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Evaluation and Status Report on HYDROCOIN at Midway

C. R. Cole

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Prepared for the U.S. Department of Energy
under Contract DE-AC06-76RLO 1830

Pacific Northwest Laboratory
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EVALUATION AND STATUS REPORT ON HYDROCOIN AT MIDWAY (HYDROCOIN .. an international project for studying groundwater hydrology modelling strategies)

C. R. Cole

December 1986

Prepared for
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Pacific Northwest Laboratory
Richland, Washington 99352

SUMMARY

The U.S. Department of Energy (DOE) is participating in the international hydrologic code intercomparison (HYDROCOIN) project organized by the Swedish Nuclear Power Inspectorate (SKI) for the purpose of improving our knowledge about the influence of various strategies for ground-water flow modeling for the safety assessment of final repositories for nuclear waste. The HYDROCOIN project consists of three levels of effort: Level One is concerned with verifying the numerical accuracy of codes, Level Two is involved with validation of models using field experiments, and Level Three is concerned with sensitivity and uncertainty analysis.

The need for the HYDROCOIN project emerged from an earlier international study for the intercomparison of computer codes for radionuclide transport (INTRACOIN). The HYDROCOIN project began in May 1984 with a group of fourteen organizations from eleven countries participating; currently twenty organizations are involved. Five teams from DOE's Office of Civilian Radioactive Waste Management (OCRWM) are participating in the HYDROCOIN project, and this document presents the results of a review of this participation and an analysis of the benefits of OCRWM participation in the first 2 years (i.e., through May 1986) of the 3-year HYDROCOIN project. Efforts on the seven Level One cases are nearly complete. Level Two problems have been formulated and are in final draft form, and Level Three problems have been identified and are in first draft form.

This report details the motivation, need, and benefits from HYDROCOIN through a 1) chronological synopsis of the project's progress to date, 2) brief description and intercomparison of preliminary Level One results prepared by OCRWM participants, and 3) discussion of OCRWM contributions and plans for HYDROCOIN Level Two and Three efforts.

The important national and international need for verified and validated performance-assessment technology to judge the safety, suitability, and acceptability of various underground nuclear waste disposal options has provided the basic area of common interest for the earlier INTRACOIN and current HYDROCOIN efforts. With the most likely route for disposed radionuclides to return to

the biosphere being through dissolution and transport by ground waters, the performance-assessment technology required for evaluating geologic disposal options and sites will include ground-water flow modeling. This complicated process involves using computer codes in conjunction with site characterization data and an interpretation process known as conceptual modeling. The importance of these codes and the ground-water modeling process to performance assessment requires 1) benchmarking and verifying the codes, 2) evaluating and demonstrating the applicability of the modeling process for describing the results of experiments at both the laboratory and field scales (validation), and 3) investigating and evaluating various methods and approaches for determining the importance of different phenomena and parameters (sensitivity analysis) and for establishing the uncertainties associated with the performance assessments obtained through this modeling process for both current and future conditions (uncertainty analysis). The three levels of the HYDROCOIN project address these important ground-water modeling issues.

Benefits of participating in HYDROCOIN Level One (verification and benchmarking) have included the following:

- insight and experience in the difficult process of formulation and selection of relevant verification and benchmark problems which will prove of value as part of four OCRWM Office of Geologic Repository (OGR) projects' ongoing verification and benchmarking efforts. The Salt Repository Project's (SRP) layered salt benchmark problem (Case 6) has been improved. Case 4 has proved to be a useful verification problem for all the project teams by providing one of the only analytical solutions involving buoyancy as well as a test for pathlines. Case 5 has provided SRP with an important salt site benchmark problem for testing the ability of codes for handling variable density problems with very steep concentration gradients. Cases 1 and 2 provide useful equivalent porous-media fracture-flow problems.
- a means for code intercomparison for complex benchmark problems where no analytical solution exists to provide the correct result. Through HYDROCOIN, results are available from a variety of codes representing various numerical approaches taken by independent modeling teams.

Case 5 was of particular benefit to SRP because it illustrated a difficulty with standard finite element approaches for density-dependent problems. As a result, the consistent velocity formulation used in the two-dimensional SUTRA code (Voss 1984) was incorporated into SRP's code. Cases 2, 4, and 7 have provided beneficial information concerning discretization strategy and various mass balance and residuals methodologies. Code intercomparisons indicated common difficulties associated with the interpolation of results between nodes and with the generation of path- and streamlines. Identification of these difficulties has resulted in code improvements and problems for Level Three to resolve the source of these difficulties.

- a unique organizational structure for code verification and benchmarking. The HYDROCOIN organization and structure draws from a wide variety of capable participants with enough diversity in interests and needs that appropriate problems of mutual interest can be and have been formulated and selected. Additionally, sufficient participation with an ample variety in code types in each of the Level One cases has given this effort the required credibility. While this set of HYDROCOIN benchmarks does not satisfy all of the needs of any of the OGR projects, it does provide a base level of key verification and benchmarking credibility. It also identifies codes against which future benchmark comparisons would be especially beneficial.
- a means for development of code credibility and a forum for the exchange of technical information on ground-water modeling strategies. The wide variety of participating groups, which includes regulatory agencies, universities, and consultants as well as other peer groups from various countries, provides a measure of credibility to the HYDROCOIN benchmarking effort that would be hard for DOE to achieve otherwise. The unique HYDROCOIN organizational structure and the diversity of participants and interests in conjunction with the focus provided by a common set of modeling problems also provide an excellent forum for technical exchange and a means for OCRWM

participants to present and compare their performance-assessment approaches with those being used by their peers.

Participation in the early planning and discussion stages of Level Two has provided useful insights regarding the difficulties associated with validation. Both the Nevada Nuclear Waste Storage Investigations (NNWSI) Project and SRP have formulated Level Three sensitivity uncertainty problems that will provide direct benefits to their projects. Given the relative difficulty of the issues addressed by Levels Two and Three, the potential benefits of participation are even greater than they were for Level One. Maximum benefits come from full and consistent participation by the project teams in the workshops and coordinating group meetings. The value of the HYDROCOIN workshops and coordinating group meetings is related to the quality of the technical discussions, the openness and sharing of successful new ideas and approaches, and more importantly the candid discussions of failures.

ACKNOWLEDGMENTS

This work, performed by Pacific Northwest Laboratory as part of the Performance Assessment Scientific Support (PASS) program, was supported by the U.S. Department of Energy's Office of Civilian Radioactive Waste Management (OCRWM), under Contract DE-AC06-76RLO 1830. Pacific Northwest Laboratory is operated by Battelle Memorial Institute for the U.S Department of Energy. I would also like to acknowledge the participation and efforts OCRWM's four Office of Geologic Repositories (OGR) project teams whose work has been discussed and compared in this report. These project teams and team leaders include:

- The Basalt Waste Isolation Project (BWIP), Peter M. Clifton
- The Crystalline Rock Project (CRP), A. Berge Gureghian
- The Nevada Nuclear Waste Storage Investigations (NNWSI) project, Robert W. Prindle
- The Salt Repository Project (SRP), Sumant K. Gupta

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INTRODUCTION

The U.S. Department of Energy (DOE) is participating in an international study for hydrologic code intercomparison (HYDROCOIN). This study is organized by the Swedish Nuclear Power Inspectorate (SKI) with participation by the Organization for Economic Cooperation and Development's Nuclear Energy Agency (OECD/NEA). The purpose of the HYDROCOIN project is to improve our knowledge about the influence of various strategies for ground-water flow modeling for the safety assessment of final repositories for nuclear waste. HYDROCOIN is a 3-year project consisting of three levels of effort with the following objectives:

- Level One is concerned with verifying the numerical accuracy of codes by code intercomparison and by comparing code results with analytical solutions.
- Level Two is an approach to model validation consisting of comparisons of model predictions with available experimental results.
- Level Three investigates the importance of uncertainties inherent to the modeling and site characterization process through sensitivity and uncertainty studies.

The need for the HYDROCOIN project emerged from an earlier international study for the intercomparison of computer codes for radionuclide transport (INTRACOIN). This study was initiated by SKI in 1981 and concluded in 1984. In May of that year the international HYDROCOIN project began. It was originally composed of a study group of fourteen organizations from eleven countries (Canada, France, Federal Republic of Germany, Finland, Japan, the Netherlands, Norway, Sweden, Switzerland, the United Kingdom, and the United States). Currently, twenty organizations are participating in the HYDROCOIN project. Appendix A contains a more detailed description of the HYDROCOIN organization, taken from the latest progress report (SKI 1986).

Five teams from DOE's Office of Civilian Radioactive Waste Management (OCRWM) are participating in the HYDROCOIN project. These teams and their respective team leaders are as follows:

- The Basalt Waste Isolation Project (BWIP), Peter M. Clifton
- The Crystalline Rock Project (CRP), A. Berge Gureghian
- The Nevada Nuclear Waste Storage Investigations (NNWSI) project, Robert W. Prindle
- The Salt Repository Project (SRP), Sumant K. Gupta
- The Performance Assessment Scientific Support (PASS) program, Charles R. Cole.

C. R. Cole of the PASS program is coordinating DOE's OCRWM participation in HYDROCOIN and is the DOE's representative to the Coordinating Group that directs the HYDROCOIN study.

The purpose of this document is to review and report on the status of DOE's OCRWM participation in the first 1.5 years of the 3-year HYDROCOIN project. Level One efforts are nearing completion (a draft of the Level One report was made available at the May 1986 workshop held in Tokai, Japan). Level Two problems have been formulated and are in final draft form, and Level Three problems have been identified and are in first draft form.

Detailed progress reports on the overall HYDROCOIN project (SKI 1984, 1985, 1986) are available. The first section of this report details the motivation, need, and perceived benefits from HYDROCOIN. A chronological synopsis of the project's progress to date follows, with discussions focused on contributions made by the OCRWM participants to the HYDROCOIN Level One, Two, and Three efforts. The next section of the report presents a brief description and intercomparison of the preliminary Level One results prepared by OCRWM participants. The final section is an analysis of the specific benefits that have resulted from DOE's participation by OCRWM's four Office of Geologic Repositories (OGR) projects and its PASS program in Level One efforts. Plans for continued involvement in Levels Two and Three along with an analysis of potential benefits are also described.

HYDROCOIN - MOTIVATION, NEED, AND APPLICATION TO OCRWM ACTIVITIES

Nuclear waste management is an important national and international concern that has fostered various successful international cooperative programs. As experience has shown, these cooperative efforts are successful when common technical interests and needs bring the parties together because of the perceived and real benefits obtainable from the exchange (Rusche 1986). The important national and international need for verified and validated performance-assessment technology to judge the safety, suitability, and acceptability of various underground nuclear waste disposal options has provided the basic area of common interest for the earlier INTRACOIN and current HYDROCOIN efforts.

The most likely route for disposed radionuclides to return to the biosphere is through dissolution and transport by flowing ground waters. As a result, performance assessments for evaluating geologic disposal options and sites will require ground-water flow modeling. This complicated process involves using computer codes in conjunction with site characterization data and an interpretation process known as conceptual modeling. The importance of these codes and the ground-water modeling process to performance assessment requires that we:

- develop, test, and demonstrate a methodology for checking the numerical accuracy of these codes over the ranges of parameters, kinds of geometries, and types of boundary conditions, and for the various phenomena and interactions likely to be encountered in repository safety assessments. The parts of this process that involve comparing numerical code results with analytical solutions are commonly referred to as verification, and the parts that can only be achieved via code intercomparisons are referred to as benchmarking. The obvious benefit of exchange is in the area of benchmarking, since it requires intercomparison of code results on common problems. Additional areas that benefit from exchange include selecting and formulating appropriate verification and realistic benchmarking problems, and investigating the means for evaluating and comparing these code results for the more realistic benchmarking problems.

- evaluate and demonstrate the applicability of the modeling process for describing the results of experiments at both the laboratory and field scales (validation). Earlier INTRACOIN project efforts indicated that many field situations, especially at larger scales, allow too many interpretations for validation in the traditional sense. As a result, at least two aspects of validation must be addressed. One aspect involves selecting sufficiently complete data sets and well-defined experiments at either the lab or the field scale that can be used to validate, in the traditional sense, our mathematical description of the physical processes involved in ground-water hydrology. A second aspect involves building confidence in the total ground-water modeling process described above. Relevant hydrologic experiments will be selected whose data sets are incomplete. Confidence in the way data are interpreted and codes are applied to assess performance is then generated by the application of codes through the ground-water modeling process by the various project teams.
- investigate and evaluate various methods and approaches for determining the importance of different phenomena and parameters (sensitivity analysis), and for establishing the uncertainties associated with the performance assessments obtained through this modeling process for both current and future conditions (uncertainty analysis).

OCRWM has ongoing efforts that address these important areas of performance assessment at each of their four OGR projects and the PASS program, as do other nations investigating geologic disposal. Issue complexity and the perceived benefit of a cooperative effort (inferred from the success and benefits of the earlier and similar INTRACOIN project) fostered the current HYDROCOIN project for addressing and improving our collective knowledge concerning these three issues.

SYNOPSIS OF HYDROCOIN PROJECT PROGRESS

FIRST WORKSHOP

The HYDROCOIN project began in May 1984. The first workshop and coordinating group meeting, hosted by SKI, was held in Stockholm, Sweden, on 22-25 October 1984. O. Hormander of SKI opened the meeting with some enlightening perspectives that captured the essence, need, and importance of HYDROCOIN. His opening remarks included some disturbing findings from the Swedish Nuclear Fuel Supply Company's report on the final storage of spent nuclear fuel: **"It is disturbing that we don't know how good our barriers are. As a result we must use conservative values. Sensitivity studies** [I assume he also meant uncertainty studies] **are crucial to the program. In the INTRACOIN effort, matrix diffusion appeared as an important phenomenon. HYDROCOIN has to cope with the difficulties of dealing with water movement in low permeability rock, which may be a difficult task for mathematical models. We must find out how to model this phenomenon and how good these models are. This is a difficult problem that can benefit from interactions between scientists and researchers around the world."**

Seven proposed Level One cases had been formulated by the HYDROCOIN project secretariat and distributed before the meeting so that project teams could review the proposals and begin preliminary simulation efforts. Each of the HYDROCOIN project teams made presentations concerning

- the codes they would be using
- pre- and postprocessing packages, which are important to the understanding of the analysis and presentation of hydrologic code results
- preliminary Level One (verification and benchmark) results
- proposed Level Two data sets, ideas on the scope and needs for HYDROCOIN Levels Two and Three, and proposals for additions and/or modification to the Level One verification and benchmark problems.

Twelve HYDROCOIN project teams each worked on at least one of the seven Level One problems before the first workshop. The BWIP team presented results for Cases 1, 2, and 4; the SRP team presented results for Cases 1 and 2.

Formulation of well-defined meaningful benchmark problems is a difficult process that is benefited when preliminary testing is done by those not originally involved with formulation. Ambiguities can be discovered and resolved early by this preliminary testing, which allows the problem definition to be improved before all project teams spend time devising their own, typically different, resolutions.

The seven Level One cases that were presented and discussed at the first workshop follow. A brief description of their status after the workshop is also given.

Case 1 -- transient flow from a borehole in a fractured permeable medium. Eight project teams including BWIP and SRP presented preliminary results that indicated the problem was well formulated. Some variations were suggested (e.g., considering flux into the matrix and fractures; additional permeability contrasts).

Case 2 -- steady-state flow in a rock mass intersected by fracture zones. Eleven project teams, including BWIP and SRP, presented preliminary results. There were some discrepancies probably related to the interpretation scheme (quadratic vs. linear) used. Some variations were suggested as desirable (e.g., considering potential plots, streamlines and travel times, flows, mass balance and/or error analysis, and parameter variations to differentiate the split between matrix and fracture dominance). The secretariat was charged with specifying streamline starting locations and mass balance measures.

Case 3 -- saturated-unsaturated flow in a layered sequence of rocks. Five project teams presented preliminary results. This problem posed difficulties for all project teams because of ambiguities concerning initial and boundary conditions and unrealistic characteristic curves for relative permeability and capillary pressure versus saturation. The NNWSI project team was charged with reformulating more realistic curves and with posing a simpler one-dimensional problem with the new characteristic curves.

Case 4 -- thermal convection in a saturated permeable medium. Three project teams, including BWIP, presented preliminary results. The problem definition was to be expanded by the secretariat to include pathlines and distributed before the next workshop.

Case 5 -- steady-state flow in a hypothetical basalt basin. No project teams presented preliminary results. This case was rejected at the first workshop and replaced by a very interesting and important variable-density problem dealing with salt plumes around a salt dome formulated by the Technical University of Berlin (TUB) project team.

Case 6 -- steady-state flow from a hypothetical bedded-salt repository. Two project teams presented preliminary results. This case was also rejected at the first workshop and replaced with an SRP-formulated benchmark problem for bedded salt. The SRP project team presented this case formally, distributed a handout, and discussed preliminary results using two different codes. It was suggested that this problem could also serve as a base problem for extension to Level Three for sensitivity and uncertainty calculations.

Case 7 -- saturated two-dimensional flow through a shallow land disposal facility in argillaceous media. One project team presented preliminary results.

Appendix B contains a brief description of the seven HYDROCOIN Level One verification (Cases 1 and 4) and benchmark (Cases 2, 3, 5, 6, and 7) problems.

Discussions and proposals for Level Two were limited, and Level Three was discussed briefly. Understanding "validation" was the central issue in the Level Two discussions. Should a validation data set and problem only test the validity of the equations we use to represent the physics and thus be limited to well-characterized systems? Or should validation data sets and problems be a test of the entire modeling process? If the latter were the case, then validation data sets should include more realistic data sets and problems where the incomplete nature of the system characterization efforts results in uncertainty in the following factors: the conceptual model, the spatial-temporal distributions of system parameters and system responses, and the uncertainty in the equations we use to describe the various phenomena and their interactions. HYDROCOIN was challenged to assess how far we can go in the quantification of validity for any real site, given the spatial and time scales of interest and the inherent uncertainty that is likely to exist in site characterization and conceptual model formulation. The PASS program team suggested that all Level Two problem formulations for HYDROCOIN be required to identify

1. the particular aspect of validation the data set and proposed problem addresses

2. the method or measure for judging when or if validation is achieved.

Additional concerns over the level of effort that might be required for some of the proposed validation problems, particularly the more realistic ones, prompted the additional requirement that

3. the proposal for a validation data set and problem include an estimate of the level of effort involved in undertaking the validation problem, as well as an outline or proposed approach to this problem consistent with obtaining the validation goals.

A. Larsson of SKI and chairman of the HYDROCOIN Coordinating Group indicated that every project team would not need to do every problem, given the level of effort and the fact that baselined codes would be used. A variety of Level Two data sets were presented for initial consideration, but only a data set on the Cornish granite heater experiment proposed by the United Kingdom was adopted as a Level Two problem.

The brief discussions dealing with Level Three involved expanding the Level Three effort to include both uncertainty and sensitivity. The regional benchmark problem (Level One, Case 6) presented by SRP was suggested for use in an expanded form as one of the sensitivity problems for the Level Three effort. This problem expansion could be used to determine the sensitivity of the results to the inclusion of repository heating and brine flow as well as parameter variations and heterogeneity. These discussions emphasized the need for the Level Three efforts to deal with the question of uncertainty and various approaches for the quantification of uncertainty as well as parameter and phenomena sensitivity.

An important feature of the earlier INTRACOIN project, promoting interchange and understanding between the experimentalists and modelers, has been continued into the HYDROCOIN project. A field trip to the Stripa mine was scheduled by SKI. Stripa has been the site of underground experiments important to nuclear waste disposal since the Swedish American Co-operative Program, which took place between 1977 and 1980. Phase I and Phase II of the current International Stripa Project are located at the site, under the auspices of the OECD/NEA. The various Stripa experiments were explained during the field trip, and the underground sites of the experimental setups were visited. This was a very informative and worthwhile experience. Most modelers, who rarely become involved with the actual experiments, benefited greatly from observing the real scale of the experiments and the rock itself.

SECOND WORKSHOP AND ADJUNCT SYMPOSIUM

Both DOE and NRC hosted the second HYDROCOIN Workshop 15-18 May 1985 and a Coordinating Group Meeting on 22 May 1985. During 20-21 May 1985 they also cosponsored an adjunct symposium titled "Symposium on Groundwater Flow and Transport Modeling for Performance Assessment of Deep Geologic Disposal of Radioactive Waste: A Critical Evaluation of the State of the Art." All three meetings were held in Albuquerque, New Mexico.

Twenty-six people from seven countries participated in the HYDROCOIN field trip to the Waste Isolation Pilot Project (WIPP) facilities (19 May 1985) organized by SNL and DOE-Carlsbad. The field trip included presentations and underground tours of the heater, thermal-mechanical, waste package, and hydrologic experiments.

