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Sandia National Laboratories
Albuquerque, New Mexico 87185

'85 NOV 21 A9:15

November 15, 1985

Dr. M. S. Nataraja
Engineering Branch
Division of Waste Management
U.S. Nuclear Regulatory Commission
7915 Eastern Avenue
Silver Spring, MD 20910

Dear Dr. Nataraja:

The enclosed monthly report summarizes the activities during the month of October for FIN A-1755.

If you have any questions, please feel free to contact either myself at FTS 844-8368 or E. J. Bonano at FTS 844-5303.

Sincerely,

R. M. Cranwell

R. M. Cranwell
Supervisor
Waste Management Systems
Division 6431

RMC:6431:jm

Enclosure

Copy to:
6400 R. C. Cochrell
6430 N. R. Ortiz
6431 R. M. Cranwell
6431 E. J. Bonano
6431 K. K. Wahi
6431 L. R. Shipers

3619

PROGRAM: Coupled Thermal-Hydrological-Mechanical Assessments and Site Characterization Activities for Geologic Repositories

FIN#: A-1755

CONTRACTOR: Sandia National Laboratories

BUDGET PERIOD 10/85-9/86

DRA PROGRAM MANAGER: M. S. Nataraja

BUDGET AMOUNT: 175K

CONTRACT PROGRAM MANAGER: R. M. Cranwell

FTS PHONE: 844-8368

PRINCIPAL INVESTIGATOR: E. J. Bonano

FTS PHONE: 844-5303

PROJECT OBJECTIVES

To provide technical assistance to NRC in the assessment of coupled thermal-hydrological-mechanical phenomena and site characterization activities for high-level waste repositories.

ACTIVITIES DURING OCTOBER 1984

Activities and Accomplishments

The effort during October concentrated on formulating and solving Teknekron's benchmark problems using the STEALTH 2D Code, as requested by the NRC. Krishan Wahi travelled to Oakland, California to meet with Douglas Vogt (Teknekron) and Michael Gross (SAIC) to establish the scope of work, "groundrules," and a schedule for the completion of SNLA's effort in assisting Teknekron. A trip report is attached that documents the agreements reached in that meeting. To date, Problems 2.4, 2.8, and 2.9 have been completed. The results obtained are in good-to-excellent agreement with the analytical solutions for these thermal problems. Problem 3.2 (a circular tunnel in an elastic-plastic medium) is nearly completed, the results so far look very promising. Figures 1 through 7 illustrate the results for the problems attempted thus far. Some effort was devoted to reviewing the BWIP ES-I and ES-II Documents, in preparation for the planned meetings with NRC and BWIP in the near future.

The previously modified analytical solution to consider a 3-dimensional temperature distribution in a half space due to an embedded finite-volume heat source was extended to consider nonhomogeneous boundary conditions on the plane surface boundary. Both specified constant flux and constant temperature boundary conditions were considered. These boundary conditions were then included as input options in the computer code used to evaluate the temperature in the half space. The analytical solution for the temperature distribution in an infinite composite medium due to an embedded finite-volume heat source was also developed and incorporated into the 3-dimensional temperature model. The composite-media solution was verified using the 2-dimensional STEALTH code. Agreement between the two solution methods was quite good, with temperatures differing by less than 4% for the cases considered. This difference can be attributed to two factors: the simulation of a semi-infinite region by a finite computational region in STEALTH and the 2-dimensional versus 3-D character of the models. Several test cases were considered in order to examine the effects of various assumptions on the resulting temperature distribution due to a finite-volume heat source. The results of this comparison are presented in Attachment 1. A final report will be prepared to describe all the details of the analytical solution and the resulting computer model.

A report for Krishan Wahi's trip to the Coupled Processes Symposium at LBL September 18-20, 1985 is included as Attachment 2.

Travel

K. Wahi travelled to Oakland, California on October 8, 1985 and met with D. Vogt (CorStar) and M. Gross (SAIC) to coordinate SNLA's assistance to NRC in using the STEALTH Code. (See attachment 3.)

Problems Encountered

None.

