would expect that this might entail use of an elementary volume with linear dimensions on the order of 10 m or larger,

while near-field calculations are required to be accurate at least down to the scale of 1 m. Thus treating fractures by an effective porosity approach may be useful for regional calculations, but the validity of the method for near-field calculations is highly questionable.

Another approach to modeling flow in fractured media is to assume an "equivalent" array of uniformly spaced identical fractures. The periodicity of the equivalent array enables one to perform calculations with relative ease. Spurious effects are introduced by the assumed periodicity, however, so one would expect at best to obtain useful approximations for average values of quantities within regions encompassing many cells. To be useful in the near-field problem, therefore, the spacing of the fracture lattice would have to be much less than 1 m. It is not immediately obvious whether such a requirement is consistent with the scale of the fractures to be expected in the neighborhood of a repository. An alternate approach would be to model flow through individual fractures that could be spaced at any interval.

USGS has done some work on fractures induced by blasting or differential heating but has, as yet, done no near-field modeling in this area either. On the experimental side, there has never been available a large scale example of fractured crystalline rock. The USGS believes that blasting does not fracture the surrounding medium over large distances; e.g. the blast induced

shock wave does not create major fracturing problems in competent granite. The differential heating problem has been experimentally studied "locally" (in small regions) by placing heat sources in rock and observing the local fracture system. Thermally induced stress caused by differential heating may be an important fracture mechanism; theory predicts fractures that are many meters in length. This problem can be ameliorated by aging the waste before placing it in the repository, reducing the density of stored waste, and increasing the canister spacing.

Some remarks of Robertson on the pros and cons of host formations for waste repositories are as follows:

Salt

- (1) Plasticity increases as temperature increases, an advantage.
- (2) Heat draws brine toward the heat source; i.e. leads to potential leaching problems.
- (3) Salt flows before fracturing, an advantage.
- (4) Salt tends to heal its fractures, an advantage.

Shale

- (1) In soft, poorly-cemented shales plastic deformation occurs at ambient temperatures.
- (2) Plasticity and temperature effects are not well understood. Respec is studying some of these problems.
- (3) Competent shales deform along fractures; i.e. do not really undergo plastic flow.

Clay

- (1) Chemical alteration occurs at $\approx 100^{\circ}\text{C}$.
  - (2) Plasticity and temperature effects are not well understood.
- Respec is also studying these problems.

Granite

- (1) Chemical alteration occurs at a few hundred degrees centigrade.
- (2) Stressed granite will fracture before it undergoes plastic flow.

Stevens is interested in rock mechanics and expressed the opinion that near-field effects are important; in particular thermal effects, rock mechanics, hydrology, and waste transport. Stevens is working on the Earth Science Technical Plan for Mined Geologic Disposal of Radioactive Waste, a document mentioned in Chapter VII of this report. Stevens is reviewing heater experiments, spent fuel experiments, etc.

The USGS has a modest effort in rock mechanics. They are conducting some study work and also have a program for evaluation and calibration of instruments. In the latter program stresses are imposed on material and various instruments are used to measure the stresses. The USGS is studying experimental techniques for obtaining information about fractures at large distances from the mining face, acoustical and electromagnetic techniques are being explored.

Work of interest in rock mechanics is being performed at several places among which are the following:

- (1) USGS (mentioned above)
- (2) Sweden. They are developing smooth wall blasting methods and make use of charge placement and charge shaping techniques.
- (3) ARPA - smooth blasting development work.
- (4) NORAD - smooth blasting development work.
- (5) Nevada Test Site (NTS) - smooth blasting development work.
- (6) Lawrence Livermore Laboratory is participating in a program that involves remining into underground nuclear bomb test sites.
- (7) Lawrence Berkeley Laboratory is involved in rock mechanics.
- (8) The Respec Company does rock mechanics studies.
- (9) The University of Minnesota has a program on the rock mechanics of the Columbia plateau area.

REFERENCES

Papers of interest for the near-field repository problem were given at the International Symposium on the Underground Disposal of Radioactive Wastes at Otaniemi near Helsinki, July 1979. Some papers of interest are:

- 9-1. N.A. Chapman, Mineralogical and Geochemical Constraints on Maximum Permissible Repository Temperatures.
- 9-2. H. Beale, et al., Thermal Aspects of Radioactive Waste Disposal in Hard Rock.

- 9-3. A.S. Kunstman, et al., Studies on the Optimal Disposal of Radioactive Wastes with Special Attention to the Thermal Influence on Surrounding Salt Bed and to Economical Aspects.
- 9-4. K. Araki, et al., Preliminary Research on Geological Isolation of High Level Radioactive Waste in Japan Atomic Energy Research Institute.

SANDIA LABORATORIES (NRC-FUNDED BRANCH)

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The Fuel Cycle Risk Analysis Division of Sandia is funded by NRC to develop a methodology for assessment of the long-term risks from disposal of radioactive wastes in deep geologic media. The analytical methods and data developed in the study are expected to form the basis for a portion of the NRC repository licensing procedure (Ref. 10-1).