Tom Nicholson of the NRC and C. R. Cole from the PASS program were the technical organizers and cochairpersons for the joint DOE/NRC technical symposium. The contributions of the symposium's two invited guests, Dr. Thomas Pigford of the University of California at Berkeley and Dr. Shlomo P. Neuman of the University of Arizona, helped ensure the success of the symposium. Proceedings of the joint symposium have now been published (PNL 1986). This document includes 26 presentations and a transcribed discussion session moderated by Dr. Neuman. Appendix C contains the table of contents for these proceedings.

Eighteen presentations on Level One results were made at the second workshop by the various HYDROCOIN project teams, including all four DOE OGR project teams. In the 6 months since the first workshop, the following actions had been taken: the NNWSI team formulated a Case 3a one-dimensional problem, which eventually became a Level Three problem; the secretariat added pathline computations to Case 4; Case 5 was reformulated by the TUB team; and the SRP team completed formulation of the Level One, Case 6 problem. These new problem formulations were distributed to the participants by the secretariat. In total, 55 Level One calculations were reported by the various project teams by the end of this second workshop and indications were that 20 additional calculational efforts were under way. All completed Level One cases had been solved by a minimum of five different project teams and codes. No further modifications of the Level One problems were made or recommended at the second workshop. Responses to the challenges of the Level One problems have been positive and have motivated changes and improvements in project codes (particularly pre- and postprocessing routines), pathline-streamline algorithms, and density-dependent flow.

Two presentations were made on preliminary Level Two results for thermal convection and conduction around the Cornish heater experiment. These two preliminary efforts indicated a need for information on the natural pressure gradient around the heater.

The following proposals for Level Two problems were made:

- a laboratory thermal convection experiment in a medium consisting of glass beads (by BWIP and PASS)

- a model calibration type of validation problem for a data set for a fractured monzonitic gneiss block at Chalk River, Canada (by the Canadian team)
- an unsaturated flow problem involving drainage for an extensive data set obtained in near-surface loams of central valley California (by NRC)
- a hot-water injection experiment that had been performed at Auburn University during 1979-1983 (by SRP and PASS, with support from Chin Fu Tsang from the University of California Berkeley Laboratory).

Additionally, the NNWSI unsaturated problem that had been prepared for Level One, Case 3a was recommended as a Level Two problem instead.

Validation again generated much Level Two discussion regarding its meaning and what can be achieved. The following paragraphs give a summary of the HYDROCOIN discussion on validation (taken from an August 1985 memo on Level Two proposals by B. Grundfelt of the HYDROCOIN secretariat).

> **Validation Aspects - Two different uses of the term "validation" as used in the HYDROCOIN context were identified, namely:**
>
> - **validation of the mathematical description of the physical processes involved in ground-water hydrology**
> - **the building of confidence that we apply models correctly in order to obtain relevant answers to the questions we raise in performance assessment.**
>
> **Both of these aspects can be included in Level Two, but they may require different type of experiments.**
>
> **In order to be able to validate a mathematical model of a physical process, the experiments must give independent data for calibration and validation. It is reasonable to believe that this criterion can be fulfilled in laboratory experiments only.**
>
> **In the field situation, the experiments generally leave too many degrees of freedom to allow validation of the mathematical model of the physical processes. Hydrological flow models are, however, applied to field**

situations. It is therefore necessary to build up confidence in the way the models are applied and in the way we interpret field data.

In conclusion we should aim at defining test cases based on:

- laboratory experiments suitable for validation of the physical models, i.e., they should offer data for calibration of the model as well as independent experimental data on predicted variables and
- field experiments for building confidence in the way data are interpreted and the models are applied.

At the end of the second coordinating group meeting, only the Cornish heater experiment and the NNWSI unsaturated flow problem were recommended for Level Two.

Discussions on Level Three resulted in the definition of Level Three objectives and an agreement on the strategy to be employed as well as the geological media to be considered. The primary objective of Level Three is to explore appropriate ways of using hydrogeological models in performance assessments, considering the uncertainties in present and future hydrogeological conditions. Secondary objectives are to 1) perform sensitivity and uncertainty analyses for realistic scenarios, 2) compare different methodologies for sensitivity and uncertainty analysis, and 3) act as a forum for exchanging ideas and information. The strategy to be employed involves specifying a reference or base case complete with a well-defined performance measure. Level Three problems also require the specification of a large number of possible sensitivity variations and the specification of ranges and/or statistical descriptions for parameter values. Methodologies for sensitivity and uncertainty would not necessarily be specified, which would allow different approaches to be taken and later compared by the various project teams. An attempt will be made to define Level Three problems for 1) near-surface disposal of intermediate and low-level waste in argillaceous media, 2) disposal of high-level waste in fractured crystalline rock, 3) disposal of high-level waste in bedded salt (extension of SRP's Level One, Case 6 problem), and 4) disposal of high-level waste in an unsaturated zone (e.g., disposal in tuff being studied by NNWSI).

THIRD WORKSHOP

The third semiannual workshop and coordinating group meeting hosted by OECD/NEA was held 18-21 November 1985 at the OECD headquarters in Paris, France. The objectives of this workshop were to review and discuss

- any additional Level One (verification-benchmarking) results
- preliminary Level Two (validation) results and additional Level Two problem proposals
- problems proposed for Level Three (sensitivity and uncertainty)
- the draft Level One report and initial compilation of Level One result comparisons compiled by the secretariat
- the tentative agenda for completing the Level One report as well as the time schedules for the Level Two and Level Three efforts.

SKI additionally reported on the status of discussions and negotiations related to their proposed new INTRAVAL project. INTRAVAL is an international cooperative effort for evaluating the validity of different mathematical models aimed at describing the transport of radionuclides in the geosphere.

The field trip to Limoges, France, was hosted by P. Raimbault of Commissariat a l'Energie Atomique/Institut de Protection et de Sureté Nucléaire (CEA/IPSN). Presentations were made by CEA-IPSN staff on both completed and planned experiments in the granite rock of the region. We visited the site of the heater experiments and the uranium mine where hydrology studies are being performed. Hydrologic and thermal-mechanical experiments at these sites are aimed at developing the understanding and methodology (including the instruments) for measuring various properties in low-permeability media. These experiments help determine how measurements at the small scale can be made, interpreted, and extrapolated to the larger scale. CEA/IPSN would like to achieve these objectives for both natural and disturbed environments.

Thirteen Level One presentations were made at the workshop including one by A. B. Gureghian for CRP. Generally, the same three difficulties recurred:

1. Case 5 appears to be one of the most difficult Level One problems to solve.
   - Controversy at this meeting centered on the validity of the convection rolls indicated by some of the project team results and by some preliminary results by C. Voss of the United States Geological Survey (USGS). A meeting was organized by TUB (and attended by S. K. Gupta of the SRP) to address the issues surrounding Case 5 and to develop logical extensions to Levels Two and Level Three to resolve the important issues posed by Case 5. Case 5 has initiated an additional controversy regarding the appropriateness of the equations used by most codes to describe variable-density flow involving dense brines. This issue was raised in studies undertaken by Rijksinstituut voor Volksgezondheid en Milieuhygiene (RIVM) as a result of the difficulties various teams were having with Case 5. New mass-averaged equations for use with Case 5 were presented by RIVM. These equations, soon to be published in Water Resources Research, are currently being tested by RIVM through a set of laboratory experiments.
2. Prediction of pathlines (Case 4) and streamlines (Case 2) was again a consistent source of deviation in Level One results. Auxiliary codes used to calculate path- and streamlines and to estimate travel times (particle trackers) prove more successful with the path- and streamline trace prediction than with the travel-time estimation.
3. Boundary conditions have continued to be a source of difficulty just as they were in the earlier INTRACOIN efforts. Boundary conditions for Cases 3, 6, and 7 continued to pose a consistent Level One difficulty and a new boundary condition difficulty arose concerning Case 6 at this workshop. The Swiss project team reported a problem with a section of the infiltration boundary condition for Case 6 near to and

east of the north-south running river. In this section, the specified infiltration rate exceeds the infiltration capacity of the media. The participating teams concluded that if finer grids had been used by the linear interpolation computer codes, the same Case 6 boundary condition problems would have been discovered. The Swiss code uses quadratic elements, which results in a nonlinear allocation of total infiltration among the nodes that in turn enhanced the ability of the Swiss to detect the error in the infiltration boundary condition of Case 6.

The secretariat presented the plots showing the currently compiled results for the seven Level One problems and the first draft of parts of the Level One report. An improved summary of the Level One results and problem status was prepared from the subsequent discussion and is included here:

Case 1 -- All results for the base case looked good. It was agreed that the optional permeability and flux calculations should be included in the report on Level One.

Case 2 -- Results for the potentials were good; however, the streamlines and travel times showed deviations. There seemed to be convergence as finer grids were used. The Swiss suggested that the values at nodal points between at least one pair of codes using the same grid be compared directly. The inter-node interpolation problem associated with postprocessor codes would thus be illustrated.

Case 3 -- This case has had very small participation, and no new comments were made.

Case 4 -- Good agreement on the scalars (i.e., temperature, pressure, and density) was achieved, but the common difficulties discussed above existed in the pathlines.

Case 5 -- This case proved to be the most difficult. The various differences in results were discussed above. The secretariat suggested that the project teams that undertook this problem give their opinions to the secretariat for inclusion in the Level One report. C. Voss of the USGS will be given the results calculated by the participants.

Case 6 -- Results were generally good except for the small section of infiltration boundary, noted by the Swiss, that was not realistically specified. Work will continue on this boundary-condition difficulty because this case will be extended to Level Three.

Case 7 -- This case as well as the results were generally good, with the exception of the boundary-condition difficulty discussed earlier. Work will continue because this case will also be extended into Level Three.

The secretariat made an initial comparison of results. A more consistent use of symbols on the comparison plots was suggested so that, as much as possible, each code has a consistent symbol. It was also suggested that the importance of proper boundary-condition specifications be specifically addressed, since it was also a problem in the INTRACOIN effort.

Two presentations of preliminary Level Two results on the NNWSI unsaturated problem proposed at the second workshop were made by the team from Japan and the United Kingdom. The results looked good; however, because actual field data might not be available (there was no NNWSI participation at the workshop), we agreed to make this a Level Three problem.

Some new measurements were made available on Level Two, Case 1 (the Cornish granite heater experiment). The original conceptual model for the heater experiment, which attributed the consistently higher temperatures near the top of the heater to convection-cell formation, had been challenged. The challenger had hypothesized that this temperature distribution could also be the result of forced convection because there were no data to refute this hypothesis. Results of potential measurements in borehole C at the site support, at least in principle, this alternate conceptual model. Therefore, the possible conceptual models are 1) a thermal-convection cell, 2) generally upward flow toward the quarry and forced convection, or 3) some combination of these.

During a session chaired by S. K. Gupta of SRP, five new Level Two problems were presented and the meaning of validation was discussed. In selecting appropriate Level Two problems, the secretariat reminded us that Level Two constraints are different than Level One constraints because Level Two

- involves more work per case
- requires different kinds and mixes of expertise
- does not require that every group treat every case
- requires pilot groups for each case.

Each of the five Level Two problems suggested for continued consideration was assigned to a pilot group to further formulate the problem descriptions. Table 1 categorizes the estimated months of effort, number of groups interested in participating, length and time scale addressed, validation aspect addressed, and the type of model required. Each pilot group was asked to formulate a statement explaining what was going to be achieved by the validation exercise and identifying a means or measure for judging the success of the exercise.

During the strategy session, animated Level Two discussions focused on the meaning of validation and what can be accomplished with the HYDROCOIN Level Two cases. There were detailed comparisons of the proposed Level Two cases, and the final selections and rejections of cases were made after the realistic ambitions and the attributes of each were discussed. The concerns regarding validation led to a further discussion of whether one validates codes or models. The group supported K. Andersson's plea to use the International Atomic Energy Agency (IAEA) definition of validation, which in the waste management context is as follows:

> **A conceptual model and the computer code derived from it are "validated" when it is confirmed that the conceptual model and the derived computer code provide a good representation of the actual processes occurring in the real system. Validation is thus carried out by comparison of calculations with observations and experimental measurements.**

P. Goblet, Ecole des Mines (EdM-France), added the following important comment about validation:

TABLE 1. Status of Recommendations Concerning Proposed HYDROCOIN Level Two Cases at the Close of the Third Workshop

Title, Brief Description, and Status of the Problem Formulation	Pilot Group[a,b]	Estimated Man Months of Effort	Interested Groups[c]	Length and Time Scales	Validation Aspect	Model Type[d]
CASE 1 CORNWALL - Heater experiment in near-surface fractured granite. Initial problem formulation complete.	AERE-Harwell	2-4	RIT,AERE, NAGRA, JAERI,CRP	10s of m, years	Thermal convection	Flow transport (2-D)
CASE 2 "ELDER" - Thermal convection problem (laboratory scale). Initial formulation sent out as alternate Level One, Case 1. Rayleigh numbers 50-200, may be important to salt dissolution.	TUB	1	TUB,RIVM, SRP, PASS	1 m, days	Thermal convection cell (analogy to salt)	Flow transport density (2-D)
CASE 3 CHALK RIVER - Gneiss block surrounded by fracture zones(Canadian data set of Ken Raven). Initial formulation to be distributed mid-Jan 1986.	KEMAKTA	3-12	CEA-IPSN,SKB, NAGRA,CRP, SNL-NRC JAERI,AERE	100-200 m, steady state, and days	Real world interpretation and characterization + porous media-fractured	Flow (2 and 3-D)
CASE 4 PICEANCE BASIN - Regional groundwater 3-D flow in low permeability anisotropic rock of Colorado. Problem formulated. Additional USGS file reports and maps to be supplied by NRC to interested parties.	SNL-NRC	2-4	SNL-NRC, NRC-staff, SRP,CEA-IPSN, RIVM,SKB, NAGRA	100 km, steady state	Regional modeling - low permeability rock. (model calibration)	Flow (3-D)
CASE 5 CENTRAL VALLEY - Unsaturated zone, layered, agricultural drainage problem. Problem formulation complete.	NRC-staff	1-2	NRC-staff, AERE	2 m, days-months	Drainage with real field data sufficient for calibration-validation	Unsaturated flow (1-D)

(a) Each pilot group will formulate what will be achieved relative to validation and how the success of the effort should be judged.

(b) Pilot groups: AERE = Atomic Energy Research Establishment, Harwell United Kingdom; TUB = Technical University of Berlin, Berlin, Federal Republic of Germany; KEMAKTA = KEMAKTA Consultants Co., Stockholm, Sweden; SNL= Sandia National Laboratories, Albuquerque, New Mexico, USA; NRC = U.S. Nuclear Regulatory Commission, Washington D.C., USA.

(c) Interested groups: RIT = Royal Institute of Technology, Stockholm, Sweden; NAGRA = Nationale Genossenschaft fur die Lagerung Ratioaktiver Abfalle, Baden, Switzerland; JAERI = Japan Atomic Energy Research Institute, Japan; CRP = Crystalline Rock Project, Chicago, Illinois, USA; RIVM = Rijksinstituut voor Volksgezondheid en Milieuhygiene, Netherlands; SRP = Salt Repository Project, Columbus, Ohio, USA; PASS = Performance Assessment Scientific Support Program, Richland, Washington, USA; CEA-IPSN = Commissariat a l'Energie Atomique/Institut de Protection et de Surete Nucleaire, Fontenay-aux-Roses, France; SKB = Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden; also (b) above. Current participation may be different from noted here.

(d) 1-D, 2-D, 3-D = one-, two-, and three-dimensional, respectively.

We know that our hydrologic flow models are correct for porous media for reasonable time periods for systems with water. We have years of experience. What the question is: is the applicability of our characterization methods, ability to interpret, understand and model in low permeability deep hydrologic systems.

A summary of the workshop participants' recommendations on Level Two problems is contained in Table 1. The group moved the proposed NNWSI unsaturated problem to Level Three and rejected the proposed Auburn heater experiment, because it had already been successfully worked on by several groups and because the presentation by NRC indicated that it would probably end with no definitive judgment on validation.

The final workshop session on Level Three proposals was chaired by C. R. Cole of the PASS program. The session began with an examination of the original objectives for HYDROCOIN Level Three and a discussion of additional Level Three constraints, which include the following:

- Level Three is not another verification exercise, so that every group does not need to run every problem.
- Participants have limited resources (i.e., time, staff, money), which means that if the Level Three problems are logical extensions of Level One or Level Two problems, they can be started "on the run" by those who previously participated in a Level One or Level Two problem.
- HYDROCOIN ends in 1987.
- The effort is solely a ground-water modeling exercise, which limits the performance measure to a hydrological one rather than a performance measure in terms of consequence, even though a consequence performance measure would be more useful in determining parameter importance from a sensitivity analysis point of view.
- Computer hardware capabilities could be a significant limitation when performing sensitivity and uncertainty analyses because of the large number of runs required.

The following is a brief description of the proposals for Level Three:

Case 1 -- sensitivity analysis extension of the Level One, Case 7 problem on near-surface disposal in argillaceous media. The aim of the effort is to compare different approaches to sensitivity analysis by studying this disposal system to determine the most important hydrogeologic parameters and other attributes for this waste disposal design. Performance measures, in the form of travel time and volumetric flow rate through the disposal area, were suggested. Uncertainties in site characterization (e.g., inhomogeneities, faults, boundaries) and even time-dependent uncertainties (e.g., climate, erosion) are proposed for study.

Case 2 -- the NNWSI deep, layered, unsaturated flow problem that was elevated from Level Two to Level Three in the previous session.

Case 3 -- a logical extension to the Level One, Case 6 problem. It is a sensitivity study to determine the importance of heterogeneities of various scales; the effect of including brine density driving forces; and the effects of thermal heating, grid, and the coupling between regional and local modeling scales. This case had been proposed and reviewed at the second HYDROCOIN workshop by S.K. Gupta of the SRP.

Case 4 -- a logical extension of the difficult Level One, Case 5 problem involving brine density effects. This case was not discussed in detail.

Case 5 -- a logical extension to the Level Two, Case 3 problem involving the Chalk River gneiss block or some similar fracture flow problem possibly from Sweden. This case was not discussed in detail.

Case 6 -- an extension of the Level Two, Case 4 problem involving the regional modeling of the Piceance Basin in Colorado. For this case, the ranges in parameters in conjunction with a calibrated Level Two model will be used in sensitivity and uncertainty analyses.

Case 7 -- a sensitivity study to determine the sources of error in particle tracking and to determine the sensitivity of flow path and travel time accuracy tracking parameters. It is designed to address some of the issues regarding auxiliary code problems related to particle tracking.

Table 2 contains a description of the status of Level Three formulations, responsible pilot groups, and schedule.

The HYDROCOIN effort has been running slightly ahead of schedule, and interest has been excellent. The overall time schedule for the HYDROCOIN effort as adopted at the third workshop is as follows:

	Level One	
Compiled results	-	November 1985
Draft report	-	May 1986
Final draft	-	September 1986
Published report	-	November 1986
	Level Two	
Decisions on remaining cases	-	November 1985
Case definitions	-	January 1986
Calculational attempts	-	May 1986
Results	-	November 1986
Draft report	-	May 1987
Final report	-	September 1987
Published report	-	November 1987
	Level Three	
Decision on structure	-	November 1985
Case definitions complete	-	May 1986
Early results	-	November 1986
Final results	-	May 1987
Draft report	-	November 1987
Final report	-	January 1988
Published report	-	March 1988

TABLE 2. Summary of HYDROCOIN Level Three Problems

Title, Brief Description, and Status of the Problem Formulation	Pilot Group[a]	Interested Groups[b]	Length and Time Scales
CASE 1 Extension of Level One, Case 7. Problem formulated and distributed.	AERE-Harwell	AERE,ATKINS, BGS,TUB, CEA-IPSN,NRC, JAERI,SRP	25 m by 300 m, steady state, and transient
CASE 2 NNWSI layered, deep unsaturated flow. Problem partially formulated and distributed.	NNWSI	NNWSI,NRC, BGS,AERE, JAERI	600 m, steady state, and transient
CASE 3 Extension of Level One, Case 6. Problem to be formulated.	SRP	SRP,NAGRA, CEA-IPSN, RIVM,JAERI, TUB	regional-local, steady state, and transient
CASE 4 Extension of Level One, Case 5. Problem to be formulated.	TUB	TUB,CEA-IPSN, SNL-NRC, SRP,CRP	900 m by 300 m, steady state, and transient
CASE 5 Crystalline Rock - either an extension to Level Two, Case 3 (Chalk River gneiss block) or a Swedish data set or both. Problem to be formulated.	KEMAKTA	KEMAKTA,CRP, SKB,AECL, NAGRA, CEA-IPSN	100 - 200 m, steady state, and transient
CASE 6 Extension to Level Two, Case 4 (Piceance regional modeling). Problem formulated and distributed.	SNL-NRC	SNL-NRC, RIVM,SRP, ATKINS,TUB	regional (100 km), steady state
CASE 7 Particle tracking sensitivity study. Initial formulation complete and distributed (additional aspects being formulated).	SNL-NRC	SNL-NRC, CRP,SRP, NAGRA,JAERI, BGS,RIVM,EdM, SKB,ATKINS	various scales, steady state

(a) Pilot groups: AERE = Atomic Energy Research Establishment, Harwell, United Kingdom; NNWSI = Nevada Nuclear Waste Storage Investigation project, Las Vegas, Nevada, USA; SRP = Salt Repository Project, Columbus, Ohio, USA; TUB = Technical University of Berlin, Berlin, Federal Republic of Germany; KEMAKTA = KEMAKTA Consultants Co., Stockholm, Sweden; SNL= Sandia National Laboratories, Albuquerque, New Mexico, USA; NRC = Nuclear Regulatory Commission, Washington, D.C., USA.