Figure 1. Temperature History at Center of Slab

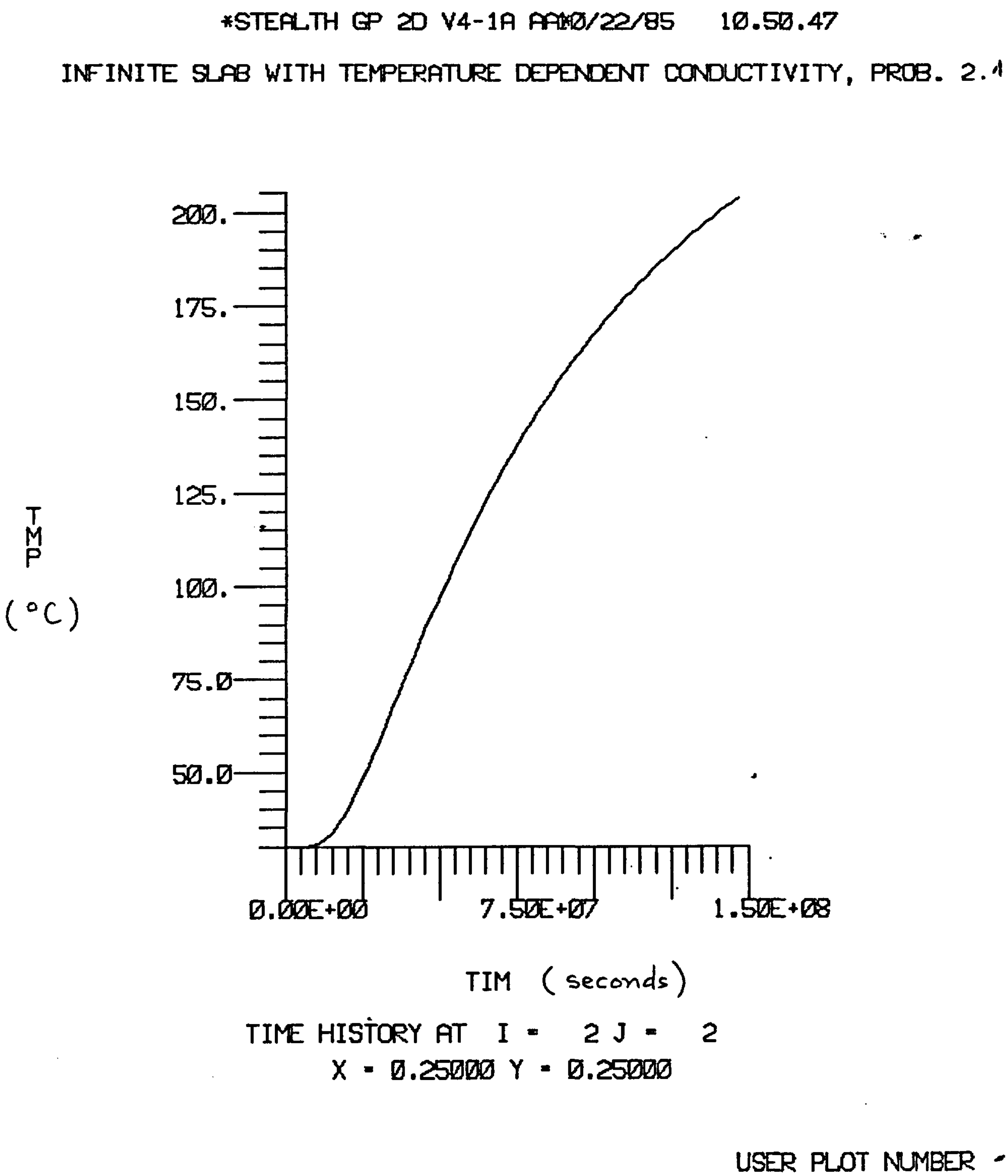
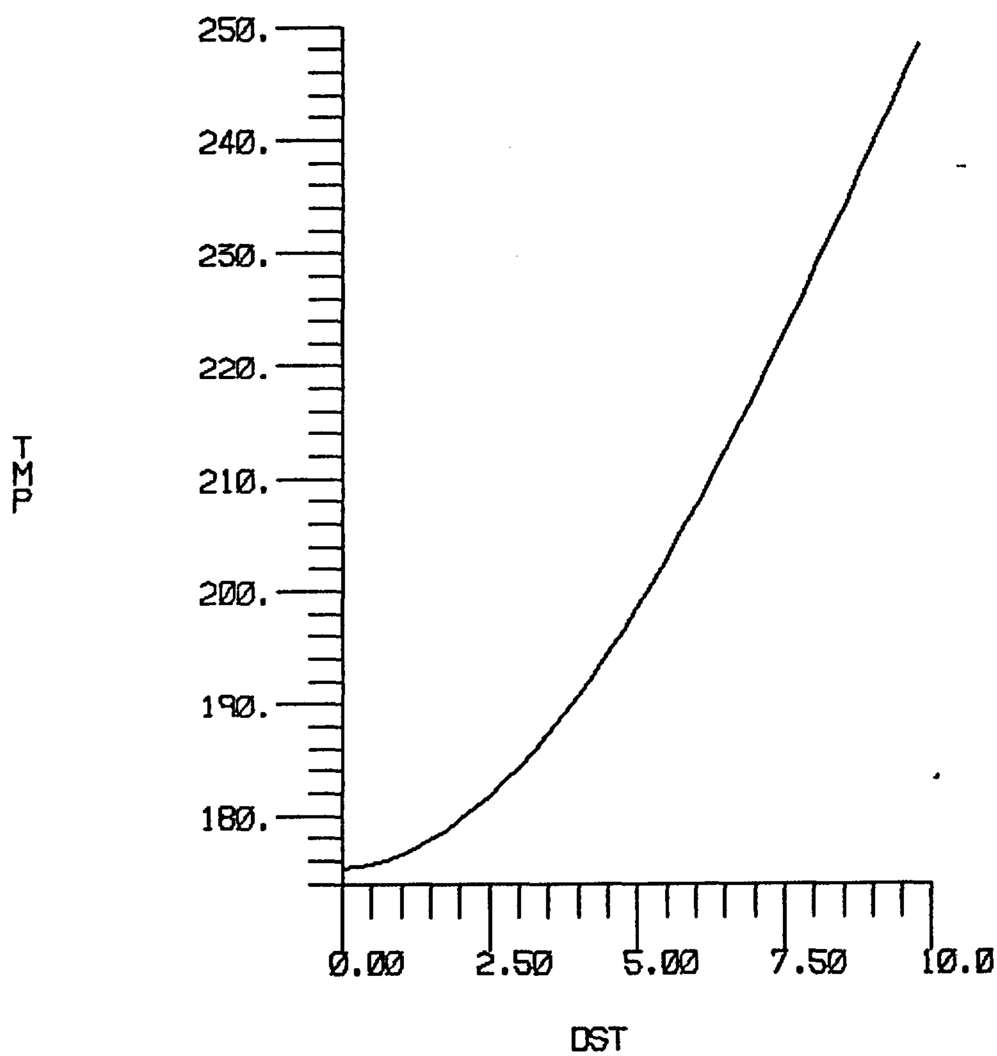


Figure 2. Temperature Distribution in Slab at 30,000 hrs.