The primary analytical tool used in the Sandia hydrological calculations is the Sandia Waste Isolation Flow and Transport (SWIFT) code. This is a finite difference code developed by Intera Corp. for Sandia. The SWIFT code is a modification of the Survey Waste Injection Program (SWIP) code. SWIP was also formulated by Intera, then a subsidiary of Intercomp., for the USGS Water Resources Division to model liquid waste disposal in deep saline aquifers. SWIP is three dimensional, and solves the coupled equations of flow and conservation of energy and solute mass. The SWIFT modification consists of adjoining the equations governing radioactive decay and radionuclide transport to the equations already in SWIP.

Both SWIP and SWIFT include heat conduction and advection, and the convection effects arising from the variation of water density with temperature and pressure. Likewise, the concentrations of salt, and of the radioactive solutes included in SWIFT, are subject to

both diffusion and advection. Both codes use finite-difference methods, and may be exercised in either the one-, two or three-dimensional mode.

Most of the SWIFT calculations performed by this group up to the present relate to a hypothetical bedded salt reference site. The site comprises a repository mined in a salt bed, which in turn is imbedded in a layer of shale. The shale layer rests on a layer of sandstone that lies on bedrock, the latter assumed to be impermeable. Above the shale layer is another layer of sandstone, part of which extends to the surface, and part of which is covered by a thin layer of shale which is overlain by a glacial aquifer. These layers are all tilted slightly with respect to the horizontal. The formation is symmetrical with respect to a vertical plane, so the entire formation represents a basin. A river flows along the floor of this basin. There are also dry river beds on each side of the symmetry plane. The rate at which radionuclides enter solution can be controlled by either a leach-limited or solubility-limited source.

At the present time Sandia is using SWIFT only for regional flow and transport calculations, as the preceding discussion implies. Campbell believes that SWIFT could be used for some detailed near-field calculations, but that machine storage could become a problem.

Even if machine storage were not a consideration, however, Campbell is not convinced that one should begin the study of a repository site with such detailed near-field calculations. He believes that one runs the risk of being smothered with output, while failing to gain little real understanding of the problem. He favors instead the formulation of rather simple models to be used for a number of exploratory calculations before performing detailed calculations. These permit one to develop an intuitive feel for the problem, and provide a basis for determining which effects and parameters are important, and how the various phenomena are coupled. An example of this type of study is the DYNAMO simulation used by Sandia to study the geological stability of the bedded salt reference-system.

In the DYNAMO calculations a number of coupled phenomena are identified, and the behavior of each is characterized in a lumped-parameter rate equation. In general, the rate equations are coupled together because the behavior of each variable is coupled to the variation of some or all of the other variables. DYNAMO solves the set of coupled rate equations, and thus permits one to investigate failure scenarios simply and efficiently.

Sandia is also formulating a simple network flow and radionuclide transport (NWFT) model. The intent is to use NWFT and SWIFT jointly. SWIFT can be used to determine the effects of any

particular depository breachment scenario on the fluid flow field and radionuclide migration path. NWFT can then be applied to reproduce the migration path and to evaluate the effects on radionuclide discharge of variables which alter the radionuclide source rate or migration time.

REFERENCE

- 10-1. James E. Campbell et al., Risk Methodology for Geologic Disposal of Radioactive Waste: Interim Report, Sandia SAND 78-0029, NUREG/CR-0458, Oct., 1978.

XI

SUMMARY AND CONCLUSIONS

Everyone we contacted in our survey believed the near-field flow problem to be an important one, and one that has not been adequately studied up to the present time. All agreed that, in principle at least, the flow problem comprises many complex, coupled phenomena. These include dissolution, sorption, chemical reactions, thermal fracture, fracture flow, convection, heat conduction, etc., and the temperature dependence of various rate constants and equilibrium constants. Not only are these phenomena and their interrelationships not well understood per se, but the data base required for quantitative studies is also sadly deficient.

In view of this situation, there are those who believe that the best way to approach the problem is by first making measurements, preferably in situ, to extend the data base while at the same time studying the individual phenomena to gain a better understanding of each of these. The rationale here is that a direct attack on the repository flow problem in the absence of a firm data base and thorough understanding of the phenomena involved would yield very little useful information. An exemplar of this point of view is the LBL group.

A second school of thought is that the problem is so complex that the initial effort should be devoted to identifying the most important phenomena and the most urgently required data. The procedure here would be to perform parametric studies based on

rather simple models. One hopes that such studies will show that the effects of some phenomena are relatively unimportant, that some couplings are negligible, or that some parameters need not be known with great precision. This raises the possibility that the problem can be simplified considerably, and that a needlessly elaborate measurement program can be avoided. RHO, BNW and Sandia appear to be proponents of this point of view.

Our own opinion is that progress will be optimized if both lines of attack are pursued, provided that the efforts are well coordinated and there is an efficient exchange of information throughout the community. The detailed, meticulous studies will provide the data and knowledge that will eventually be required, and lessen the probability that some important effect is overlooked. The model studies will contribute to an intuitive understanding of the problem, help guide the detailed research program, and provide useful interim information. We believe that the interplay between the two types of programs promises to produce meaningful results more quickly and efficiently than would a sequential approach, regardless of the order of the sequence.