(b) Interested groups: ATKINS = Atkins Research and Development, Epsom, Surrey, United Kingdom; BGS = British Geological Survey, Nottingham, United Kingdom; CEA-IPSN = Commissariat a l'Energie Atomique/Institut de Protection et de Surete Nucleaire, Fontenay-aux-Roses, France; JAERI = Japan Atomic Energy Research Institute, Tokai, Japan; NAGRA = Nationale Genossenschaft fur die Lagerung Ratioaktiver Abfalle, Baden, Switzerland; RIVM = Rijksinstituut voor Volksgezondheid en Milieuhygiene, Netherlands; CRP = Crystalline Rock Project, Chicago, Illinois, USA; SKB = Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden; AECL = Atomic Energy of Canada Ltd. Manitoba, Canada; EdM = Ecole Nationale Superieure des Mines de Paris, Fontainebleau, France; also (a) above. Current participation may be different from noted here.

HYDROCOIN participants agreed on the need to inform the scientific and radioactive waste management communities as well as the general public about the HYDROCOIN and INTRACOIN efforts. Various participating groups are investigating ways to achieve this goal. SKI indicated that they will host a HYDROCOIN symposium in late 1987. T. Nicholson (NRC) and C. R. Cole (PASS) will announce the availability of the Albuquerque symposium proceedings and provide background information on INTRACOIN and HYDROCOIN in EOS, Transactions, American Geophysical Union. Each participant indicated that they will publish their project team reports.

BRIEF DESCRIPTION AND INTERCOMPARISON OF OCRWM PROJECT RESULTS FOR LEVEL ONE

The OCRWM project team results for all seven HYDROCOIN Level One cases are discussed and compared in this section to illustrate the value and benefit of participation in this code verification and benchmarking effort. Complete and detailed descriptions of Level One calculations are being prepared by the OCRWM project teams. A complete report on Level One efforts and intercomparison of results from all participating HYDROCOIN project teams is being prepared by the HYDROCOIN secretariat. Consequently, detailed problem descriptions and comprehensive intercomparison of results are not presented here. The reader should refer to Appendix B for a brief description of each case and the diagrams that illustrate geometry and boundary conditions.

Level One problems consist of a set of base case calculations and may include optional additional calculations. For each case we will 1) discuss the type of problem (verification or benchmarking), 2) indicate the OCRWM project teams that participated, their level of participation in any optional calculations, and the codes they used, 3) present a limited yet illustrative intercomparison of the base case and optional results calculated by OCRWM participants, and 4) briefly discuss differences between results, what was learned as a result of participation, and the value of the effort.

CASE 1: TRANSIENT FLOW FROM A BOREHOLE IN A FRACTURED PERMEABLE MEDIUM

The analytical solution for this verification problem allows prediction of piezometric head in both the fracture and matrix as a function of time and space. Optional calculations are provided by an additional analytical solution that predicts the time-dependent flow rates from the borehole into both the fracture and the matrix. The problem domain is a finite cylinder, 5.1 meters high with a radius of 10 meters.

BWIP, CRP, and SRP participated in the base case, which consisted of predicting piezometric head relative to the steady-state head in the borehole as a function of time and space. CRP and SRP also performed the optional flux calculations, and SRP performed the additional calculation in which the fracture transmissivity was a factor of 10 higher. BWIP participated with their

MAGNUM-2D two-dimensional finite element code (England et al. 1985); CRP used the STOKES two-dimensional and three-dimensional (i.e., axis-symmetric case) finite element code (code documentation is in progress); and SRP used the CFEST three-dimensional finite element code (Gupta et al. 1982).

The comparison between BWIP, CRP, and SRP base case results is shown in Figures 1 and 2. Figure 1 is a plot of predicted relative hydraulic head versus time at a radius of 5 meters and a depth of 5 meters, and Figure 2 illustrates predictions for relative head versus radial distance from the center of the borehole at a depth of 4 meters 100 seconds after initiation of pumping. As evidenced by the figures, the results from the three codes are in very good agreement. These results and those from the analytical solution (not plotted) also agreed very well.

Grid design emerged as an important lesson from HYDROCOIN. Solution accuracy, particularly for vector quantities, was directly related to adequate spatial discretization. A typical grid design for Case 1 is illustrated in Figure 3.

CRP results for the optional time-dependent flow calculations are shown in Figure 4. This figure shows a comparison of results for flow from the borehole into the rock matrix as a function of time calculated by two different numerical methods and for two different analytical solution methods. SRP results for these optional calculations are similar to the results CRP obtained with numerical method 2. The comparison between analytical results and SRP numerical results for time-dependent flow from the borehole into the fracture for the high fracture transmissivity case (i.e., $Tf=10^{-7}$ m^2/sec instead of 10^{-8} m^2/sec) are illustrated in Figure 5.

Results for Case 1 agreed closely with the analytical solution and with each other for both the base and optional cases. In general this problem, which was designed to test numerical codes, proved easier to solve than had been expected. The total value of the efforts on Case 1 and all that was learned is not evident from the short description presented here and the limited comparison between three OCRWM finite element codes. The full HYDROCOIN code comparison will discuss any apparent advantages of finite element methods over finite difference methods and the capability of one-dimensional fracture

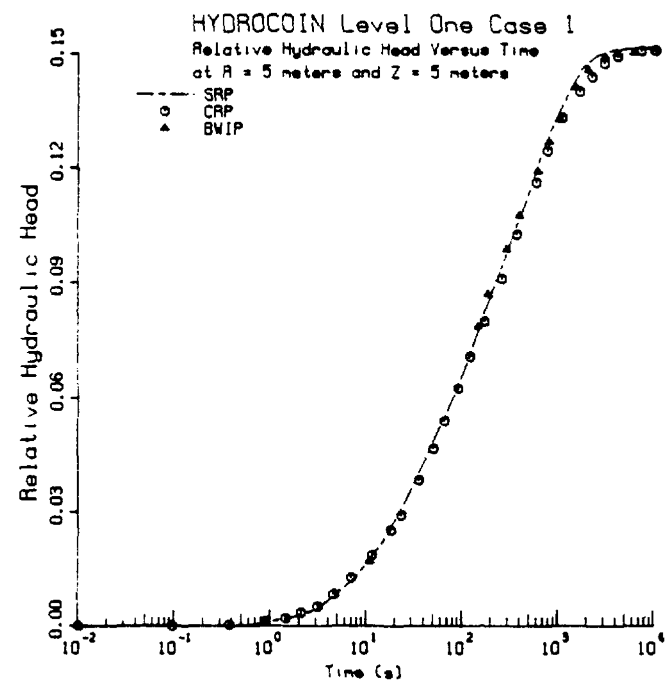


FIGURE 1. A Comparison of BWIP, CRP, and SRP Results for Relative Head as a Function of Time at the Interface Between the Rock Matrix and Fracture

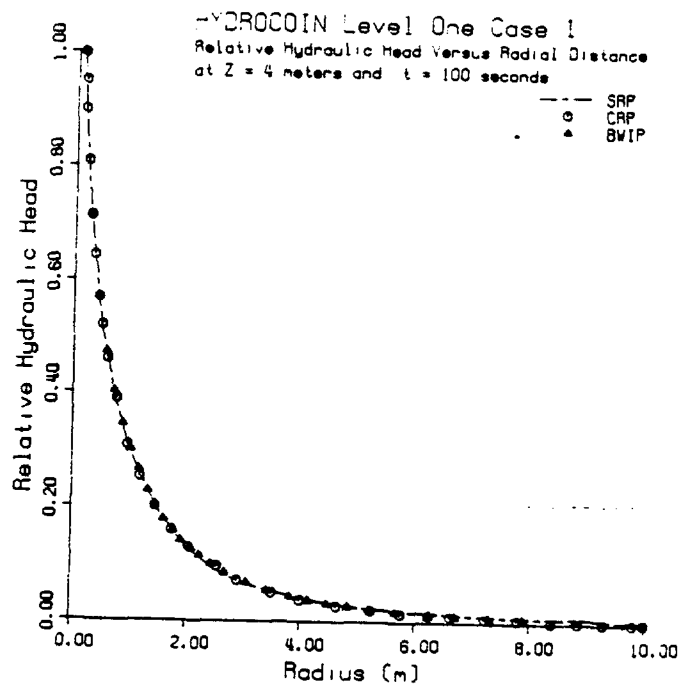


FIGURE 2. A Comparison of BWIP, CRP, and SRP Results for Relative Head in the Rock Matrix as a Function of Radial Distance from the Borehole

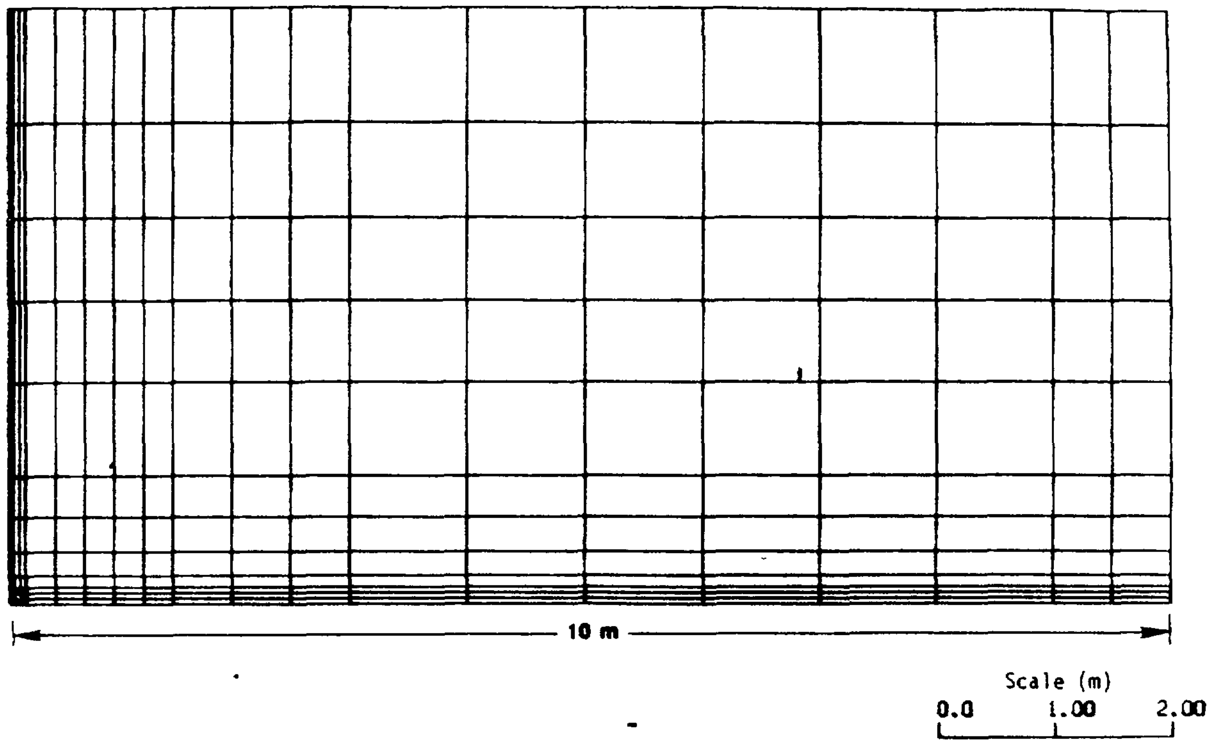


FIGURE 3. A Typical Case 1 Finite Element Grid Mesh. This figure was taken from an SRP presentation at the second HYDROCOIN workshop.

elements. The full HYDROCOIN report and the more detailed project team reports of all the participants will document more completely all that was learned. Experience gained with various grid designs and time discretization schemes will prove valuable in future performance-assessment efforts. The fine grid near the borehole and fracture-matrix interface, as shown in Figure 3, proved necessary to match the borehole inflow rates shown in Figures 4 and 5 and to match the steady-state head at the long times (104 seconds) shown in Figure 1.

A preliminary analysis of other HYDROCOIN project team results, reported at the fourth HYDROCOIN workshop, indicates that finite element and finite difference codes performed equally well on this problem. Additionally EdM used a mixed one- and two-dimensional element approach on this problem; one-dimensional elements were used for the fracture. They obtained equivalent results for reduced costs.

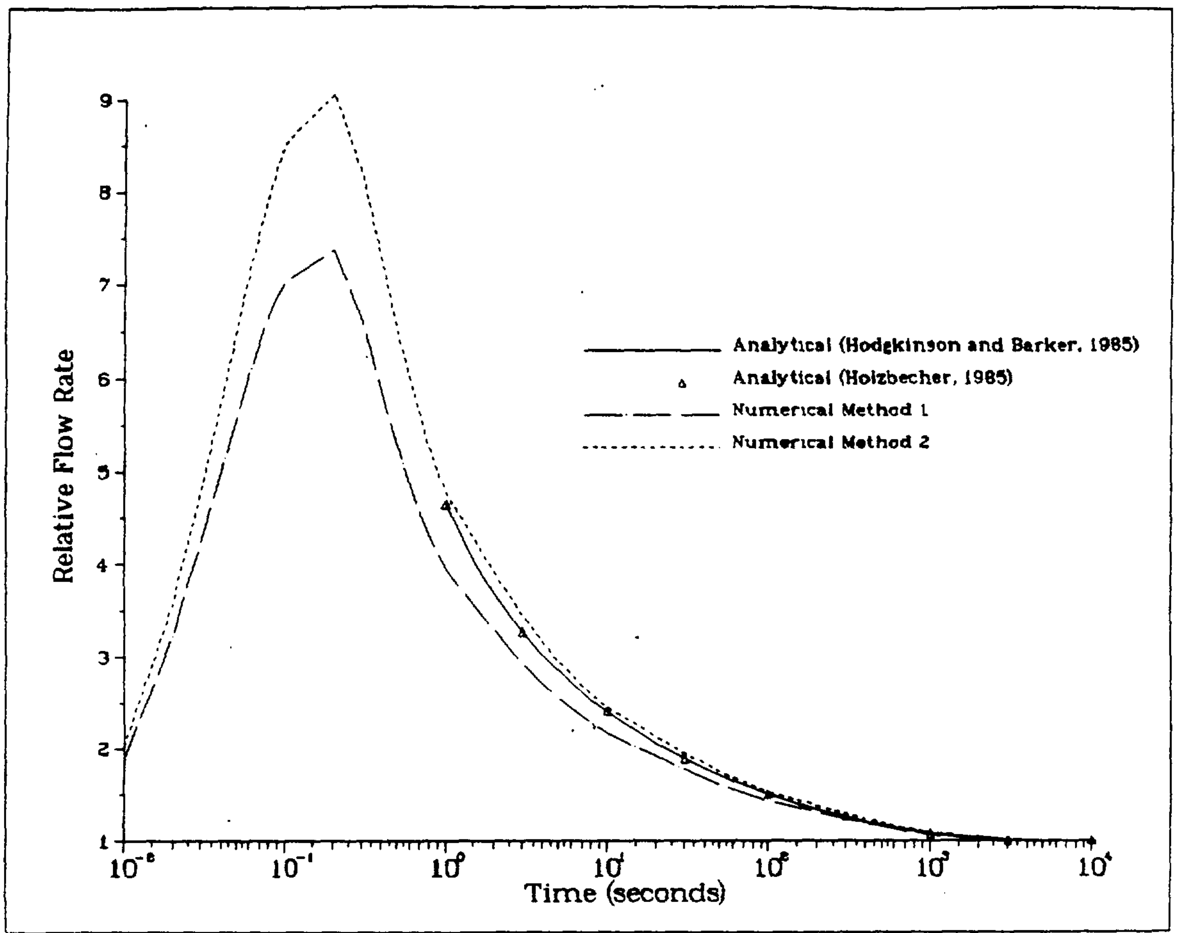


FIGURE 4. CRP Results for Time-Dependent Relative Flow Rate from the Borehole into the Rock Matrix as a Function of Time. This graph was taken from a CRP presentation at the third HYDROCOIN workshop. Results for two different numerical methods and two different analytical solution methods are shown.

CASE 2: STEADY-STATE FLOW IN A ROCK MASS INTERSECTED BY PERMEABLE FRACTURE ZONES

This two-dimensional (x-z), regional scale, steady-state, fracture zone flow, benchmark problem was designed to test the ability of codes to treat high permeability contrasts for a complicated geometry. Being a benchmark problem, no analytical solution exists and solution correctness was tested by tracking solution convergence as a function of spatial discretization as well as code intercomparison. Coarse, medium, and fine mesh solutions were calculated and

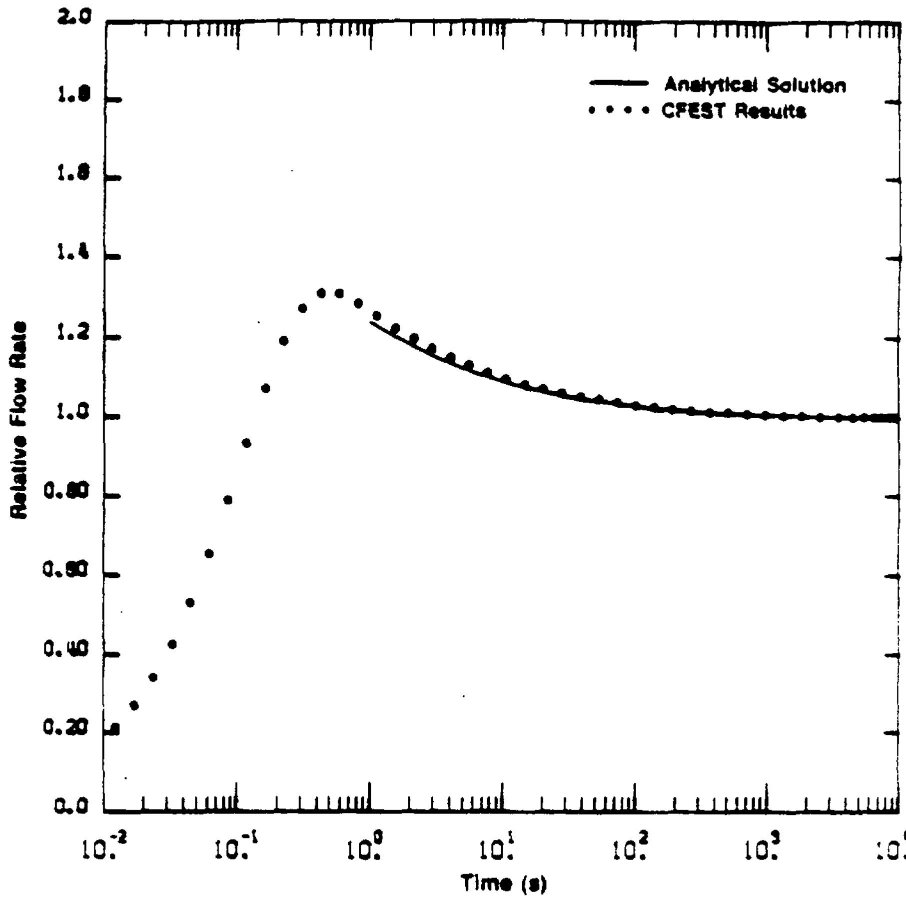


FIGURE 5. SRP Results for Time-Dependent Relative Flow Rate from the Borehole into the Fracture as a Function of Time for the High Transmissivity Optional Calculations. This graph was taken from an SRP presentation at the second HYDROCOIN workshop.

the convergence of potentials as a function of x-location at depths of z = 0 m, -200 m, -400 m, -600 m, and -800 m were compared to indicate solution convergence as a function of spatial discretization. Additionally, since it is recognized that pathlines and travel time predictions are a better measure of system performance, the starting location for four pathlines was identified. Comparisons of both trajectory and travel time were made as a function of spatial discretization. There were no optional additional calculations.