*STEALTH GP 2D V4-1A AA10/22/85 10.50.47

INFINITE SLAB WITH TEMPERATURE DEPENDENT CONDUCTIVITY, PROB. 2.4



SNAPSHOT OF ROW 2

TIME = 1.08E+08 CYCLE = 2000

USER PLOT NUMBER =

Figure 3. Temperature History at Exposed Surface

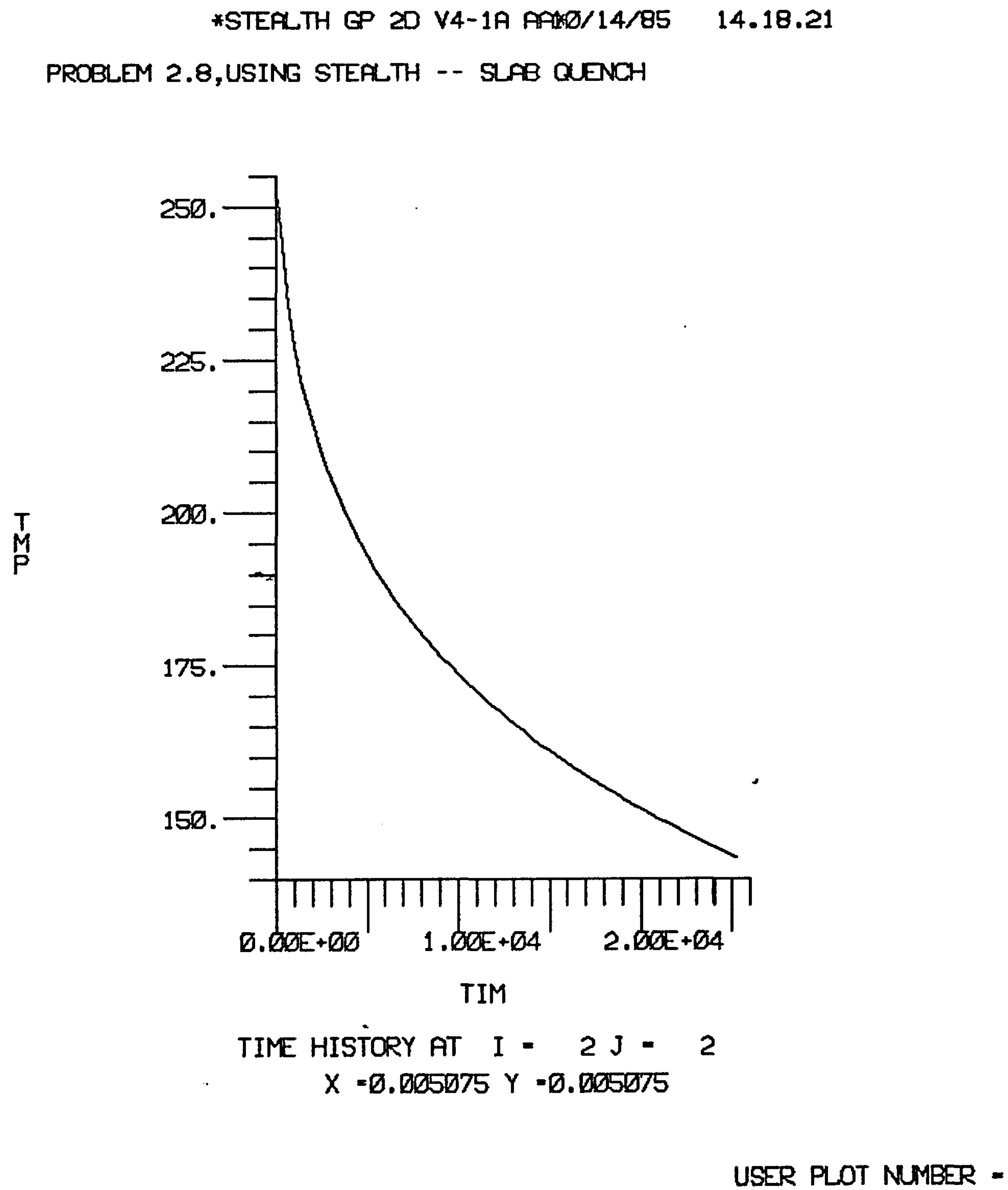


Figure 4. Temperature Distribution in Slab at 4.6 hrs.

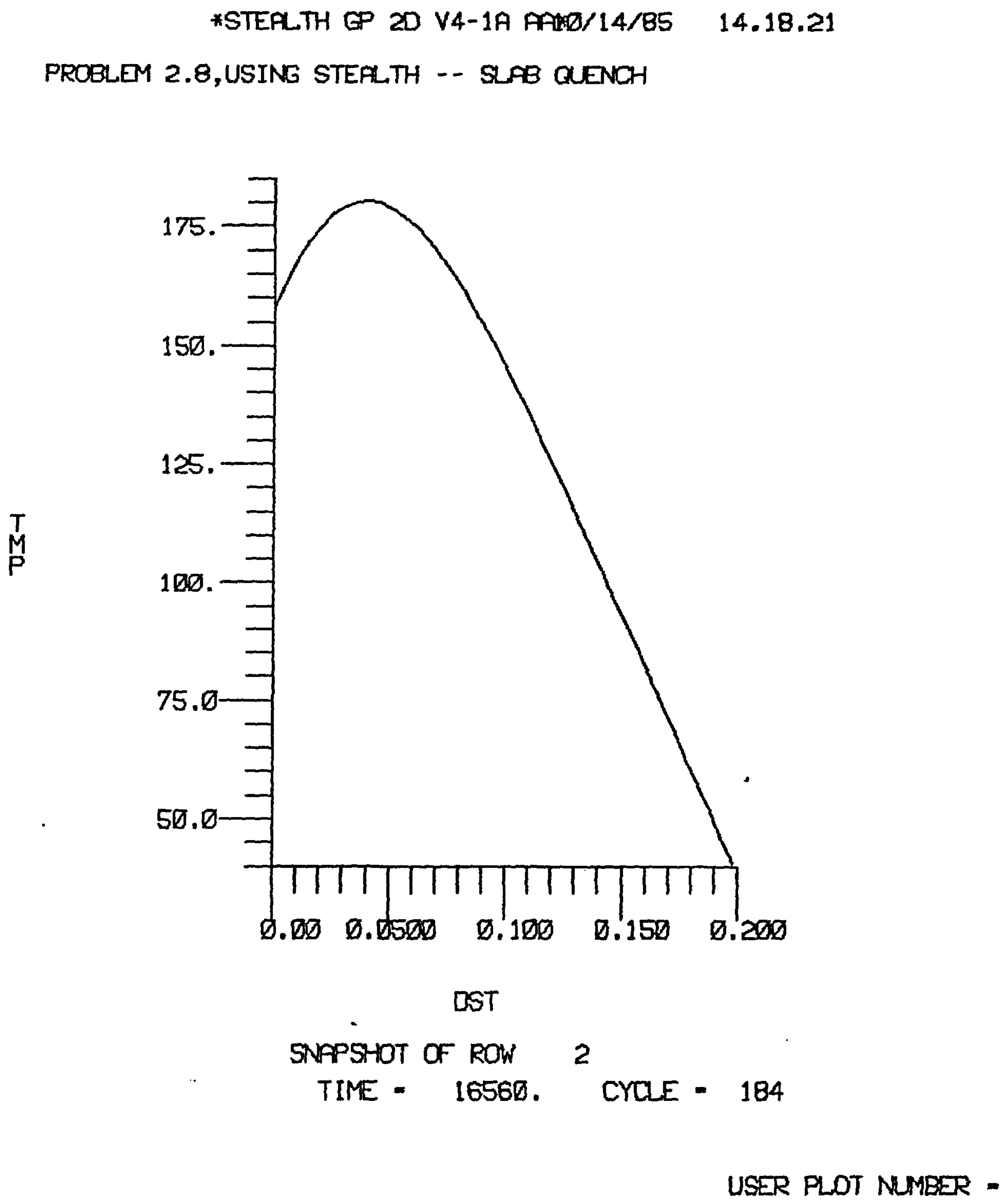
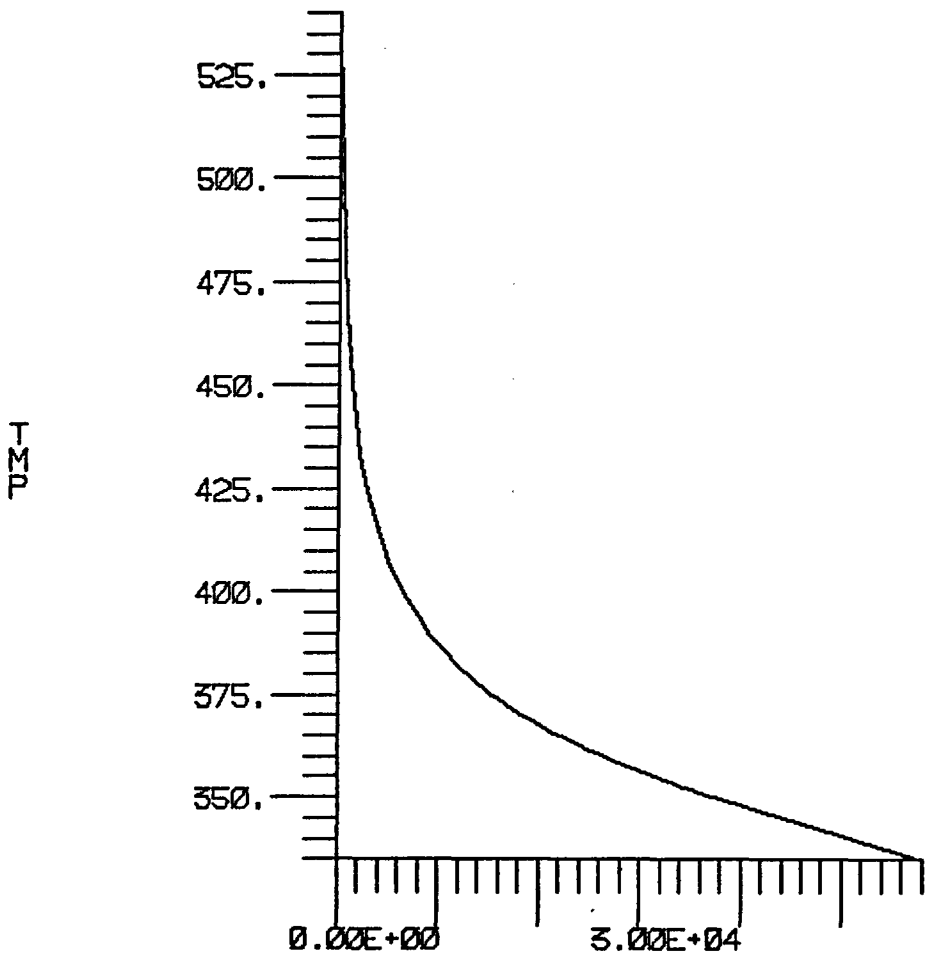