BWIP, CRP, NNWSI, and SRP participated. BWIP used their MAGNUM-2D code; CRP used the STOKES code to solve for potentials and their particle tracking code, PARTICLE, to predict streamlines (code documentation is in progress);

NNWSI used the two-dimensional, partially or fully saturated, finite element code, SAGUARO (Eaton et al. 1983); SRP again exercised the CFEST code.

A comparison plot of BWIP-, CRP-, NNWSI-, and SRP-calculated potentials at an elevation of -800 m as a function of x-location is shown in Figure 6. Because this depth proved to be the most sensitive to spatial discretization, which is appropriate given that it is the greatest distance from the specified potential boundaries, no other comparison plot of potentials will be illustrated. The full suite of comparisons will be left for the HYDROCOIN report. A typical experience with solution convergence for quadratic elements as a function of spatial discretization is illustrated by the results shown in Figure 7. Typical fine-grid potential contours for this case are illustrated in Figure 8. A comparison of CRP-, NNWSI-, and SRP-calculated streamline trajectories for the finest grids is shown in Figure 9. BWIP did not calculate streamlines because participation was limited to the first and second workshops.

The CRP presentation at the third HYDROCOIN workshop indicated that CRP did an extensive analysis of the differences between the use of linear versus quadratic elements; in the STOKES code these are user-selected options. For comparison purposes, CRP's experience with solution convergence for linear elements as a function of spatial discretization is illustrated by the results shown in Figure 10. A comparison with Figure 7, which shows convergence for the same element grids for quadratic elements, illustrates the higher accuracy of these elements. The question of using linear versus quadratic elements surfaced throughout the HYDROCOIN exercise; it was generally felt that quadratic elements offered some advantages. All of the comparisons have been based on solution accuracy versus number of elements, although the more meaningful comparison numbers would be in terms of solution accuracy as a function of number of nodes and work per node.

The finest finite element grid used by CRP (Figure 11) illustrates another recurrent HYDROCOIN boundary-condition problem. Solution singularities occur at the juncture between Dirichlet and no-flow boundaries in the upper right and upper left corners of Figure 11. These can be handled by using a narrow element along the no-flow boundary and specifying the same Dirichlet boundary

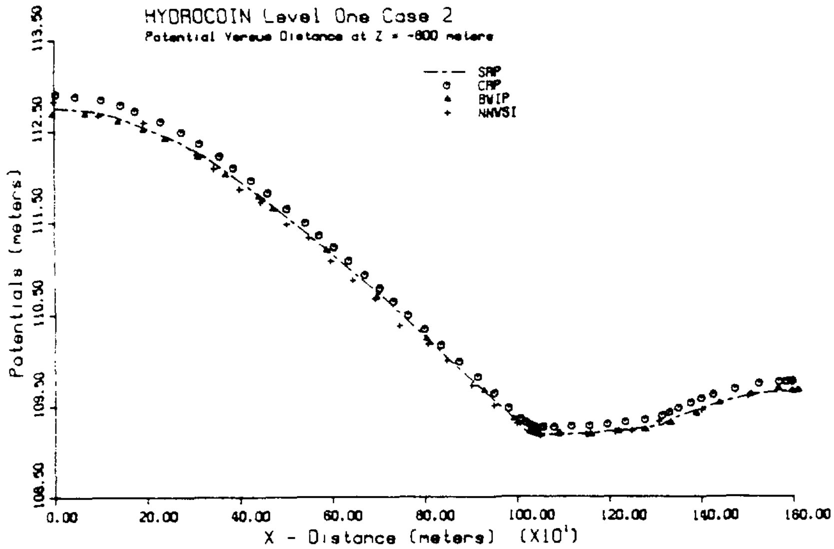


FIGURE 6. Comparison of BWIP, CRP (quadratic interpolation), NNWSI, and SRP Calculated Potentials Versus x-Location at a Elevation of -800 m for Their Finest Grids

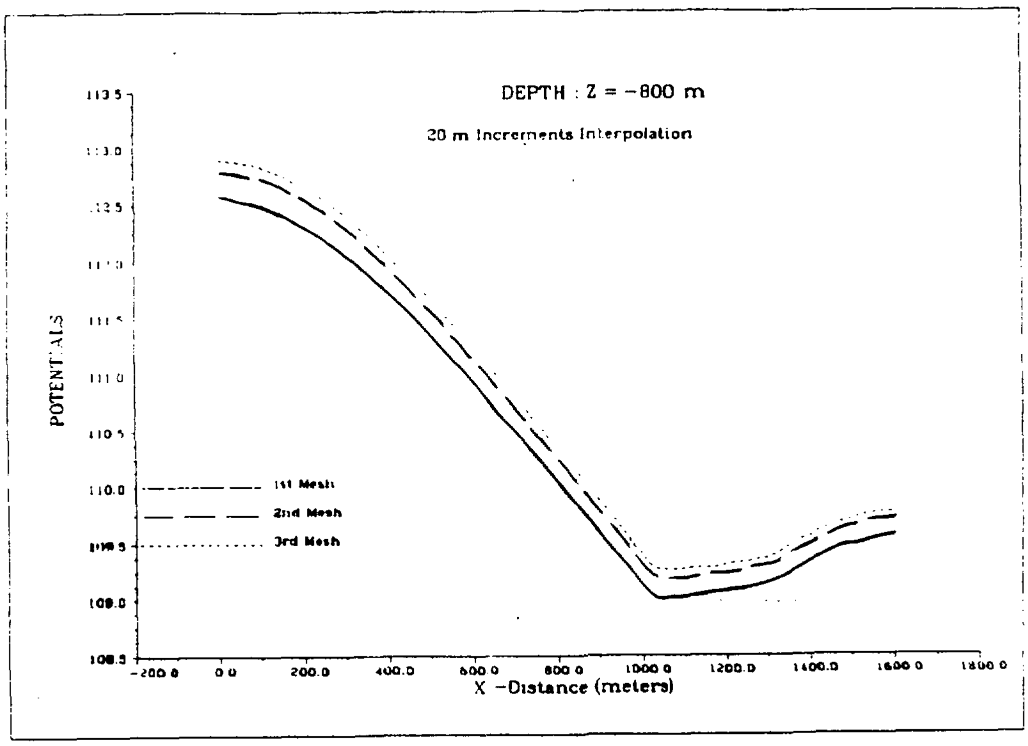
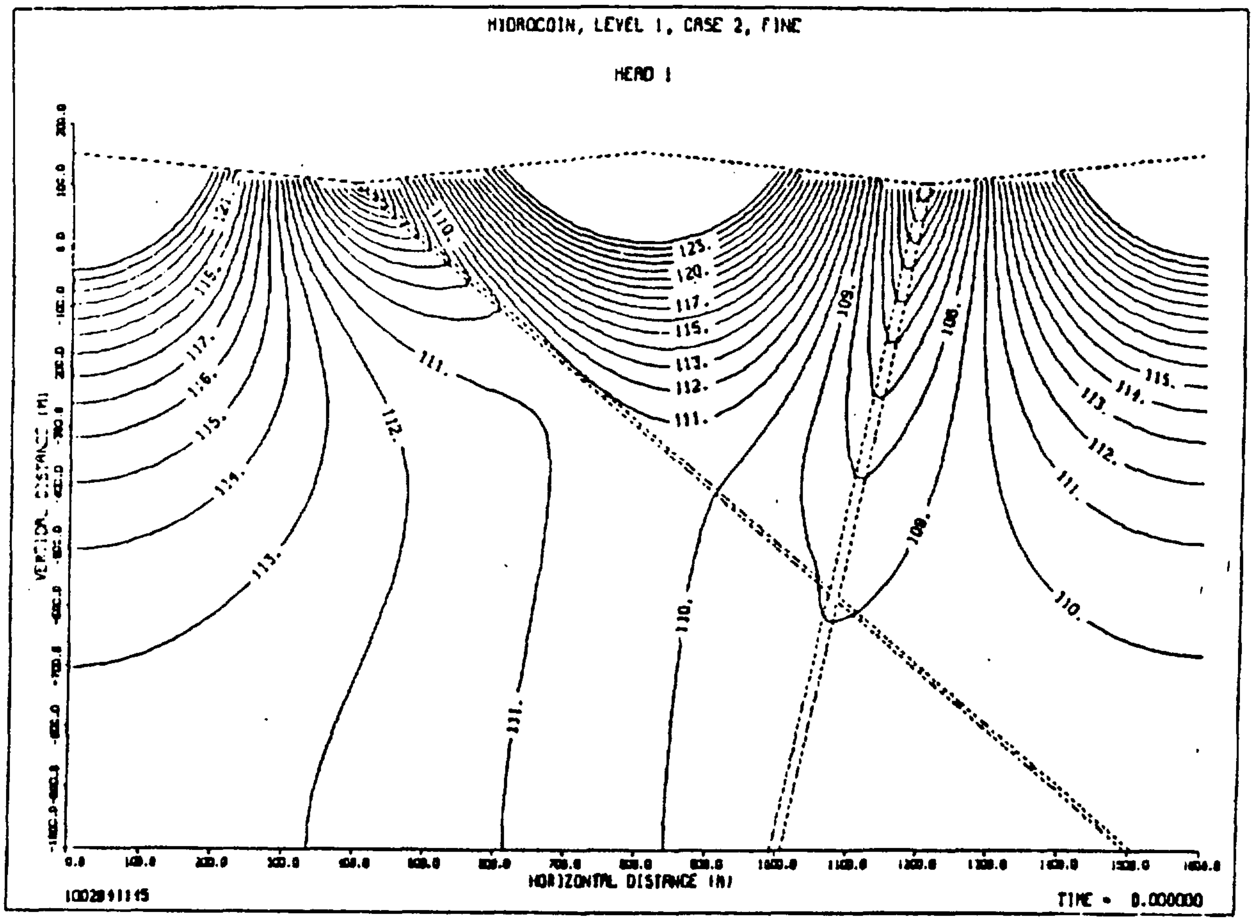


FIGURE 7. CRP Results (presented at the third HYDROCOIN workshop) Illustrating Solution Convergence as a Function of Increased Spatial Resolution. This is a plot of calculated potential versus x-location at an elevation of -800 m for three different grid meshes and quadratic interpolation.



STEADY STATE HYDRAULIC HEAD FIELD, FINE FINITE ELEMENT MESH

FIGURE 8. Fine-Grid Potential Contours Calculated by BWIP. This plot was taken from a BWIP presentation at the first HYDROCOIN workshop.

condition, thus causing flow in this corner element to be parallel to the no-flow boundary. The introduction of narrow elements along a no-flow boundary as illustrated in Figure 11 allows for flow field curvature and thus a better approximation of a no-flow boundary. I believe the CRP solution presented in Figure 6 to be better than the others as a result of the use of this discretization strategy. The importance of implementation details like this one is often overlooked even though model results can be significantly affected. Discussions regarding the effects of discretization strategy suggest that sharing of modeling techniques (the "tricks of the trade") is one of the positive aspects of the HYDROCOIN and previous INTRACOIN efforts.

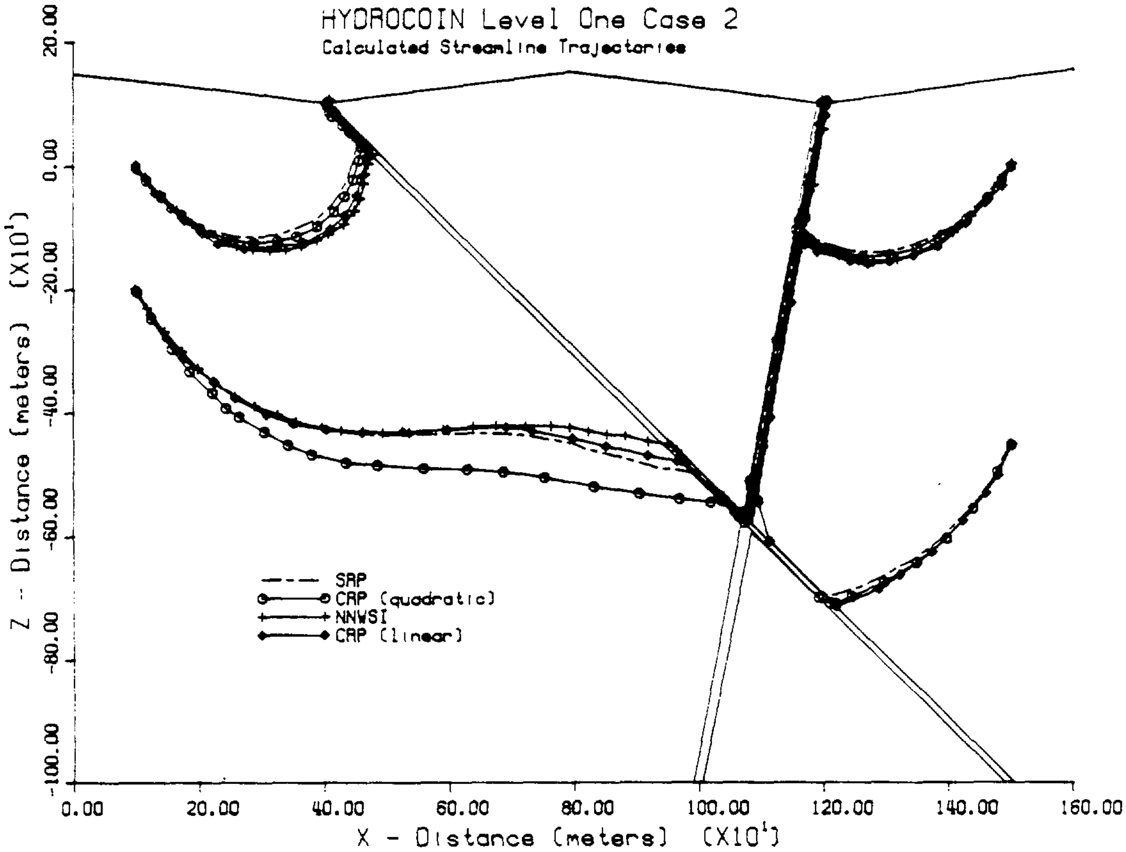


FIGURE 9. Comparison of Streamline Trajectories for the Finest Grids Calculated by CRP (using two different interpolation schemes), NNWSI, and SRP

The complicated geometry and high permeability contrasts of this problem caused difficulties for many of the auxiliary codes used to calculate pathlines and travel times. As a result of these difficulties, SRP and CRP improved their codes. These difficulties, as well as others that surfaced in Case 4 and Case 7, resulted in the Level Three problem on pathline-travel times. Case 2, like other Level One problems that included pathline-travel time calculations, illustrated that comparison of single pathline-travel time calculations is not a meaningful way to compare predictions. It would be more appropriate to identify a region of interest from which multiple pathlines (equally spaced in the flow field) and their associated travel times are calculated. This distribution of pathlines and travel times would then be compared statistically as a part of the code intercomparison.

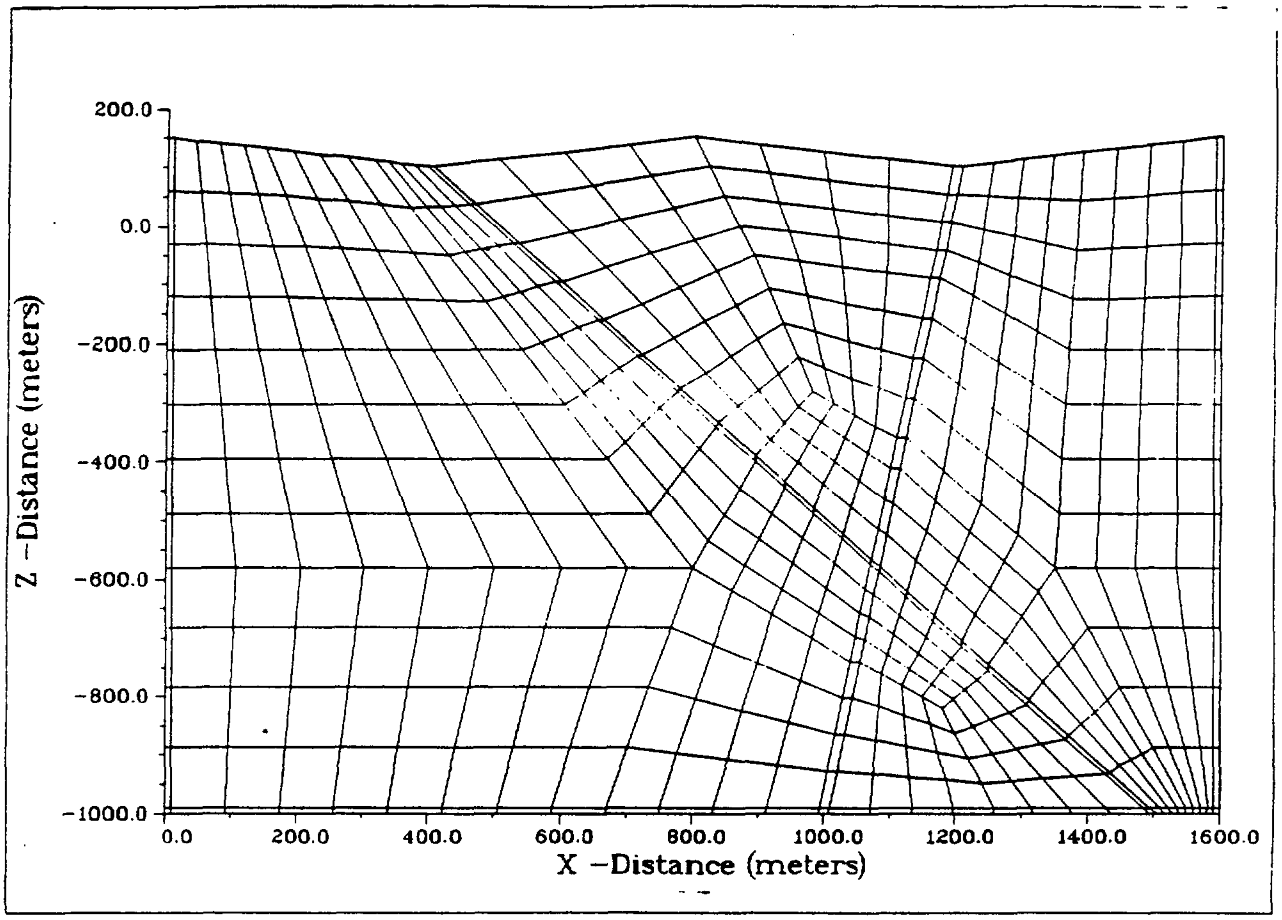


FIGURE 10. CRP's Finest Finite Element Grid, Illustrating the Use of Narrow Elements for Boundary Condition Implementation. This plot was taken from the CRP presentation at the third HYDROCOIN workshop.

The more complicated geometry of this problem served to better test the finite element versus finite difference question regarding complicated geometry and the advantage of lower-dimensional elements for the fractures. Several participants used this problem to test methods for illustrating solution convergence and distribution of mass-balance errors. The conclusions regarding these comparisons will be discussed in the HYDROCOIN report. The strong dependence of results, both in the form of predicted potentials and the more meaningful performance measures (e.g., streamlines), on the spatial discretization chosen indicates that detailed spatial discretization studies should accompany every performance calculation.

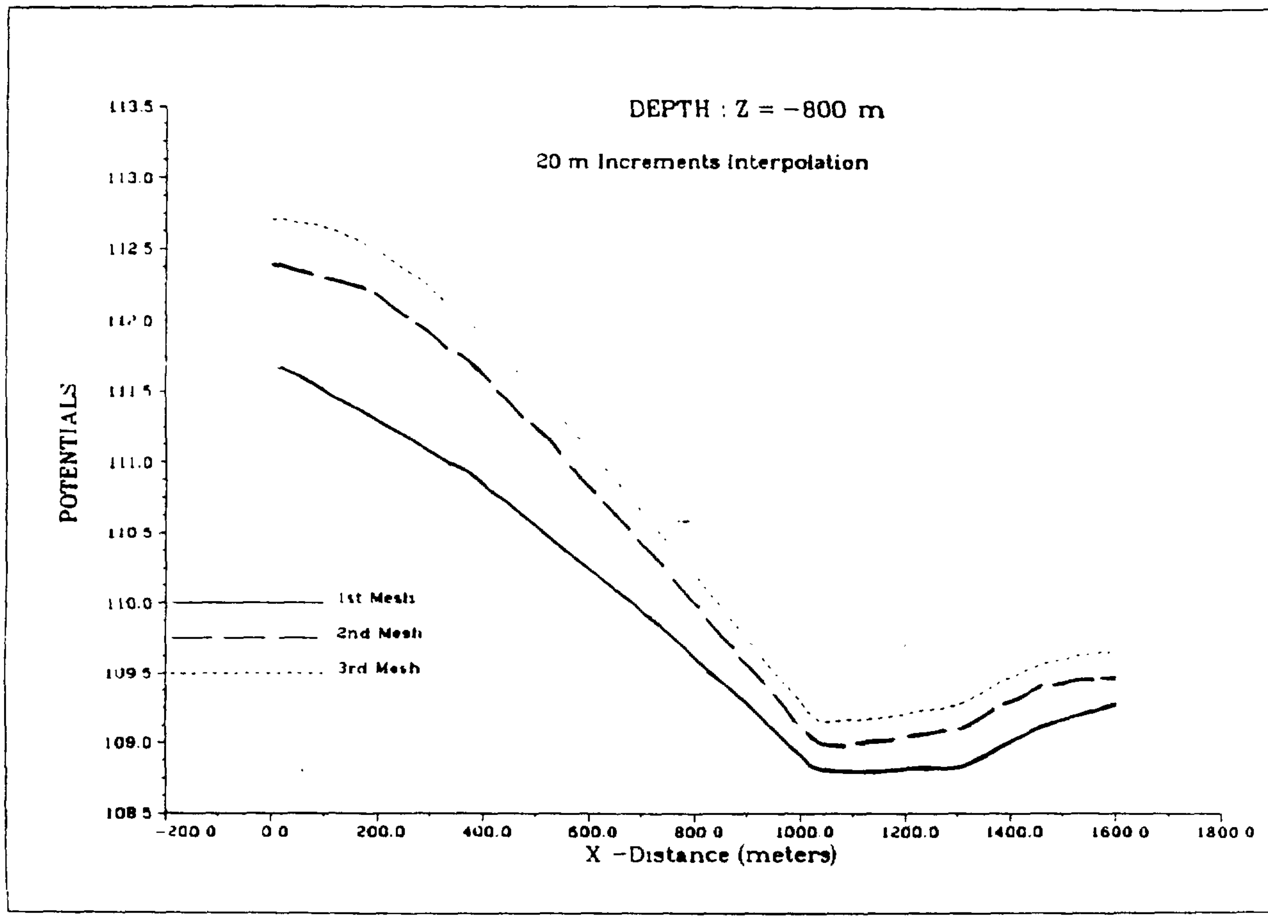


FIGURE 11. CRP Results (presented at the third HYDROCOIN workshop) Illustrating Solution Convergence as a Function of Increased Spatial Resolution. This is a plot of calculated potential versus x-location at an elevation of -800 m for three different grid meshes and linear interpolation.

Analysis of other HYDROCOIN project team results, reported at the fourth HYDROCOIN workshop, indicates that coarse grids and finite difference codes may be inadequate for this kind of problem. The analysis also indicated that one-dimensional fracture element approaches can be used successfully for potentials but that no team was able to use them for streamline calculations.

CASE 3: SATURATED-UNSATURATED FLOW THROUGH A LAYERED SEQUENCE OF SEDIMENTARY ROCKS

The purpose of this benchmark problem, which is based on the ground-water system observed at a Swiss site being investigated for disposal of intermediate-level waste, was to test the ability of numerical codes to determine the position of the water table in a layered sedimentary sequence where the layers have totally different hydraulic properties.

Among the OCRWM teams only NNWSI participated in this case, using their SAGUARO code with its saturated-unsaturated capabilities. Case 3 was tackled by only a few HYDROCOIN participants and each one, including NNWSI, had to alter the characteristic curves that represent the material properties to achieve any kind of solution. The Case 3 problem definition calls for comparison of the steady-state location of the water table and comparison of transient results as the system proceeds to steady-state. By altering the characteristic curves, NNWSI was able to obtain an approximate solution for the steady-state location of the water table, which, as shown in Figure 12, compared reasonably

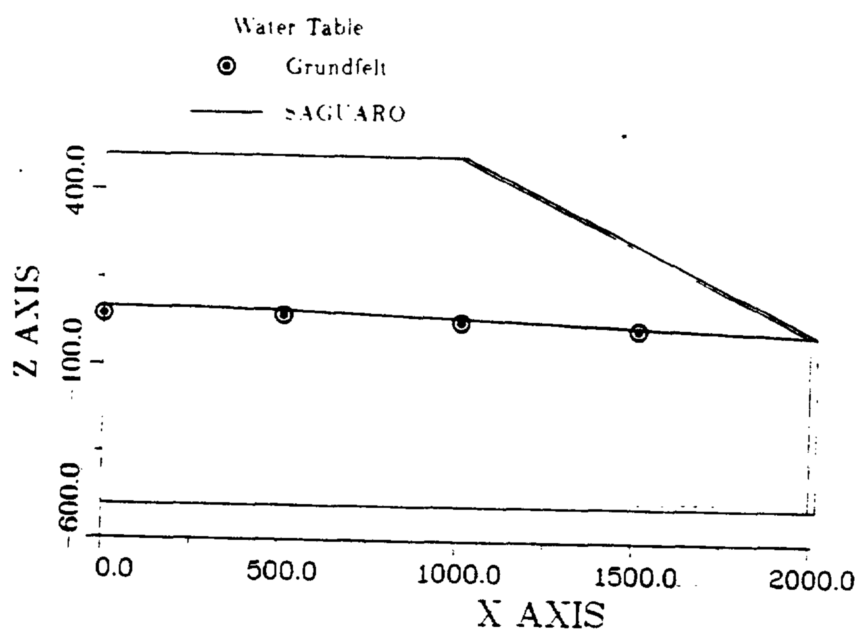


FIGURE 12. A Comparison of NNWSI Calculated Steady-State Water Table Location With Results Presented by Grundfelt (1984). This figure was taken from the January 10, 1986, NNWSI status report submitted to the HYDROCOIN secretariat.

well with the solution calculated by Grundfelt (1984). Case 3 proved to be a much more difficult problem than had been envisioned. The major difficulties were most likely related to the unrealistic characteristic curves, which were extrapolated from a limited amount of field data.

CASE 4: TRANSIENT THERMAL CONVECTION IN A SATURATED PERMEABLE MEDIUM

The analytical solution for this important verification problem describes time-dependent buoyancy-driven flow in a saturated, permeable, homogeneous, isotropic medium resulting from a decaying heat source. This highly idealized spherical repository problem provided a means to test a code's ability to predict the vertical driving forces that decrease travel time to the biosphere. The analytical solution allows prediction of temperature, pressure, and pathlines everywhere within the cylindrical polar coordinate system for which the solution is defined. The spherical repository is located in an infinite, permeable medium that has an exponentially decaying heat source. Problem definition called for comparison of calculated pathline trajectories and the associated travel times as well as temperatures and pressures at specified times as a function of space coordinates and at specified space locations as a function of time.

BWIP, CRP, NNWSI, and SRP participated in this case. BWIP used the PORFLO code (Kline et al. 1983) but did not perform the pathline-travel time calculations because of their limited participation. PORFLO is a two-dimensional, integrated finite difference code for modeling ground-water flow, heat transfer and mass transport. CRP used the STOKES code; NNWSI used the SAGUARO code; SRP used the CFEST code.

Figures 13, 14, and 15 are included to illustrate the typical problem geometry and spatial distribution of temperature and dynamic pressure that is calculated for this case. Figure 13 is the radial (r-z) grid used by the SRP team to solve this problem. Figures 14 and 15 are contour maps of temperature and dynamic pressure results at a time of 100 years and depict the region of elevated temperature due to repository heating and the presence of the buoyancy driving force, as indicated by the dynamic pressure contours. In these figures, the temperature contour interval is 10°C and the dynamic pressure contour

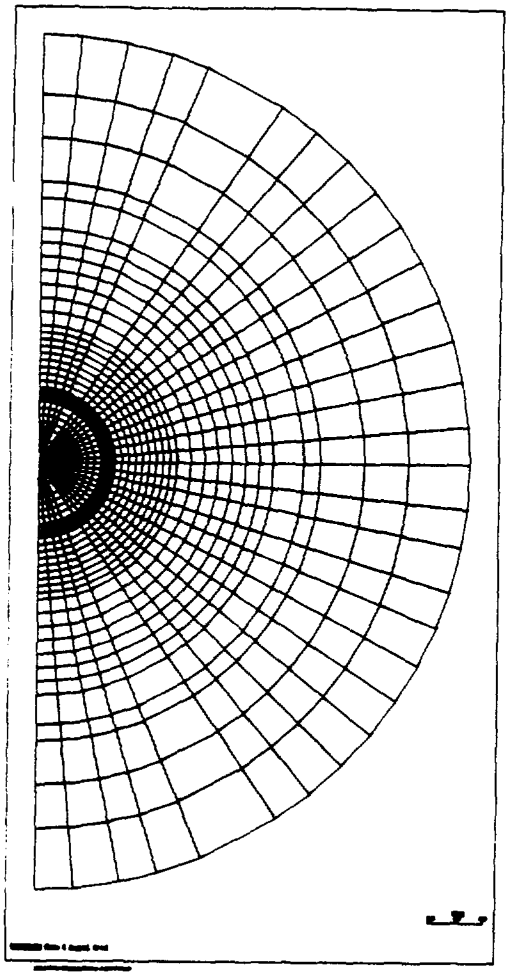


FIGURE 13. The Radial (r-z) Grid Utilized by SRP for Case 4. This figure was taken from their presentation at the fourth HYDROCOIN workshop.

interval is 2000 Pascals. The comparison between BWIP, CRP, NNWSI, and SRP calculations of temperature versus vertical distance at a radius of 0 meters and at times of 50, 100, 500, and 1000 years is shown in Figure 16. The comparison between BWIP, CRP, NNWSI, and SRP calculations of temperature versus time at vertical distances of 0, 125, 250, and 375 meters and at a radius of 0 meters is illustrated in Figure 17. The comparison between BWIP, CRP, NNWSI, and SRP calculations for dynamic pressure versus vertical distance at a radius of 0 meters and at times of 50, 100, 500, and 1000 years is depicted in Figure 18. Figure 19 is similar to Figure 18 but shows only CRP, NNWSI, and SRP calculations in order to allow for a closer comparison of these results.

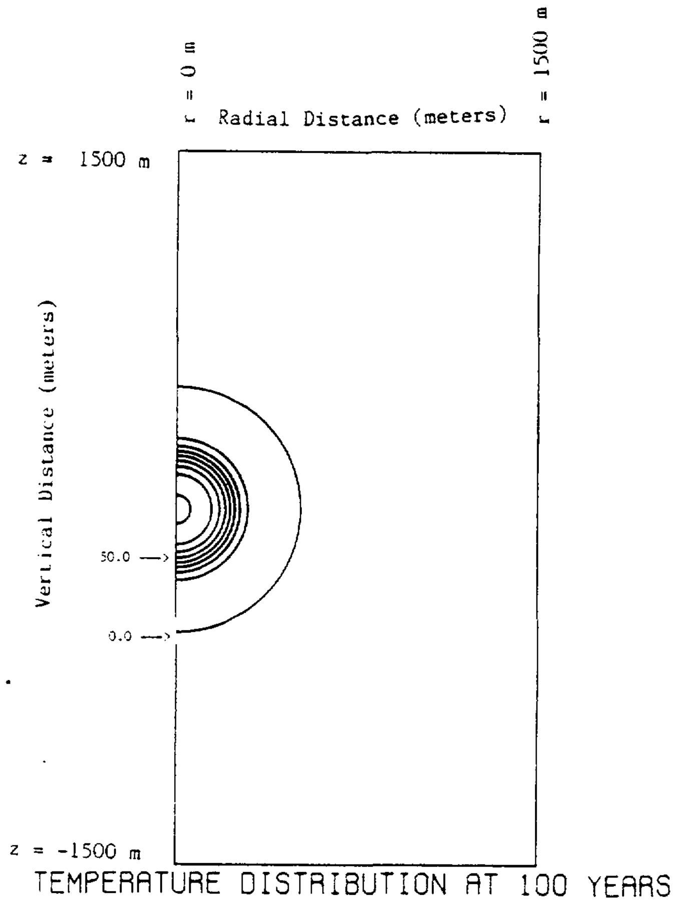


FIGURE 14. Contour Maps of SRP Temperature Results for Case 4 at a Time of 100 Years With Equally Spaced Temperature Contours of 10°C. This figure was taken from SRP results presented at the fourth HYDROCOIN workshop.

Similarly, Figure 20 illustrates BWIP, CRP, NNWSI, and SRP calculations for pressure versus time for vertical distances of 125, 250, and 375 meters at a radius of 0 meters; Figure 21 illustrates just the CRP, NNWSI, and SRP calculations. Figure 22 illustrates the CRP-, NNWSI-, and SRP-calculated pathline trajectories as well as the analytical solution for three pathlines initiated at a time of 100 years from locations r = 0 meters and for z = 0, 125, and 250 meters respectively.

The agreement between CRP-, NNWSI-, and SRP-calculated temperatures and pressures as a function of time and space is excellent, as is the agreement of these results with the analytical solution, which is not shown. The slight

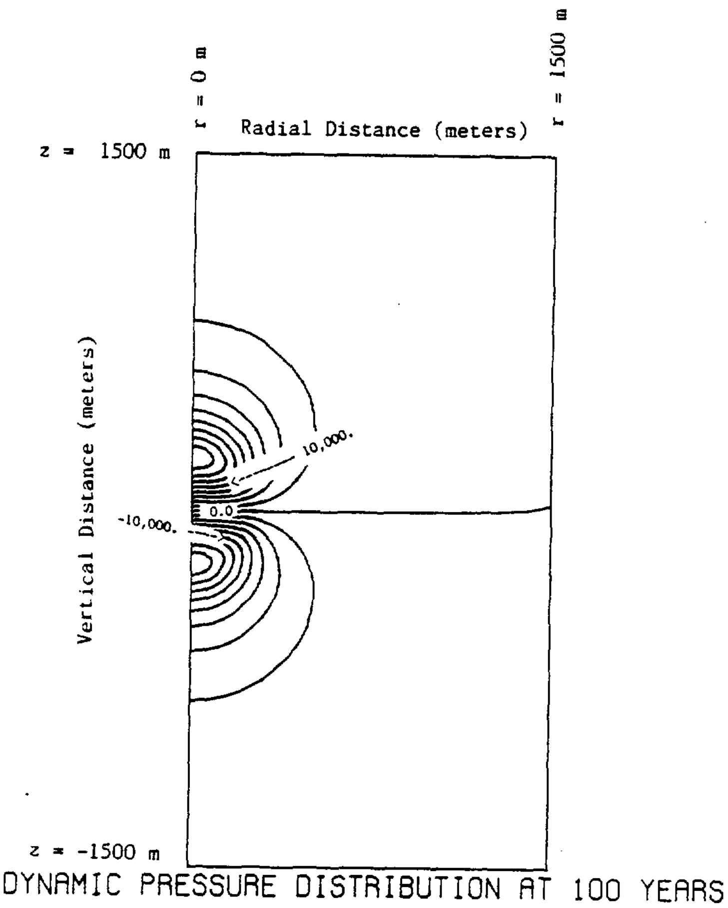


FIGURE 15. Contour Map of Dynamic Pressure Results for Case 4 at a Time of 100 Years With Dynamic Pressure Contour Spacing of 2000 Pascals. This figure taken from SRP results presented at the fourth HYDROCOIN workshop.

deviations in these results are probably related to the spatial and time discretizations used and to the methods used to establish boundary conditions that approximate the infinite medium of the analytical solution with a finite spatial grid.

The deviation of the BWIP temperature and pressure results is related to two factors. The first factor, which explains the deviation in the temperature results, is that the heat source in the BWIP modeling was cylindrical instead of spherical. That is why the temperature comparisons shown in Figures 16 and 17 are relatively good everywhere except at the edge of the repository (250 meters), where the deviation between spherical and cylindrical approximations

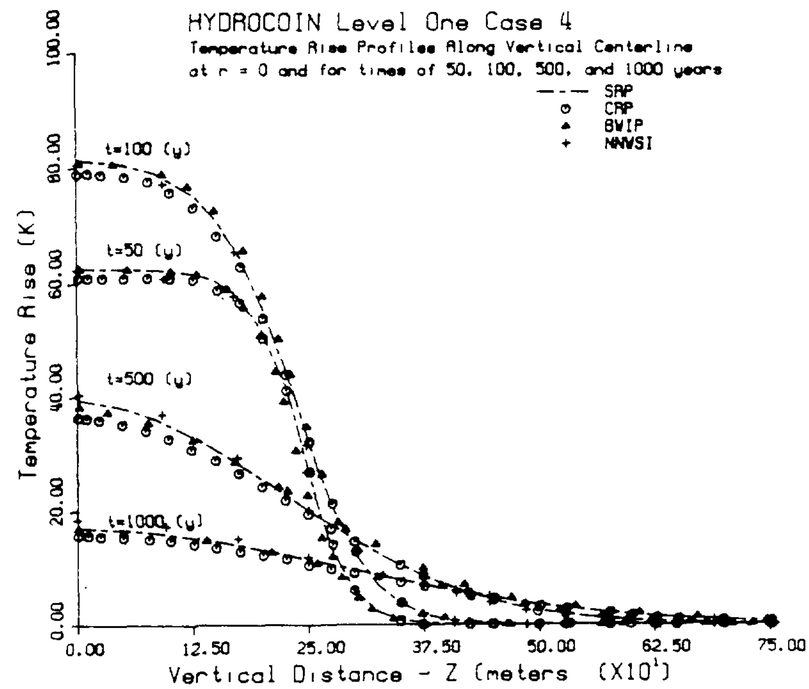


FIGURE 15. Comparison Between BWIP, CRP, NNWSI, and SRP Calculations for Temperature Versus Vertical Distance at a Radius of 0 m and at Times of 50, 100, 500, and 1000 Years

for the heat source geometry is greatest. The large deviations in pressure results should have no effect on the calculated temperature rise since temperature is only a result of conduction (i.e., temperature calculations are decoupled from pressure calculations). SRP had similar geometry problems initially and as a result added a grid-generation capability to handle the arbitrary r-z geometries needed to address this problem.

The second factor that explains the deviations in the BWIP calculations of pressure versus time (Figure 18) and pressure versus distance (Figure 20) calculations is that the analytical solution used in this case assumes a linear relationship between the density of water and temperature; the PORFLO code used by BWIP assumes an exponential relationship. BWIP recognized these difficulties and reported them at the first HYDROCOIN workshop. They also suggested that variations of this same problem could be utilized for more realistic benchmark comparisons in which the temperature and pressure equations were more fully coupled than in the current verification problem. BWIP presented some

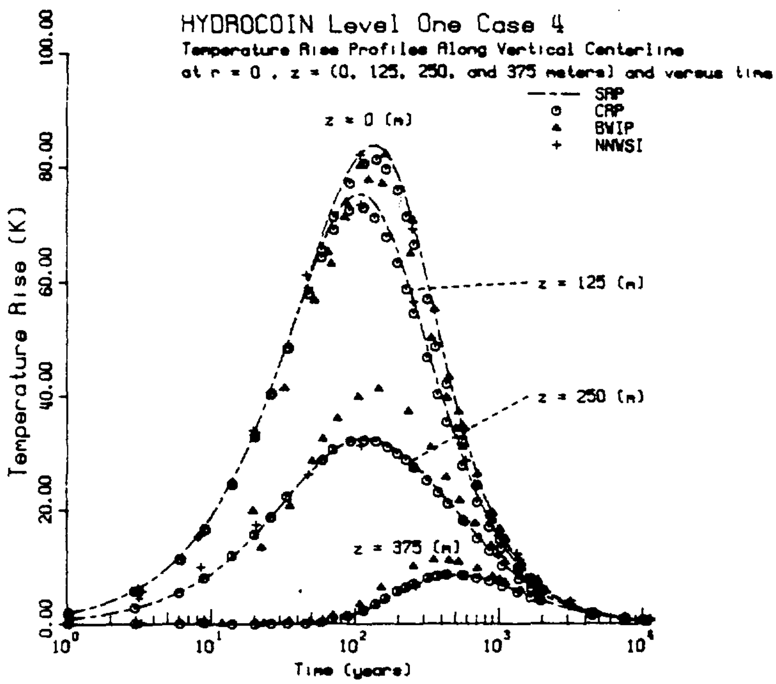


FIGURE 17. Comparison of BWIP, CRP, NNWSI, and SRP Calculations for Temperature Versus Time at Vertical Distances of 0, 125, 250, and 375 m and at a Radius of 0 m

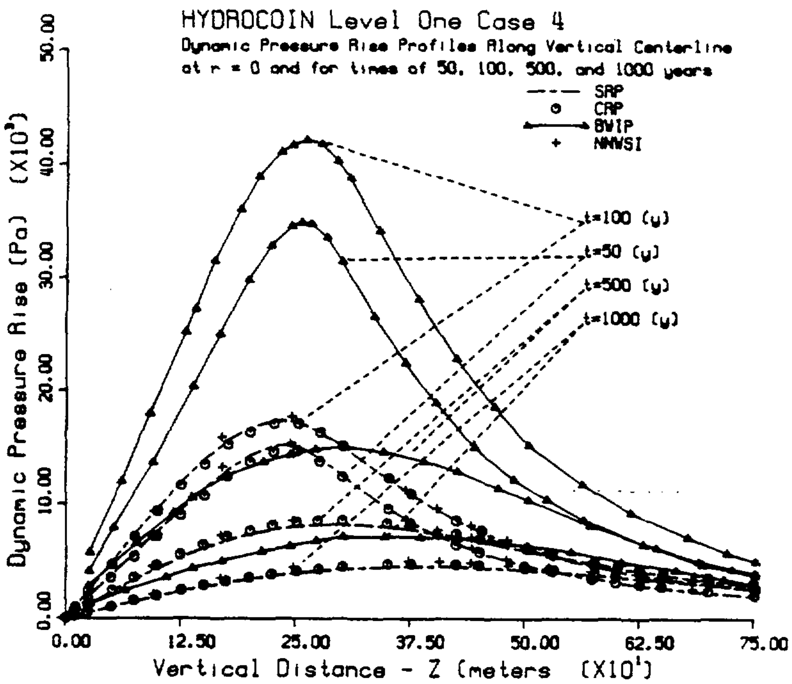


FIGURE 18. Comparison Between BWIP, CRP, NNWSI, and SRP Calculations for Dynamic Pressure Versus Vertical Distance at a Radius of 0 m and at Times of 50, 100, 500, and 1000 Years.