Figure 5. Temperature History at Exposed Surface

*STEALTH GP 2D V4-1A AA10/21/85 14.14.02

PROBLEM 2.9,USING STEALTH -- SLAB RADIATION



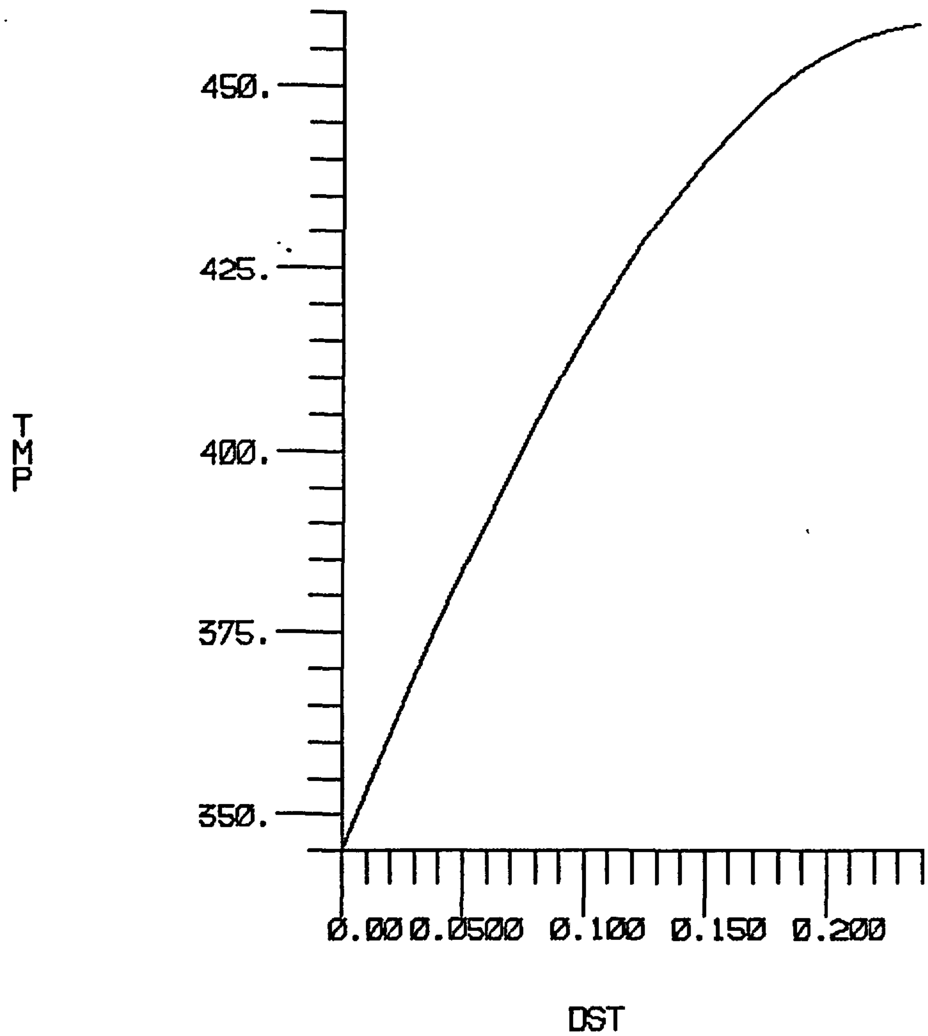
TIME HISTORY AT I = 2 J = 2
X =0.012500 Y =0.012500

USER PLOT NUMBER =

Figure 6. Temperature Distribution in Slab at 12 hrs.

*STEALTH GP 2D V4-1A AA10/21/85 14.14.02

PROBLEM 2.9, USING STEALTH -- SLAB RADIATION



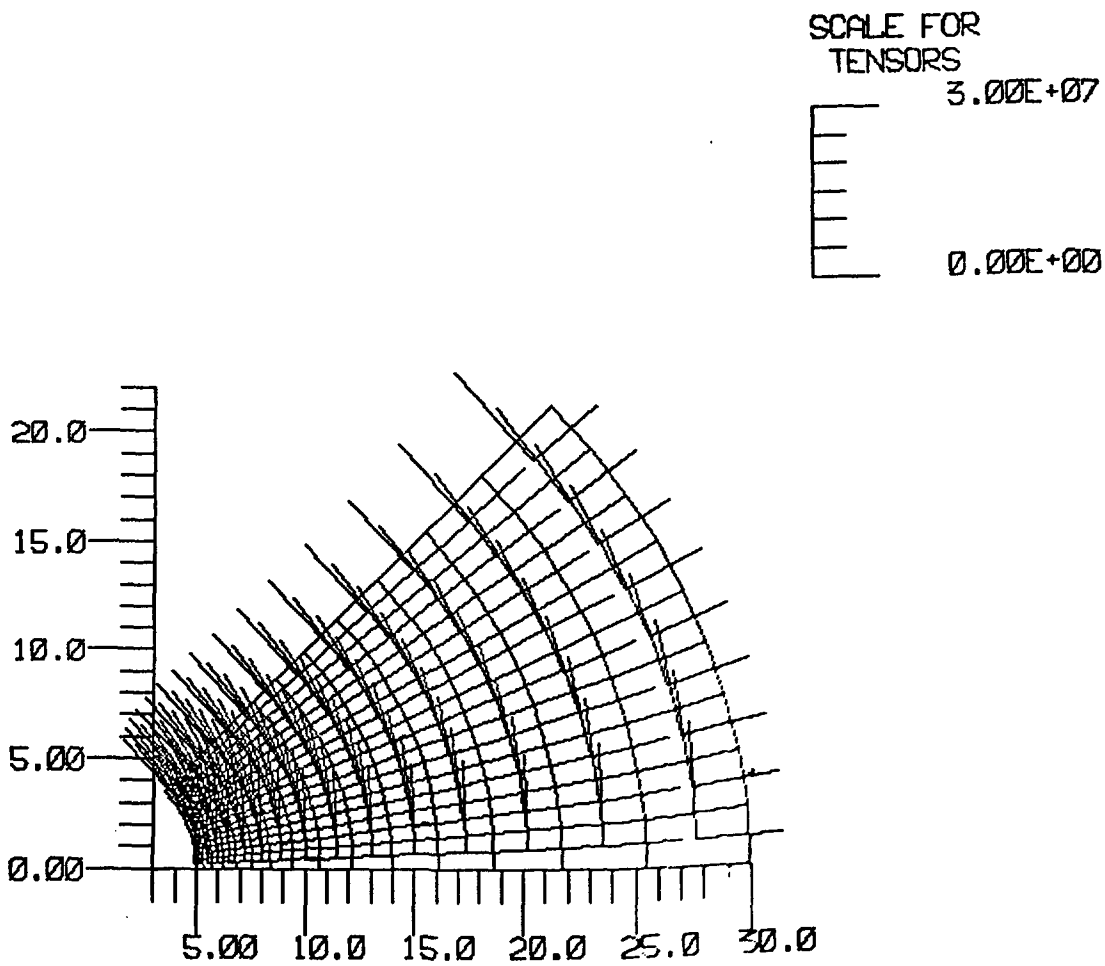
SNAPSHOT OF ROW 2
TIME = 43218. CYCLE = 304