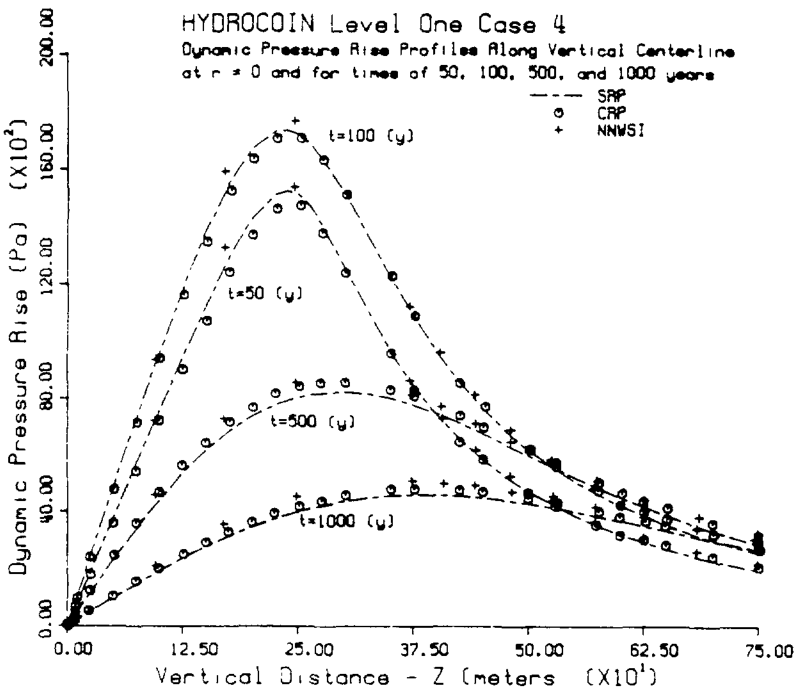


FIGURE 19. Closer Comparison Between CRP, NNWSI, and SRP Calculations for Dynamic Pressure Versus Vertical Distance at a Radius of 0 m and at Times of 50, 100, 500, and 1000 Years

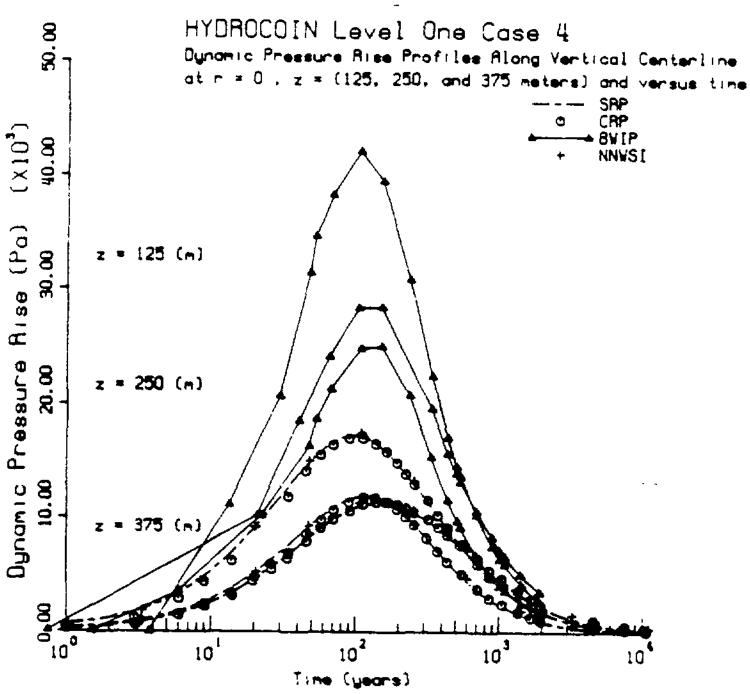


FIGURE 20. Comparison Between BWIP, CRP, NNWSI, and SRP Calculations for Pressure Versus Time for Vertical Distances of 125, 250, and 375 m at a Radius of 0 m

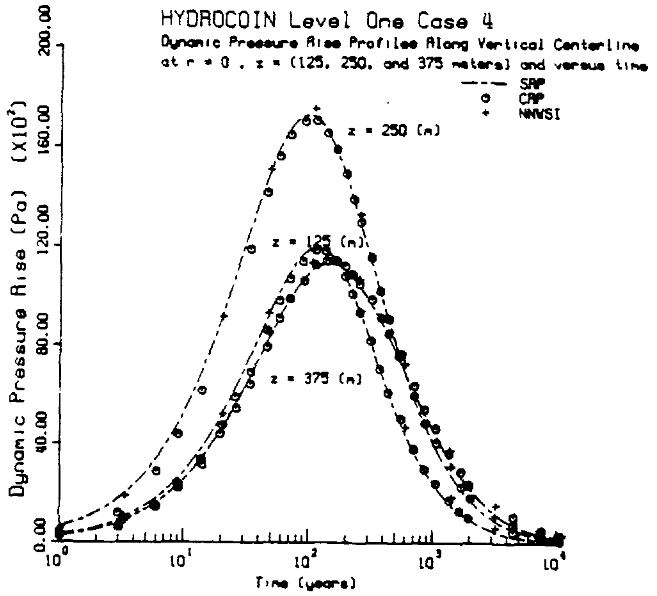


FIGURE 21. Closer Comparison Between CRP, NNWSI, and SRP Calculations for Pressure Versus Time for Vertical Distances of 125, 250, and 375 m at a Radius of 0 m

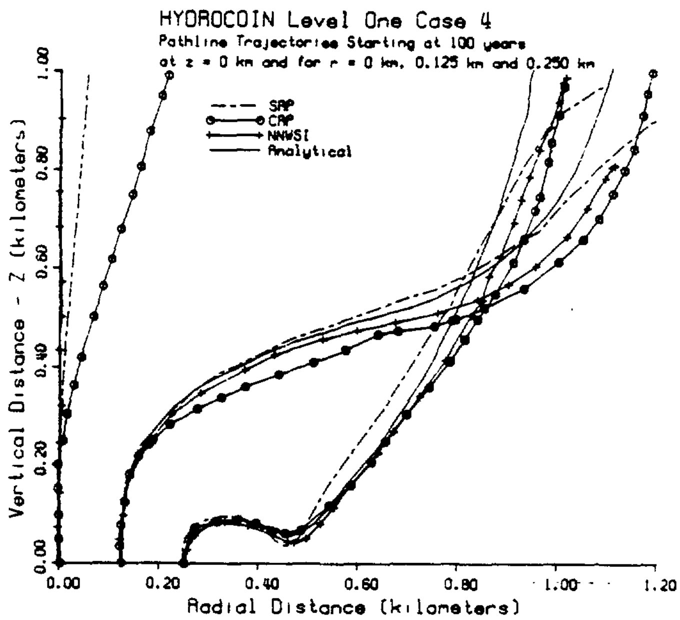


FIGURE 22. CRP, NNWSI, and SRP Calculated Pathline Trajectories and the Analytical Solution for Three Pathlines Initiated at a Time of 100 Years from Locations r = 0 m and for z = 0, 125, and 250 m

initial benchmark results illustrating the effect of different amounts of coupling at the second HYDROCOIN workshop, the last workshop in which they were able to participate.

The pathline trajectory comparisons of Figure 22 illustrate a common pattern in HYDROCOIN and the earlier INTRACOIN results. We can predict scalar quantities such as temperature, pressure, or head with little deviation, but have much greater difficulty with vector quantities such as fluxes, velocities, and stream- or pathlines. SRP studied the effects of various spatial and temporal discretizations and concluded that much of the difficulty appears to be directly related to the spatial and temporal discretizations utilized. For example, the deviation from vertical (the analytical trajectory) of the trajectory of the pathlines of Figure 22 that start at r = 0 m and z = 0 m is directly related to the size of the first angular discretization, the linear element interpolation scheme, and the left no-flow boundary that arises from problem symmetry. Problems at this boundary are similar to the no-flow boundary problems already discussed for Case 2. Other difficulties are directly related to the interpolation schemes used and to the methods by which velocities are calculated from the scalar quantities calculated as solutions to the partial differential equations. These problems with correct pathline and streamline calculation have resulted in a Level Three problem to determine the source of these difficulties.

CASE 5: SALT WATER DISTRIBUTION IN A SATURATED POROUS MEDIUM

Case 5 is benchmark problem designed to test the ability of a code to predict the location of the fresh water-salt water interface in a ground-water system above a salt dome. This idealized, two-dimensional, vertical (x-z) cross-section problem was patterned after a hydrogeologic setting observed near a German salt dome. It involves modeling nonlinear, steady-state flow and brine transport. Interactions between strong density gradients and the diffusion-dispersion parameters control system behavior. Understanding how isolated stagnation zones form in these systems is important for assessing the performance of proposed salt repositories.

SRP, using their CFEST code, was the only OCRWM project to participate in this case, which proved to be one of the most difficult of the Level One problems. Five other HYDROCOIN teams and C. Voss of the USGS also addressed this problem. SRP is preparing a detailed project report on their Level One efforts, so only brief, illustrative results from SRP's presentation at the fourth HYDROCOIN workshop will be discussed here. The steady-state, salt concentration (normalized 0-1.0) contours calculated by SRP are shown in Figure 23. An analysis of these contours, the calculated streamline trajectories (Figure 24), and a plot of the velocity vectors (Figure 25) indicate that two separate flow systems exist. The lower system is essentially stagnant with what little circulation that exists being dominated by density gradients and diffusion (see Figure 25). Communication across the relatively sharp salt water-fresh water interface is controlled by the system's diffusion-dispersion parameters. This communication in turn controls the degree of isolation of the lower system. No formal comparisons can be made until published team reports from the other participants are available. Results presented by AERE, Harwell, at the fourth HYDROCOIN workshop are very similar to SRP's.

Case 5 has been extremely valuable to SRP because it addresses important questions related to density-dependent flow. This case has no analytical

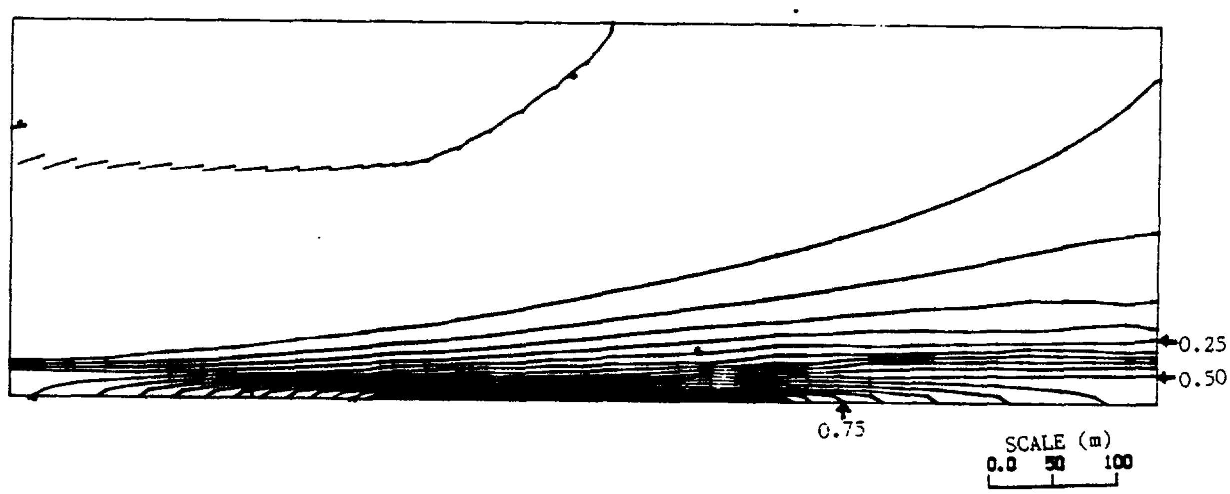


FIGURE 23. SRP-Calculated Steady-State, Salt Concentration Contours for Level One, Case 5. The contour interval is 0.05 and concentration is normalized (0-1.0). This figure is taken from SRP results presented at the fourth HYDROCOIN workshop.

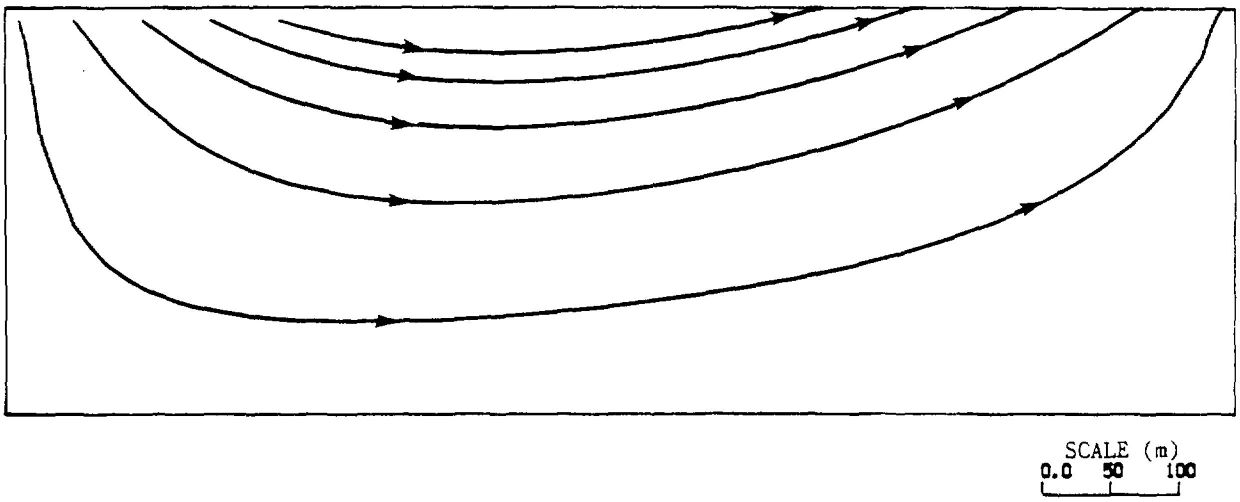


FIGURE 24. SRP's Calculated Trajectories for the Five Level One, Case 5 Streamlines. This figure was taken from SRP results presented at the fourth HYDROCOIN workshop.

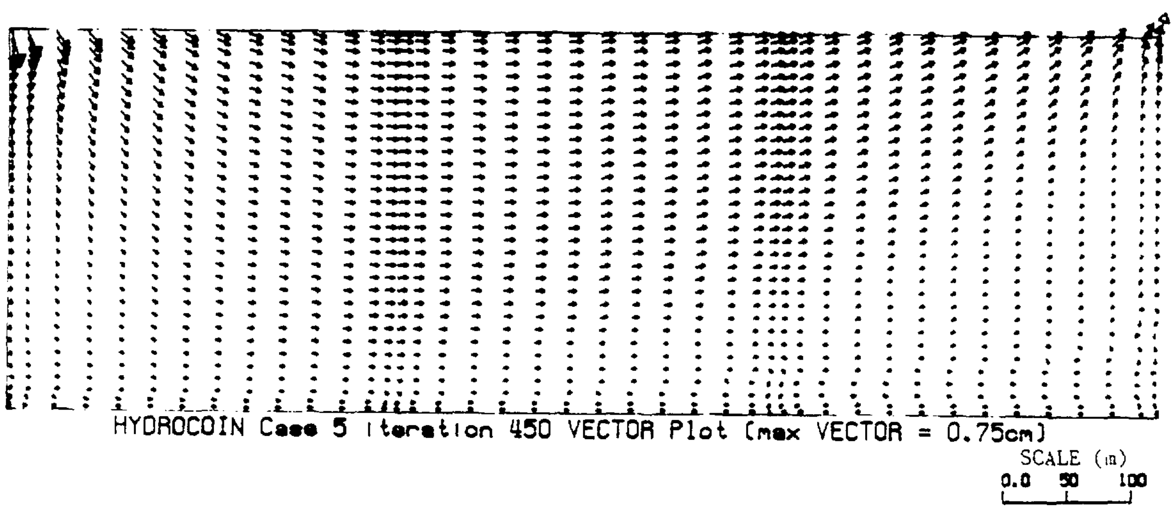


FIGURE 25. **Velocity Vector Plot Calculated by SRP for Level One, Case 5.** This **figure taken from SRP results presented at the fourth** HYDROCOIN **workshop.**

solutions and would have been extremely difficult to test without the HYDROCOIN environment. The initial SRP solution for this case, shown in Figure 26, seemed very reasonable but was wrong. This solution is the kind that would have been obtained for a system with a very high molecular diffusion

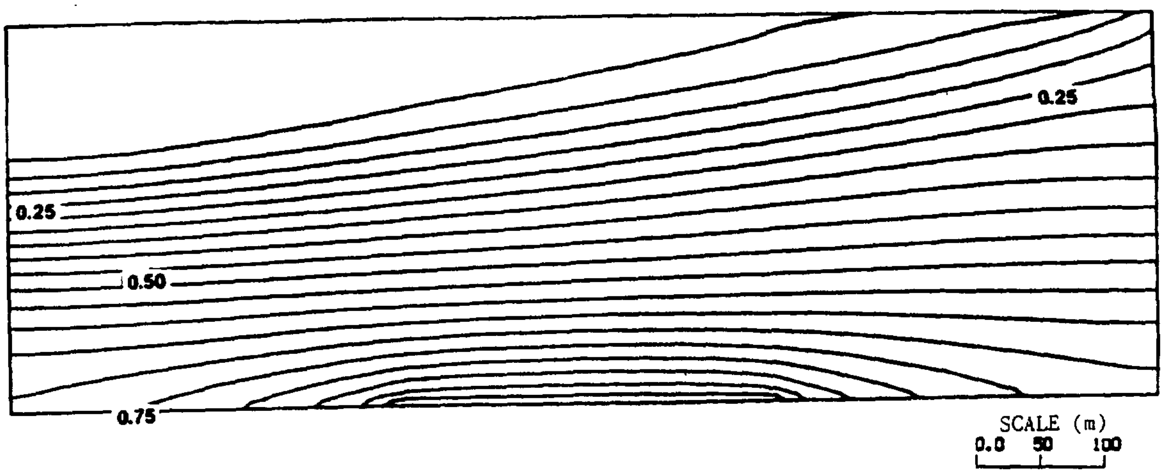


FIGURE 26. The Initial SRP Solution for Level One, Case 5 Calculated Without the Consistent Velocity Interpolation Scheme. This figure taken from SRP results presented at the second HYDROCOIN workshop.

coefficient. A comparison of this early SRP result with the solution the USGS initially obtained with their SUTRA code indicated that the source of the high artificial diffusion in the SRP's CFEST solution was a ground-water velocity interpolation difficulty that arises when modeling variable density systems. As a result, the consistent velocity approach discussed in the SUTRA code documentation (Voss 1984) was implemented in the CFEST code. The AERE team experienced a similar velocity interpolation difficulty that forced them to use a mixed interpolation scheme to allow for the appropriate balance between the gravitational term and the pressure gradient in the highly stratified regions. Quadratic interpolation was used for pressure and linear interpolation was used for salt concentration.