USER PLOT NUMBER =

Figure 7. Stress Tensor Plot Around a Circular Tunnel (elastic-plastic boundary at ~ 6.2 m using Von Mises Criterion)

*STEALTH GP 2D V4-1A AA10/31/85 10.42.57

ELASTIC PLASTIC CIRCULAR TUNNEL, PROB. 3.2



TENSORS OF STR IN GRID NO :
TIME = 10.000 CYCLE = 100

USER PLOT NUMBER =

A-1755
1628.010
October 1985

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month	Year-to-Date
I. Direct Manpower (man-months of charged effort)	1.5	1.5
II. Direct Loaded Labor Costs	18.0	18.0
Materials and Services	0.0	0.0
ADP Support (computer)	1.0	1.0
Subcontracts*	32.0	32.0
Travel	0.0	0.0
Other	0.0	0.0
TOTAL COSTS	51.0	51.0

Other = rounding approximation by computer

III. Funding Status

Prior FY Carryover	FY86 Projected Funding Level	FY86 Funds Received to Date	FY86 Funding Balance Needed
31K	156K	125K	None

*These charges seem excessive. We are investigating them and will resolve the problem in the next monthly.

Attachment 1

In order to examine the effects of various common assumptions used in the thermal analysis for the geologic disposal of radioactive waste, a simplified physical situation was considered. A repository was assumed to be located in a layer of bedded salt bounded above by a layer of shale. The repository was located 500 ft. below this salt/shale boundary. The repository was treated as a decaying heat source with an initial output of 60 kw/acre over an 1100 acre high-level waste disposal area. In the 3-Dimensional temperature model, the repository was assumed to have a square cross section and a unit depth. The heat output was allowed to decay to zero over a period of 600 years. The initial ambient temperature was assumed to be 110°F.

This physical situation was modeled using both a semi-infinite and an infinite conducting medium. In the semi-infinite medium model, a plane surface boundary was assumed to be located at the salt/shale boundary. Two types of boundary conditions were considered on this surface. In the first, the temperature on this plane surface boundary was assumed to be constant at the initial ambient value. In the second, the salt/shale interface was treated as an insulated boundary. Two cases of an infinite conducting medium were also considered. In the first, the infinite medium was assumed to be only salt. In the second, a composite medium consisting of semi-infinite salt medium bounded above by a semi-infinite shale medium was used.

The resulting temperature profiles of two points located above the center of the repository for each of these models are shown in Figs. 8 and 9. As can be seen from the figures, the choice of model type has no effect on the resulting temperature profiles for early times but as time increases a signification difference results due to the model choice. Note that the insulated boundary condition, allowing no heat loss across the salt/shale boundary, results in the highest temperatures at longer times while a specified temperature boundary resulted in the lowest. The two infinite media models resulted in temperature profiles between the semi-infinite media cases. The composite media case, where shale with its lower thermal conductivity acts as a quasi-insulator, resulted in higher temperatures at longer times than the infinite salt media case. Note also that the magnitude of the peak temperature at a point away from the repository surface depends upon the model type. Again, an insulated boundary, results in the maximum peak temperature.

In conclusion, the assumptions embedded in the thermal analysis of a geologic repository for radioactive waste can have significant effects on the resulting time dependent temperature distribution. While a period of time does exist when the different models do predict the same temperature distribution, the length of this time period depends on both the physical characteristics of the system considered and the distance from the repository. The resulting peak temperatures at a point not on the repository boundary are also significantly affected by the assumptions of the thermal analysis.

Figure 8

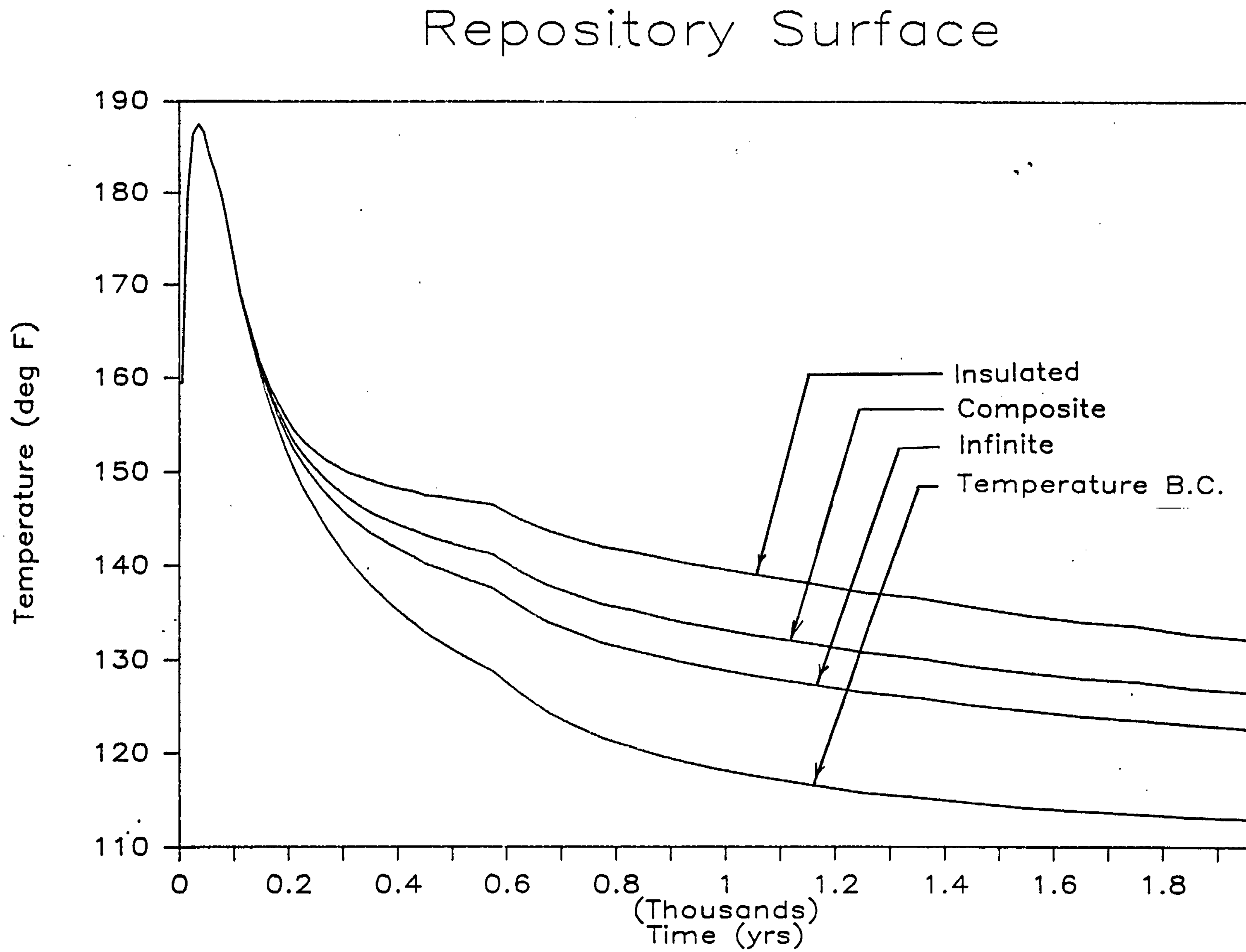
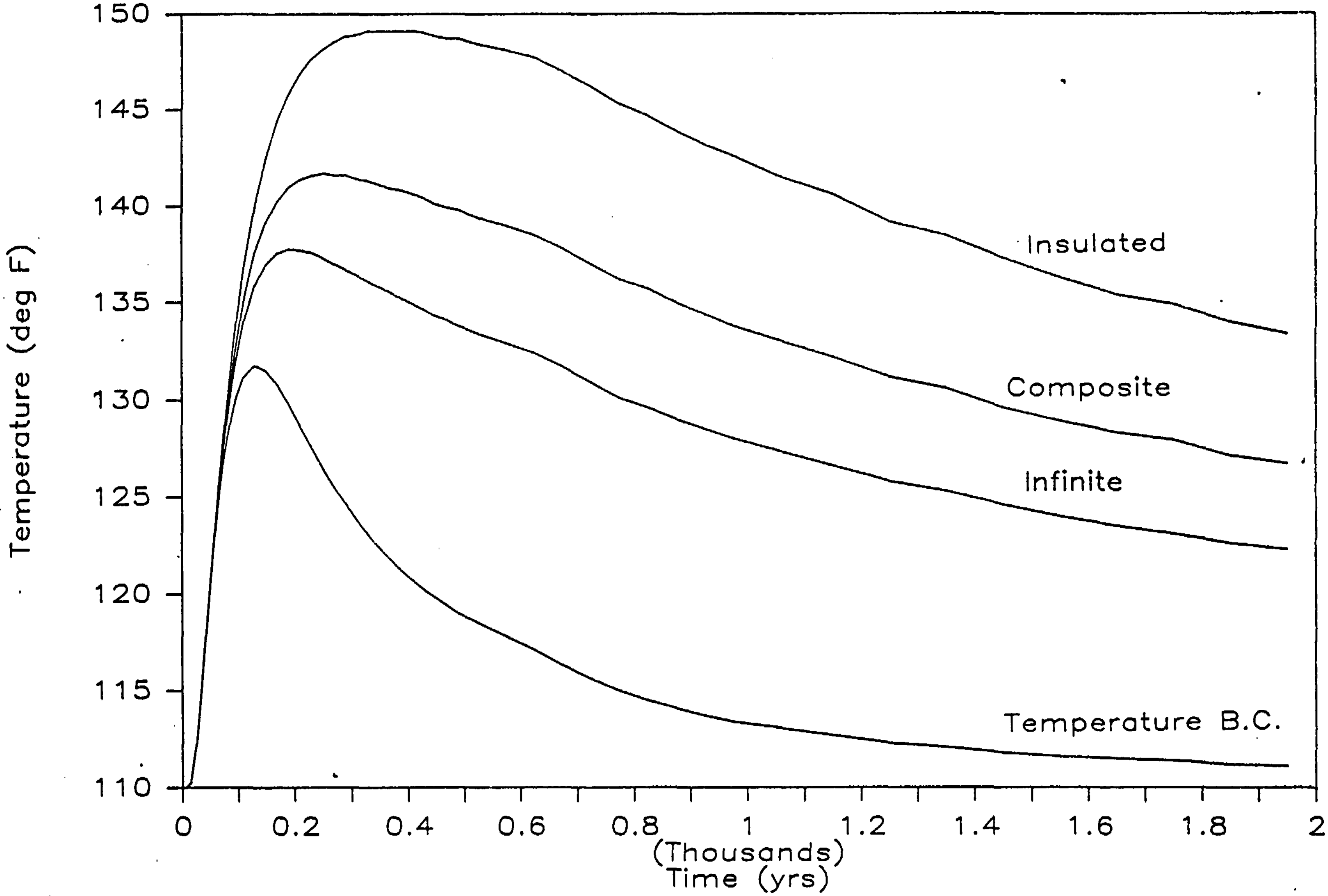

Repository Surface
190
180
170
160
150
140
130
120
110
Temperature (deg F)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
(Thousands)
Time (yrs)
Insulated
Composite
Infinite
Temperature B.C.

Figure 9

200 ft. Above Repository



Berkeley Trip Report

A symposium on coupled processes was held at Lawrence Berkeley Laboratory (LBL) in Berkeley, CA on September 18-20, 1985. The title of the symposium is "International Symposium on Coupled Processes Affecting the Performance of a Nuclear Waste Repository." At NRC's request, Krishan Wahi attended these meetings in support of the FIN A-1755 Project. The following is a chronological summary of important presentations and discussions that took place.