Analysis of this problem resulted in the preparation of a vector plotting capability for the CFEST code (Figure 25), because for variable density systems one cannot study potential or pressure contours to determine either flow direction or velocity. Participation in HYDROCOIN has resulted in many code improvements, especially in auxiliary codes for plotting, interpreting, and displaying results. SRP has already begun to use the experience with variable density systems that they gained as a result of the HYDROCOIN Case 4 and Case 5 efforts in ongoing performance-assessment studies.

This problem, like many of the others, had some boundary condition difficulties, again emphasizing the importance of careful analysis and selection of boundary conditions. The problem as originally posed should have had no salt water concentration plume, because the molecular diffusion constant was specified as zero. The system's lateral and longitudinal dispersion parameters should not allow any salt movement from the top of the salt dome, since flow can only be parallel with the top of the dome, resulting in zero vertical velocity and thus no vertical dispersion. Numerical codes, however, will predict salt movement into the system even if the diffusion coefficient is set to zero because there is always a free numerical diffusion component related to the grid spacing. Without a defined value for molecular diffusion, the amount of salt entering the system is strictly a function of grid spacing and numerical diffusion.

The Dirichlet pressure boundary condition along the top, if implemented exactly as specified, would result in solution singularities in the upper left and upper right corners. The introduction of narrow elements along the left and right sides, as discussed for Case 2, alleviates this problem. The experience of the SRP team in obtaining a solution as a result of this Dirichlet boundary indicates the need for more careful selection of boundary conditions during the conceptual modeling and boundary condition interpretation stage of performance assessment. The left end of this system represents a ground-water divide in a recharge area. The right end represents a ground-water divide near a discharge river or lake, and a reasonable conceptual model would include ground-water system recharge in between. The Dirichlet pressure boundary condition specified was meant to approximate this case, but, as shown by Figure 25, recharge occurs in less than half of the system. For the boundary conditions specified, the recharge-discharge quantities and locations are strictly a function of the current subsurface salt concentrations, which means that the definition of the system being simulated is constantly changing as one approaches steady state. If the recharge distribution were specified directly and Dirichlet boundary conditions were specified only at discharge locations, then the system definition would be fixed. The difficulties this caused the SRP team can be best described as sloshing. SRP was using a direct, iterative, steady-state approach, unlike the transient approach used by the USGS and TUB.

In this steady-state approach, initial estimates for the concentration distribution were used to update the estimates for density. For the first iteration, predicted flow in the system was from left to right. As a result of concentration-density updates, flow in the system would reverse during the next iteration, and the system would slosh back and forth as the iterations proceeded. If pressures were specified only at the discharge locations and recharge was specified elsewhere, then calculated system pressures would adjust to accommodate the specified recharge inflow. The predicted flow direction in the system would be more stable and more importantly the flux moving through the system would be constant and not a function of the iteration or time step as in the case as posed. To solve this flow system oscillation problem, SRP had to severely limit the allowable density changes that could be made on any single iteration.

CASE 6: THREE-DIMENSIONAL STEADY-STATE FLOW IN A REGIONAL AQUIFER

This benchmark problem was developed and posed by SRP and tests the ability of a computer code to model three-dimensional ground-water flow in a regional ground-water system with rock layers of highly contrasting anisotropic hydraulic conductivity, typical of bedded salt sites and basalts. This highly idealized system was constructed to include many of the features important to modeling the regional ground water of the Palo Duro Basin in Texas, USA. See Appendix B for a description of the geometry. The required output for purposes of comparison is hydraulic head along specified lines, streamlines, and flux through the salt layer.

SRP was the only OCRWM project to participate in this Level One case, and they used their three-dimensional, finite element, hydrologic flow code FE3DGW (Gupta et al. 1984). Seven other HYDROCOIN project teams participated in this case. Three teams used finite difference codes; the rest used finite element codes. SRP is preparing a detailed project report, so only brief illustrative results from SRP's presentation at the second HYDROCOIN workshop will be discussed here. Figure 27 shows an isometric view of the grid mesh used for Case 6. Figure 28 is a contour map of calculated potentials along a vertical

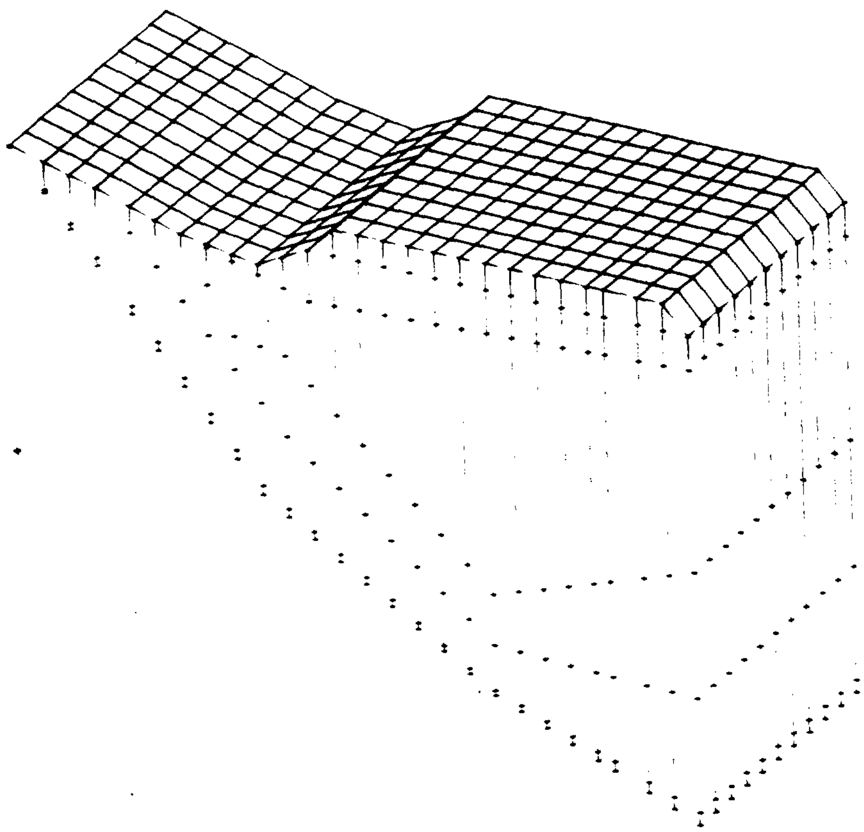


FIGURE 27. An Isometric View of the Finite Element Grid Mesh Used by SRP for Level One, Case 6. This figure was taken from SRP results presented at the second HYDROCOIN workshop.

cross-section on the southern problem boundary. Until published team reports from the other HYDROCOIN participants are available, SRP results cannot be formally compared with their results.

Initial analysis of results at the fourth HYDROCOIN workshop indicate that, while there is a spread in predicted potentials and streamline-travel time results, there is definite clustering of results. The greatest variability in potentials was near the surface, in the region where an unrealistically high infiltration boundary condition was specified. The boundary-condition problem area is noted by an asterisk in Figure 28. Another observation was that finite difference codes showed the greatest variability. This is consistent with what was learned from Case 2 regarding the relative ability of finite element codes versus finite difference codes for dealing with complex

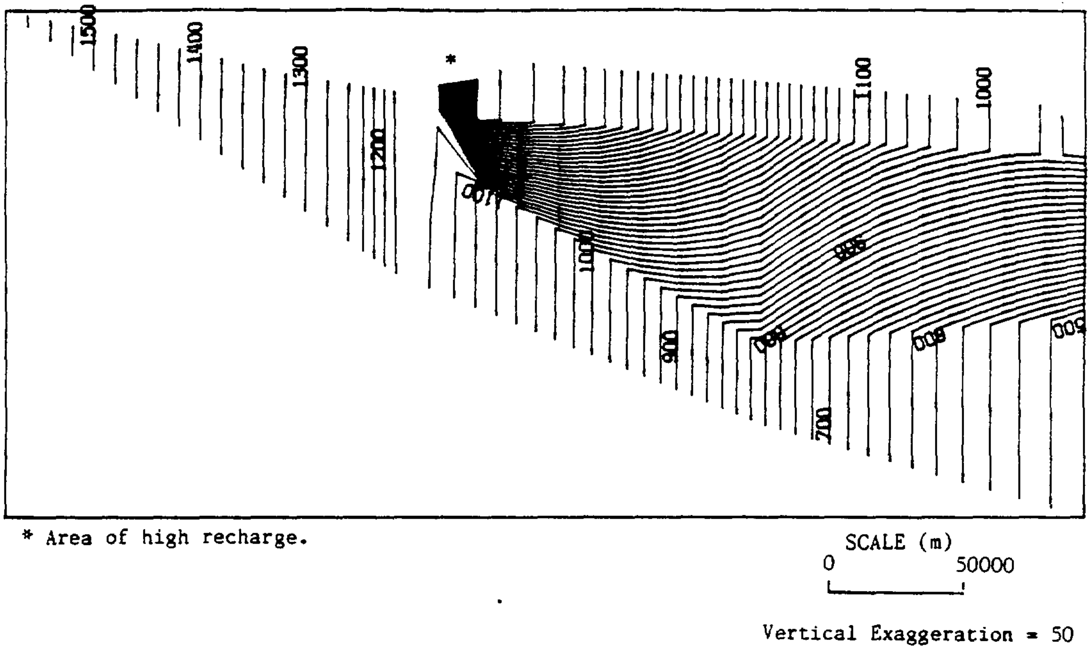


FIGURE 28. Contour Map of the Level One, Case 6 Potentials Calculated by SRP with the FE3DGW Code Along a Vertical Cross-Section on the Southern Problem Boundary. The contour interval is 25 m. This figure was taken from SRP results presented at the second HYDROCOIN workshop.

geometries and limited discretization. A solution convergence study for this problem, like that performed for Case 2, would probably indicate that the major cause of the deviations is due to inadequate spatial discretization.

SRP found that they had to double the vertical resolution of the lowest hydrologic layer to keep streamlines moving parallel to the lower no-flow boundary. Without this increased vertical resolution, the streamlines would exit the no-flow boundary. However, despite all the difficulties and variability in potentials, calculated fluxes through the salt system (an important measure of performance) varied only by a factor of two. The active participation of the various HYDROCOIN project teams in this benchmark problem has been extremely valuable to SRP. The projected participation in the Level Three extension to this problem will provide even greater benefits to SRP.

CASE 7: TWO-DIMENSIONAL FLOW THROUGH A SHALLOW LAND DISPOSAL FACILITY IN ARGILLACEOUS MEDIA

Case 7 is a benchmark problem designed to test a code's ability to model ground-water flow around a hypothetical shallow land disposal facility designed for low- and intermediate-level waste. The geometry and vertically varying hydraulic conductivity and porosity selected for this problem correspond to proposed disposal options and the hydrological setting found at several potential sites located in the United Kingdom. Fully saturated, two-dimensional ground-water flow calculations were performed along a vertical (x-z) cross-section for two disposal options involving high- and low-permeability concrete blocks. Code comparisons were made by comparing calculated trajectories and travel times for twelve different streamlines and by comparing code-predicted vertical velocities along horizontal lines at three different depths.

SRP was the only OCRWM participant that had completed Case 7 at the time this report was drafted. They utilized the CFEST code. CRP has also completed this case using their STOKES code and PARTICLE auxiliary code, but results were not available in time to be included here. Detailed reports are being prepared by the CRP and SRP teams. Only a summary of SRP results that were presented at the second HYDROCOIN workshop will be discussed here. A contour map of calculated potentials for the low-permeability concrete variation is shown in Figure 29. The calculated streamline trajectories for this low-permeability variation are illustrated in Figure 30. This problem did not pose any significant difficulty for the SRP project team. Published team reports from the other HYDROCOIN participants are not yet available, so no formal comparison of results can be made.

The results of an initial analyses of the full HYDROCOIN participation in this case were presented at the fourth HYDROCOIN workshop. This analysis indicates that twelve project teams participated in Case 7. The major difficulties with this benchmark problem were associated with the variation of permeability and porosity with depth and the implementation of an unrealistic seepage face boundary condition on the right end of the problem. In general, Case 7 results are in reasonable agreement. The largest deviations were observed for the low permeability variation and with the use of triangular elements.

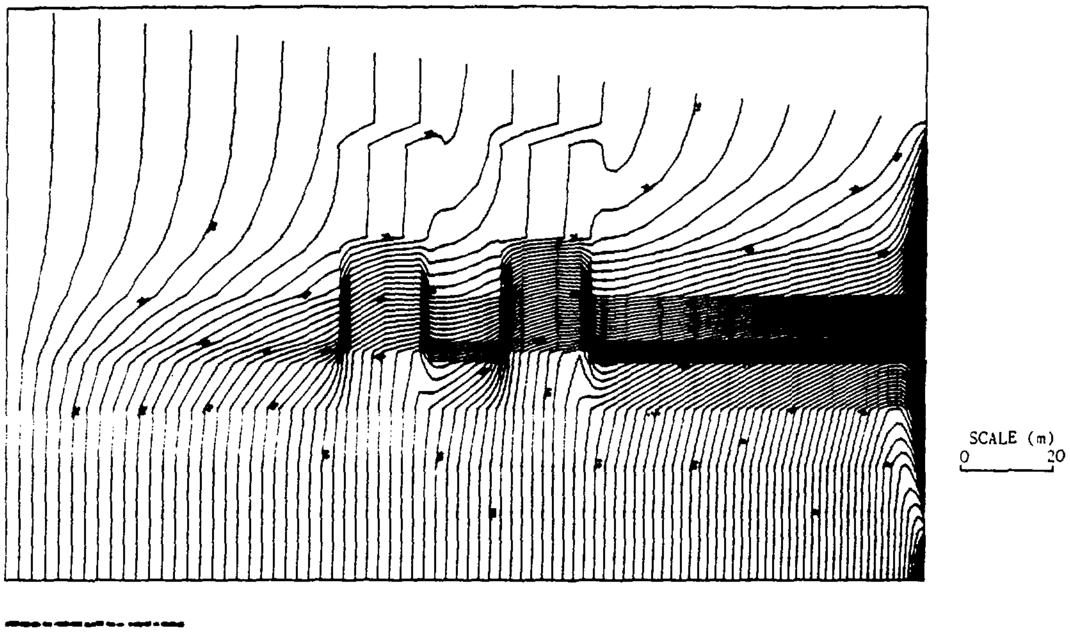


FIGURE 29. Contour Map of Calculated Potentials for the Low-Permeability Concrete Variation. The contour interval is 0.25 m. This figure was taken from SRP results presented at the second HYDROCOIN workshop.

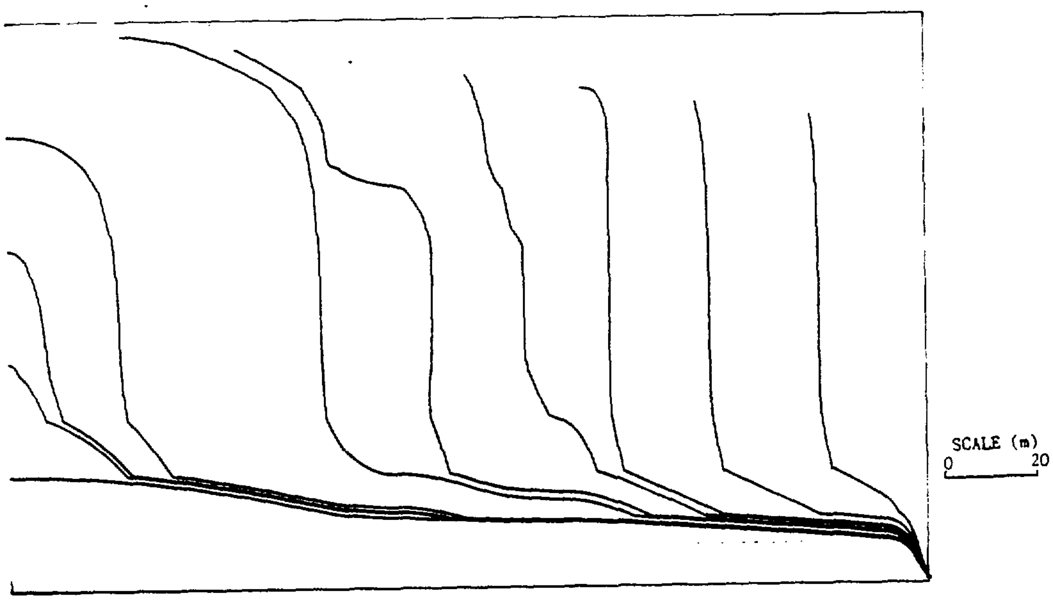


FIGURE 30. Calculated Streamline Trajectories for the Twelve Streamlines Specified in the Case 7 Problem Definition. This figure was taken from SRP results presented at the second HYDROCOIN workshop.

DISCUSSION OF RESULTS FROM LEVEL ONE AND PLANS FOR LEVELS TWO AND THREE

LEVEL ONE

The benefits to OCRWM from participating in HYDROCOIN Level One (verification and benchmarking) have exceeded the stated objectives for this level. The insights gained on the technical details of modeling from the face to face interaction of OCRWM scientists with their peers has greatly augmented the knowledge that would have been gained from strict code intercomparisons. The following enumeration lists all the major benefits complete with a short description of each.

1. Problem Formulation and Selection - Formulation and selection of relevant verification and benchmark problems is a difficult process. Participation in HYDROCOIN has provided the OCRWM participants with a great deal of insight and experience which will prove of value in their ongoing verification and benchmarking efforts. SRP's layered salt benchmark problem (Case 6) has been improved as a result of HYDROCOIN participation. Enhancements were made to the Case 6 problem formulation that required additional comparison of predicted flux through the salt. An ambiguity in the infiltration boundary condition was exposed as a result of the particular code and discretization scheme used by the Swiss. Case 4 has proved to be a useful verification problem for all OCRWM project teams by providing one of the only analytical solutions involving buoyancy as well as a test for pathlines. Case 5 has proved to be one of the toughest and most revealing of the benchmark problems. This important salt site problem, which on the surface appears very simple, would probably not have been chosen outside the forum of HYDROCOIN. This Case 5 problem, without a doubt, was proposed because of the difficulties that a similar real problem had posed. Cases 1 and 2 provide useful equivalent porous media fracture flow problems important to the CRP and the other projects that must deal with fractures and fracture zones.

Involvement with a respected peer group for the process of verification and benchmark problem formulation has proved to be a valuable experience for the OCRWM participants. This experience will continue to benefit future OCRWM verification and benchmarking efforts, which are such an important part of the continuing need to assure ourselves, the regulators, and the public concerning the numerical accuracy and applicability of our performance-assessment codes.

2. Intercode Comparison - The obvious advantage of HYDROCOIN participation is in the area of code intercomparison for benchmark problems because no analytical solution (or answer book) exists to provide the correct result. The correctness or accuracy of a code can only be judged by comparing it with the solutions computed by other codes. For the HYDROCOIN benchmark problems, a number of results are available from a variety of different codes representing various numerical approaches by independent modeling teams. This variety provides the best type of code intercomparison. Although verification problems generally provide a useful means for checking code accuracy and applicability without the need for code intercomparison, this does not always provide the complete set of information of interest. As a result of discretization and other approximations, numerical codes rarely reproduce analytical solutions exactly.

   Intercomparison of results from different codes can thus be beneficial, even for verification problems. As is the case with benchmark problem intercomparison, subtle differences between a given code and the majority of the other codes can identify potential advantages or errors either in the majority of the codes or in the deviant code. Intercomparison of results can also reveal inadequate or advantageous means of discretization or other useful information concerning numerical implementation strategy. Participation in Level One has provided benefits in each of these areas of code intercomparison. Case 5, for example, illustrated a difficulty with standard finite element approaches for density-dependent problems. As a result, the consistent velocity formulation used in the two-dimensional SUTRA code

(Voss 1984) was incorporated into SRP's code. Additionally, the SUTRA code was identified as a potentially important code for the PASS program to verify and benchmark because it can also solve unsaturated flow and transport problems important to tuff performance assessment. Cases 2, 4, and 7 have provided beneficial information concerning discretization strategy and various mass balance and residuals methodologies for evaluating the adequacy of a given grid. Problems associated with the interpolation of results between nodes and with the generation of path- and streamlines has resulted in code improvements and problems for Level Three to resolve the source of these difficulties.

3. Appropriate Organization and Timing - The organization and timing of HYDROCOIN have provided an opportunity to make progress in the area of code verification and benchmarking which, at best, could otherwise only be achieved through more costly and time-consuming efforts. The HYDROCOIN organization and structure draws from a wide variety of capable participants with enough diversity in interests and needs such that appropriate problems of mutual interest can be formulated and used. Additionally, sufficient participation with an ample variety of code types in each of the Level One cases has given this effort the required credibility. While this set of HYDROCOIN benchmarks does not satisfy the complete needs of any of the OGR projects, they do provide a base level of key verification and benchmarking credibility and also identify those codes against which future benchmark comparisons would be most beneficial.