The first part of the morning session on Wednesday (September 18) consisted of presentations by U.S. and International Agencies providing programmatic overviews and objectives. C. Klingsberg from the U.S. Department of Energy provided surprisingly little information. S. G. Carlyle from OECD Nuclear Energy Agency alluded to their role in ISIRS and CODATA, which are geochemical and thermochemical data bases. He concluded that coupled processes are a principal issue in performance assessment. P. Venet from the Commission of European Communities (CEC) described the laboratory scale and in-situ testing programs being conducted and planned for near future. In the testing done to date, the influence of brine and of stress level on creep rates has been measured. Based on field data, the effect of a magmatic intrusion on a clay body is estimated to have caused mineralogic changes to a distance of 4m and dehydration to a distance of 8m; the maximum temperature at the time of intrusion being roughly 800 degrees Celsius. Paul Witherspoon (LBL) talked about the necessity of large-scale underground testing to understand fracture flow and couplings among different processes. He reported that their work has shown that the cubic law (for fracture flow) begins to fail at 10 to 20 MPa of normal load. Shear deformation of the fracture starts to dominate, and less that 1mm of movement can cause an order of magnitude change in permeability. He showed a conceptual model which is a set of interconnected discs simulating cracks. He posed the following question to all present: "To what extent will it be necessary to carry out large-scale in-situ tests over several years in order to validate a code to sufficient degree?"

The second part of the Wednesday morning session consisted of presentations on the current field projects in the U.S. (BWIP, SRP, NNWSI). D. Dahlem from DOE provided an overview of the BWIP program which is using a systems engineering approach. A copy of his paper was available. It includes two tables that show the exploratory shaft objectives and planned tests, and hydrologic test activities. According to Dahlem, seismicity is a major concern at the Hanford Site. H. Kalia (ONWI) spoke on coupled processes addressed by the planned underground testing for the SRP. The basic objective of the proposed testing, according to Kalia, is to sufficiently reduce uncertainties arising from incomplete understanding of processes, their representation by models, and in the system parameters. A tentative set of information needs (that consider coupled processes) is presented in Table 1 of his paper; and Table 2 outlines a proposed underground test program. In answer to a question on utilizing data from other in-situ tests, the response was that ONWI would like to use data from Germany, Avery Island, and WIPP; however, he could not say how much of that would be used to support the license application. Mike Voegele (SAIC) made a presentation on behalf of DOE on the in-situ testing at Yucca Mountain, Nevada Test Site. A total of 28 tests are proposed to conduct in-situ measurements from the planned 1480-ft deep exploratory shaft. The tests are in four general categories: (1) geological characterization, (2) geomechanical characterization, (3) hydrologic and transport phenomena characterization, and (4) near-field characterization and measuring effects of thermal perturbation. Some of the proposed tests are designed to investigate coupled phenomena. A copy of this paper was available (though not included in the draft proceedings document).

The Wednesday afternoon session provided reports on international (outside the U.S.) field testing programs. A. Barbreau presented a talk on "French Field Investigations in the Underground Laboratory at Fanay-Augeres." S. G. Carlyle (OECD) reported on recent progress of the NEA Stripa Project. Results from Phase 1 and early results from Phase 2 were outlined along with possible future research under any Phase 3 of the project. The primary conclusion was that there is great difficulty in measuring detailed hydrogeochemical processes. In a large-scale heated buffer mass test (blocks of sodium bentonite), temperature, moisture content, swelling pressure, and piezometric head were measured. The results compared very well with the predicted behavior of the buffer material. The authors conclude that existing predictive flow models can be adapted to a site only by developing a detailed understanding of the hydrogeochemical processes operating at that site.

K. Dormuth (AECL) gave an overview of geotechnical experiments in the Canadian Program. The major objectives of the experimental programs are the development and validation of mathematical models soundly based on field observations. The construction of the Underground Research Laboratory (URL) in Manitoba has been used to perform hydrogeological and geomechanics experiments as well as model predictions . R. H. Heremans (ONDRAF/NIRAS) reported on the Belgian Program of disposal in a clay formation at a depth of roughly 230m. An underground facility was constructed in Boom Clay for in-situ experimentation.

The construction was started in artificially frozen soil, but the last portion of the construction project involved excavating a 20m deep shaft and a 6m long horizontal gallery in unfrozen clay, both with a diameter of 1.4m. Since late 1984, in-situ experiments have been launched in areas of corrosion testing, heat transfer and hydrology and radionuclide migration. A long-term risk evaluation has been undertaken that uses the "fault-tree" approach. The Boom Clay characteristics have been determined to be relatively constant throughout its thickness of roughly 100 m. A repository is feasible if the waste is allowed to cool off for nearly 50 years. Mineability in unfrozen clay on a larger scale remains to be demonstrated. C. McCombie (NAGRA, Switzerland) provided an overview of the Swiss Program for HLW disposal. The underground test facility at Grimsel is expected to provide data for both: a HLW repository ("Type C"), and a low and Intermediate waste repository ("Type B"). The granite at the test facility has an overburden of a few hundred meters.

The Thursday morning session consisted of three invited papers on coupled processes with emphasis in the areas of Geohydrology, Geomechanics, and Geochemistry, respectively. G. de Marsily (Ecoles des Mines, Paris) presented an overview of coupled process with emphasis in geohydrology. He estimated the energy (heat) released from the high-level waste as being 100 times that of an earthquake with a magnitude of 6.6; thus, a repository could be a potential trigger for creation of new faults. Possibility of "piping" (due to preferential dissolution) as well as clogging due to silica precipitation was mentioned. Transport of colloids may occur at velocities that are 10% to 40% higher than the ground-water velocity. His conclusions were that coupled processes are not minor effects, and these effects may be synergistic. Priorities, according to de Marsily, should be studies in: (1) large-scale T-H-M effects, (2) colloid transport in fractures, (3) T-C effects (precipitation/dissolution), (4) Thermodynamics, (5) T-H currents, and (6) dispersion and channeling. Neville Cook (LBL) presented a discussion from the geomechanics point-of-view. He believes that the excavation will cause the maximum perturbation to the in-situ environment. Formation of new fractures in the vicinity of the excavations and/or movement across pre-existing fractures may enhance the rock permeability. Previous underground experience and in-situ testing should be most valuable in identifying and understanding coupled phenomena in geomechanics. Some examples of different opening shapes and in-situ stress environments were given to illustrate the potentially adverse and beneficial situations. It was pointed out that the commonly accepted cubic-law for flow in fractures may not hold at higher stress levels. D. Langmuir (Colorado School of Mines) gave an overview of coupled processes with emphasis in geochemistry. He believes that geochemistry plays a very important role in terms of coupled effects and should receive more attention in terms of research and modeling efforts. He cited geochemical effects and parameters that can alter the hydrologic properties.

Thursday afternoon meetings consisted of a review of contributed papers by three rapporteurs (K. Preuss, B. Clark, and C. L. Carnahan) and a poster session for all contributed papers. A majority of these papers are included in the proceedings of the symposium.