4. Development of Credibility and Forum for Exchange - The wide variety of participating groups, which includes regulatory agencies from various countries and various peer groups, provides a measure of credibility to the HYDROCOIN benchmarking effort that would be hard for DOE to otherwise achieve. This same combination also provides an excellent forum for technical exchange and a means for OCRWM participants to present and compare their performance-assessment approaches with those being used by their peers. Comparisons of OCRWM efforts

with those of independent groups not only build credibility for OCRWM projects but these comparisons also help ensure that we are using the best performance-assessment approaches and techniques available. In addition to the HYDROCOIN code intercomparison report being published by the secretariat, each of the projects is publishing separate team reports, which will provide additional credibility to OGR project verification and benchmarking efforts.

The successful joint DOE/NRC "Symposium on Groundwater Flow and Transport Modeling for Performance Assessment of Deep Geological Disposal of Radioactive Waste: A Critical Evaluation of the State of the Art" was another direct benefit related to HYDROCOIN participation to date.

LEVELS TWO AND THREE

Participation in the early planning and discussion stages of Level Two has already provided useful insights about the difficulties associated with validation efforts. Continued involvement in both Level Two and Level Three is planned to varying degrees by the various OCRWM project teams (see Tables 1 and 2). Both NNWSI and SRP have formulated Level Three sensitivity and uncertainty problems that will provide direct benefit, because these problems have been defined to be useful both for the HYDROCOIN participants and for the respective OCRWM projects. Given the relative difficulty of the issues addressed by Levels Two and Three, the potential for benefits of participation are much greater than they were for Level One.

Participation by the project teams in the HYDROCOIN workshops and co-ordinating group meetings is so valuable because of the quality of the technical discussions, the openness and sharing of successful new ideas and approaches, and the candid discussions of failures. These meetings alone would justify full participation in HYDROCOIN. NRC and DOE will host the May 1987 HYDROCOIN meeting in the United States in order to allow more of the U.S. ground-water modelers to attend.

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APPENDIX A

DESCRIPTION OF THE HYDROCOIN ORGANIZATION

(TAKEN FROM HYDROCOIN PROGRESS REPORT NO. 3)

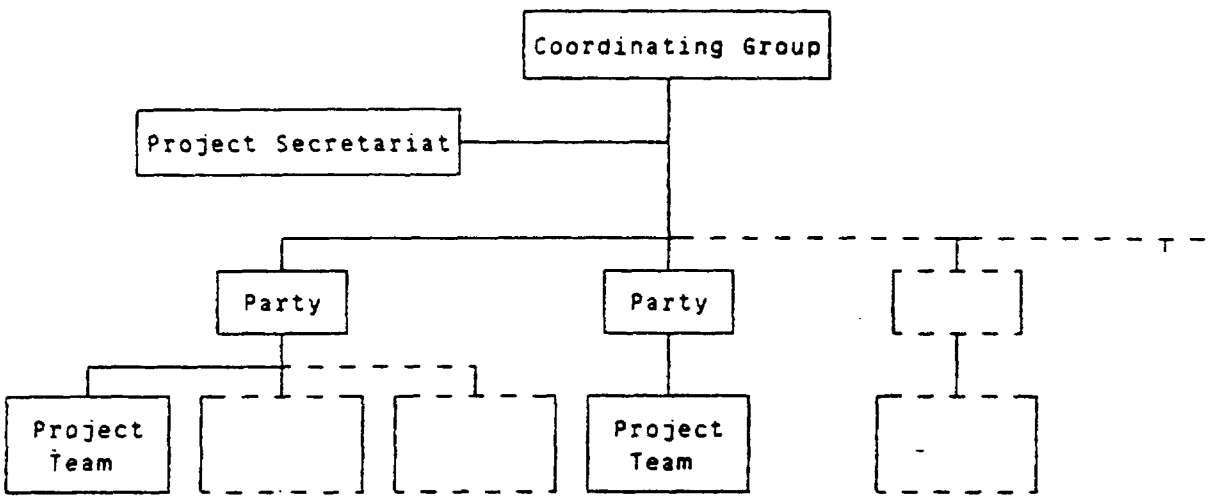
HYDROCOIN ORGANIZATION

The study is directed by a Coordinating Group with one member from each participating organization (Party) setting up the study. The Swedish Nuclear Power Inspectorate (SKI) acts as managing participant. A project Secretariat has, according to the agreement between the HYDROCOIN Parties, been set up by SKI in cooperation with the United Kingdom Atomic Energy Authority/Atomic Energy Research Establishment, Harwell (UKAEA/AERE), and with a certain economic support from the Nordic Liaison Committee for Atomic Energy (NKA). The Organisation for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA) participates in the Secretariat, Kemakta Consultants Co. participates in the Secretariat as principal investigator and the Institute for Energy Technology, Norway (IFE) participates as Nordic representative.

The Parties organize project teams for the actual project work with model calculations. Each Party covers the costs for its participation in the study and is responsible for its project team or teams including computer cost, travelling expences etc.

At suitable time intervals depending upon the progress of the study, workshops are arranged, normally in conjunction with meetings of the Coordinating Group. During the workshops problem definitions and achieved results are discussed as a preparation for decisions in the Coordinating Group.

SURVEY OF ORGANIZATION OF HYDROCOIN



<u>Managing Participant:</u>	SKI
<u>Principal Investigator:</u>	Kemakta

<u>Coordinating Group:</u>

Chairman:	A. Larsson, SKI
Vice chairman:	T. Nicholson, NRC
Secretary:	K. Andersson, SKI

<u>Project Secretariat:</u>	K. Andersson, SKI B. Grundfelt, Kemakta D.P. Hodgkinson, AERE A.B. Muller, OECD/NEA U. Tveten, NKA/IFE

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Organization for Economic Co-operation and Development/Nuclear Energy Agency (OECD/NEA)	Member of Secretariat: Org. for Econ. Co-oper. and Dev./ Nuclear Energy Agency (OECD/NEA)

APPENDIX B

A BRIEF DESCRIPTION OF THE SEVEN HYDROCOIN LEVEL ONE PROBLEMS ON VERIFICATION AND BENCHMARKING (TAKEN FROM HYDROCOIN PROGRESS REPORT NO. 2)

BRIEF DESCRIPTION OF LEVEL 1 CASES

<u>Case 1</u> Comparison of numerical solutions with an analytical solution to a problem involving transient flow from a borehole in a permeable medium containing a single fracture. The anticipated situation is given in fig. 1.

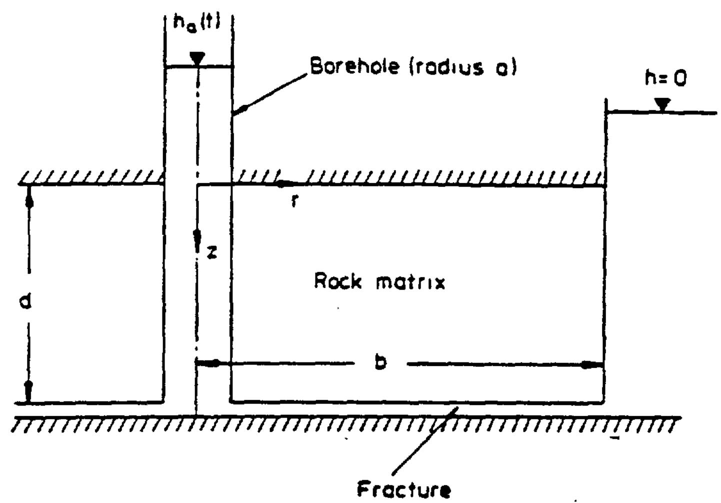

Fig. 1 Schematic diagram of test problem for Case 1.

<u>Case 2</u> Simulation of steady-state flow in a two-dimensional domain containing two permeable fracture zones. The zones are inclined so that they intersect at a certain depth. The modelled situation is shown in fig. 2.

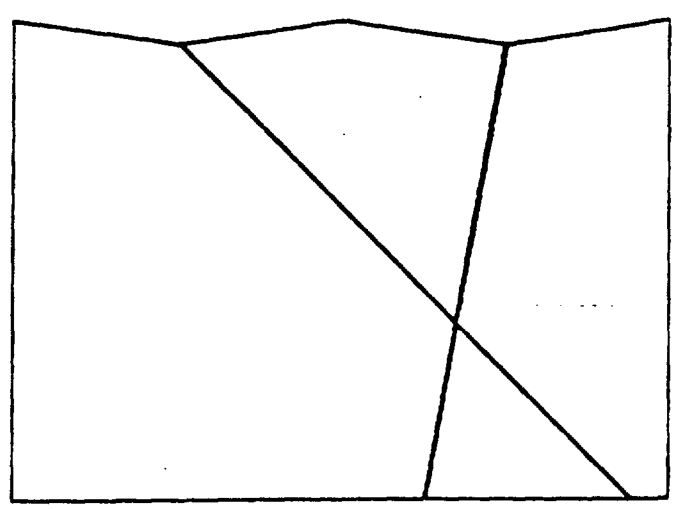

Fig. 2 The geometry of the modelled domain in Case 2. The thick inclined lines represent fracture zones with higher permeability than the rest of the domain.

Case 3 Simulation of partially saturated flow through a sequence of alternating pervious and low permeability sedimentary rocks. The boundary conditions involve a seepage face. The situation is illustrated in fig. 3.

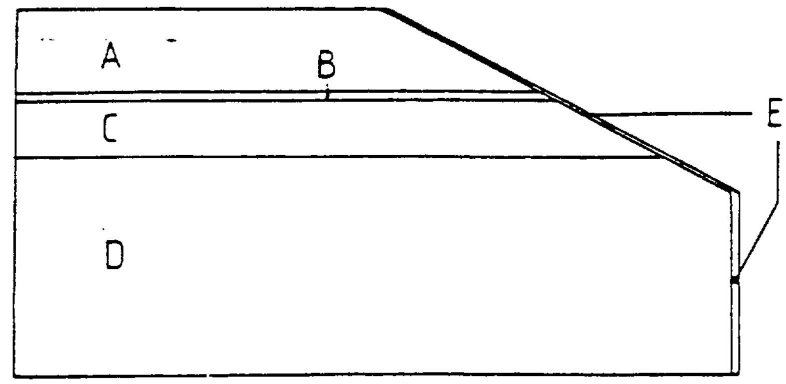

Fig. 3 The geometry assumed for Case 3. The media A and C represent pervious formations whereas media B and D are regarded as relatively impervious. Medium E is used to simulate the seepage face.

Case 4 Comparison of analytical and numerical solutions of thermal convection driven flow. The heat is evolved from a spherical source with a decaying heat output. The thermal bouyancy is the only driving force. The case is illustrated in fig. 4.

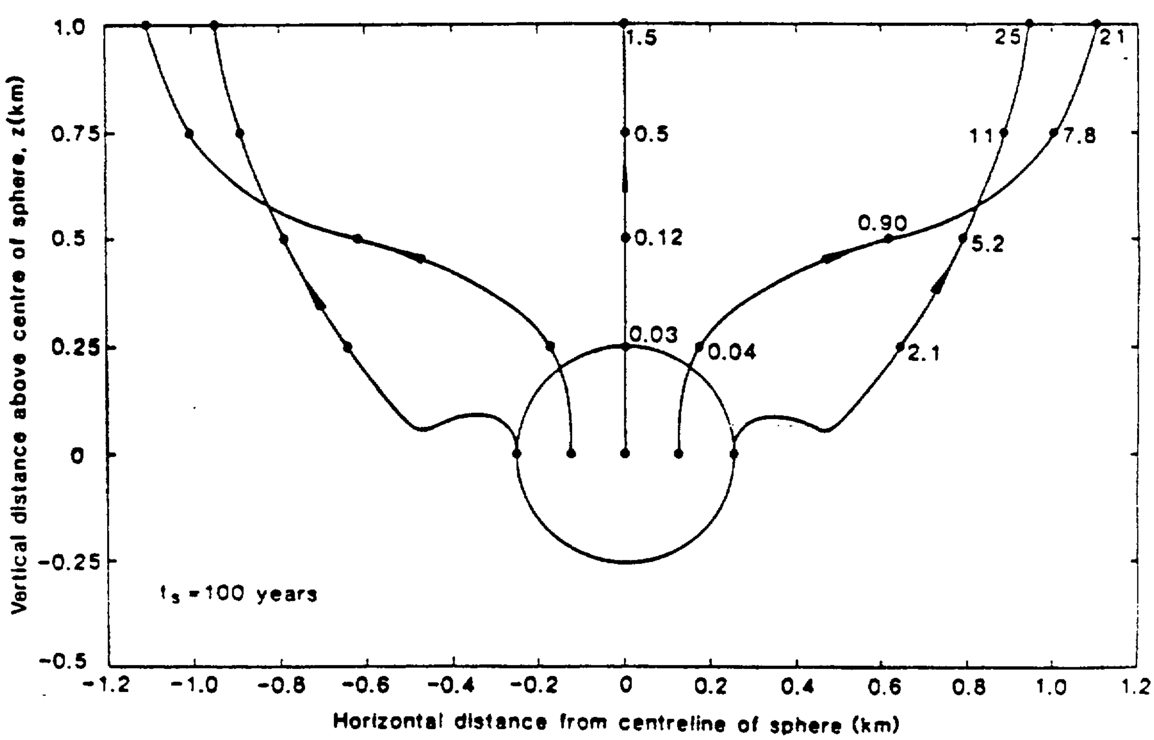

Fig. 4 Representation of the spherical heat source. Shown are also some pathlines starting after 100 years. The numbers represent approximate travel times in thousands of years.

Case 5 Simulation of water flow and salt transport in a two-dimensional domain. The fluid density is linearly dependent on the salt concentration. The domain is illustrated in fig. 5.

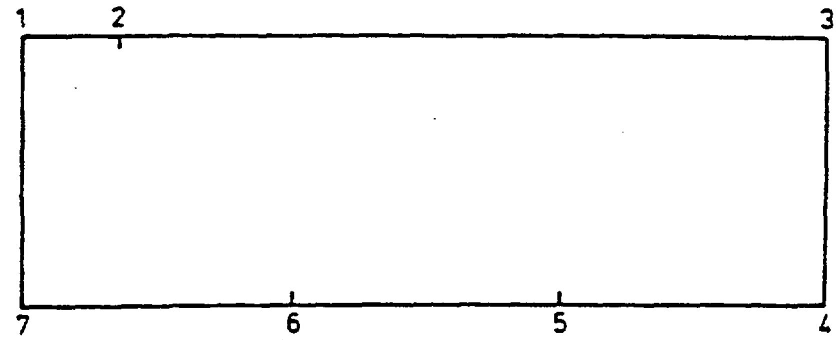

Fig. 5 Geometry of the modelled domain. The bottom boundary between the points 5 and 6 is held at a constant salt concentration.

Case 6 Simulation of steady-state flow in a three-dimensional domain representing a generic bedded salt situation. The domain is shown in fig. 6.

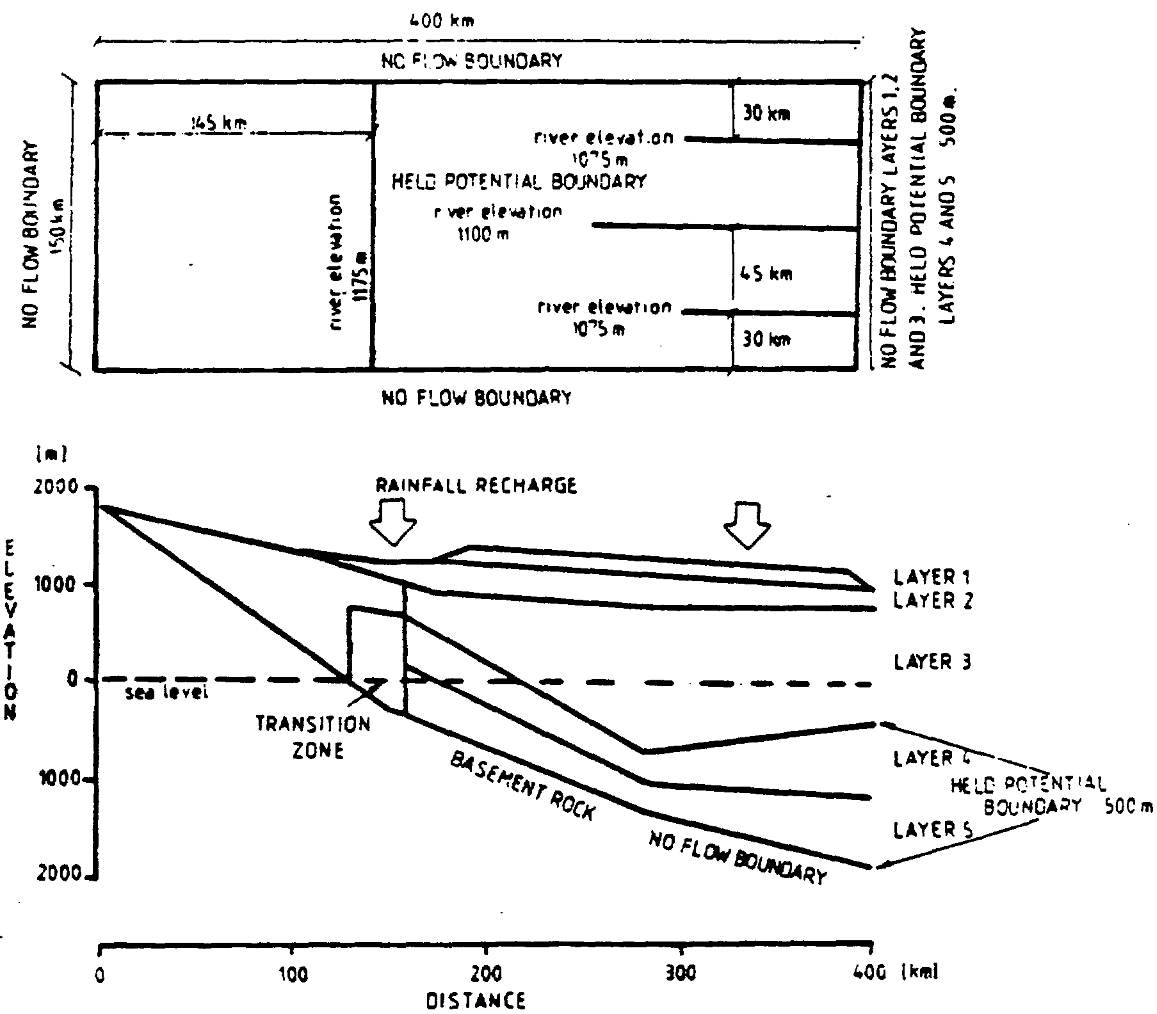

Fig. 6 Horizontal (top) and vertical (bottom) view of the modelled domain for Case 6.

<u>Case 7</u> Simulation of steady-state flow through a shallow land burial site in argillaceous media. The calculations involve saturated flow and the modelling of a seepage face. The modelled domain is shown in fig. 7.

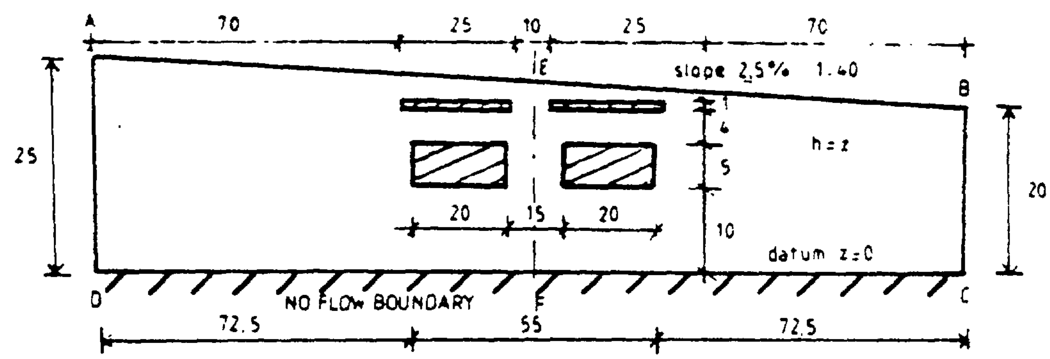

Fig. 7 Schematic diagram of the domain modelled in Case 7. The striped rectangles represent the repository and anti-intervention lids of concrete.

APPENDIX C

TABLE OF CONTENTS FROM THE PROCEEDINGS OF THE SYMPOSIUM ON GROUNDWATER FLOW AND TRANSPORT MODELING FOR PERFORMANCE ASSESSMENT OF DEEP GEOLOGICAL DISPOSAL OF RADIOACTIVE WASTE: A CRITICAL EVALUATION OF THE STATE OF THE ART

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