The Friday morning session included discussions stimulated by the contributed papers with the rapporteurs of the previous day acting as the discussion leaders. B. Clark (Leighton and Associates) commented that there was no time or money to do irrelevant experiments. C. F. Tsang brought up the subject of the Oklo reactor (a natural reactor) serving as a data base for validation. Someone from LBL elaborated further by referring to Oklo studies. He felt that it was unlikely that one could ever model the transport of elements as they have occurred at the Oklo site; however, the "fixation" of elements could be modeled with relative ease. The pressure and temperature conditions at Oklo are generally more adverse than for proposed repositories. Witherspoon questioned the applicability of block tests (typically, 2 meter cubes) to larger dimensions and repository depths in terms of predicting the system response. Dan Reeda (SNLA) referred to careful laboratory experiments being performed at Sandia in attempting to validate MYRIAH, a flow and transport code. K. Soo Kim (BWIP) claimed that the thermal response of in-situ tests at NSTF was predicted fairly accurately. K. Wahi expressed a concern about placing too much faith in field measurements with improper or inadequate instrumentation and then attempting to fit material behavior (e.g., constitutive law development) to the data. It is not uncommon to get anomalous response from sophisticated instruments. Tito Bonano (SNLA) stated that validation attempts should be categorized according to what can be validated in the lab, in the field, and "not at all". G. de Marsily reiterated the role of analog studies for validation purposes. Nerenieks (Sweden) fels that both, refined scale as well as large scale tests are needed to understand and characterize interactions among rock, rock surface area, and matrix diffusion. The largest scale experiment at Stripa for such studies is 75 m. S. Neumann (Univ. of Arizona) said that different mathematical descriptions may apply at small scale versus large scale for the same type of process. Reference was made to statistical methods as having meaningful applications. Jane Long (LBL) does not think that scaling laws will work in describing fracture flow. Commenting on relative scales for geochemical effects, Langmuir expects that precipitation and dissolution are limited to the first few meters. He mentioned the distinct possibility that radionuclides (RN's) don't follow the same travel path as the ground-water. Another participant felt that geochemistry could provide a lot of performance (i.e., an effective barrier). R. Fournier (USGS) reported that there aren't any colloids in old, natural systems; supersaturated conditions need to exist for colloids to be present. K. Preuss feels that theoretical predictability is rather limited for "real world" systems.

The Friday afternoon session was a panel discussion on "coupled Processes for a Nuclear Waste Repository". The panel consisted of leading experts in different disciplines. The members were: C. Fairhurst, R. Fournier, K. Kovari, I. Neretnieks, S. Neumann, T. Pigford, P. Witherspoon, and C. F. Tsang (moderator). Each panel member made a short presentation in his area of expertise followed by discussion and questions from the audience. Fairhurst thinks that issues of credibility are developing that need to be addressed; engineers don't feel comfortable predicting system behavior for periods beyond a hundred years or so. On the contrary, geoscientists have trouble predicting phenomena for times less than 10^5 years. He referred to the new, developing field of "Discrete Mechanics" as a hopeful way of understanding non-linear rock behavior. K. Kovari (Switzerland) warned against "orbiting" around the problem by thinking up endless combinations of coupled processes that may be interesting but do not truly interfere with designing a safe repository. Neretnieks mentioned that only a part of a fracture participates in flow which makes it very difficult to characterize and quantify the sorption phenomenon in these fractures. Under certain circumstances, chemistry can affect stress. For example, in the backfill, chemical reactions can generate swelling pressures if water infiltrates. S. Neumann believes that storativity effectively provides a coupling involving heat, fluid flow and stress. The "megapermeability" (i.e., permeability of a large rock mass) approach may be acceptable for <u>flow</u> in the far-field; however, small details can be very important. R. Fournier sees major problems that are poorly understood if the fluid temperatures are higher than 100 C. His feeling is that in hindsight anything can be modeled, but truly predictive modeling may not be very reliable. T. Pigford was in favor of taking the performance assessment approach. He said that research is not the mission or need of the national programs regarding high-level waste management. In his opinion, the DOE has to make sensible decisions now and there is a danger in waiting too long; it would be an invitation to open ended research and development. Reliablity of predictions is the most difficult part of this whole process. Yet, some of the most reliable predictions are very inexact. Adding more detail adds more parameters which tends to lower the reliability of results. His opinion is that the most reliable predictions are based on theory that can be validated, and that empirical approach is not very desirable. As a specific item, he identified detailed modeling of mass transport as a requirement. Paul Witherspoon, who is in favor of extensive in-situ testing (not necessarily at potential repository sites), posed the question of "how do you reconcile ten orders of magnitude variation in, say, hydraulic conductivity (10^{-15} cm/s to 10^{-5} cm/s) in the context of Pigford's suggestion of reliable predictions?" The other question from him was to what extent is there a need to rely on large-scale in-situ tests to validate the codes used in predictions? His list of priorities included R & D studies and efforts on: (1) waste form, (2) Copper canister (because of its excellent corrosion resistance), (3) Backfill, and (4) Rock mass characterization with respect to heat effects and hydrologic properties.

Attachment 3

Trip Report

Krishan Wahi travelled to Oakland on October 8, 1985 to meet with Douglas Vogt (CorSTAR/Teknekron) and Michael Gross (SAIC) to discuss and plan SNLA's role in assisting CorSTAR in benchmarking the STEALTH code. Each of the proposed problems was discussed at some length. For some of the problems identified as benchmark problems for STEALTH (2.6 and 2.10), it appears that STEALTH may not be well suited. So, the possibility of replacing two or three problems with other benchmark problems was mentioned. Doug Vogt will bring this up with Acres American and the NRC. The following agreements were made among the meeting participants:

SAIC will provide the most recent set of updates to STEALTH (Version 4-1A) that are currently being used for ONWI work. In addition, draft documentation for any new or modified user instructions will be provided for the geomechanics version of the code.

Krishan Wahi will provide a tentative estimate of completion dates subject to revision due to other NRC priorities for his time.

It will be sufficient to get each problem successfully started and run partially (i.e., not necessarily to final time). The input files will then be turned over to CorSTAR for them to run each problem to completion.

It is unclear at this time as to what is the best modeling approach for Problem 6.3. Some recommendations were made by Wahi which are under consideration by CorSTAR. Specifically, the issue of two-dimensional calculation(s) was debated. It was suggested that a set of 2D calculations be performed in lieu of a 3D calculation. A decision will be made in the near future.

Problem 6.1 (Project Salt Vault Simulation) will be formulated as a two-dimensional plane-strain problem. The "exponential-time" law will be used to describe creep. Instantaneous excavation and a plane of symmetry through "Pillar 2-3" will be assumed.

Sandia National Laboratories
Albuquerque, New Mexico 87185

October 29, 1985

Dear Colleague:

By now you should have received an invitation from Dr. John Randall of the U.S. Nuclear Regulatory Commission to participate in the upcoming Workshop on "Validation of Mathematical Models for Waste Repository Licensing." This workshop is to be held December 2-4, 1985 in Washington, D.C.

As mentioned by Dr. Randall, enclosed is a packet describing the workshop, its rationale, and the agenda. If you are either a speaker or a panelist, you should have also received appropriate instructions with Dr. Randall's letter.

If you have any questions or need additional information, please feel free to contact either J. D. Randall (304-427-4633), F. A. Kulacki (303-491-6603), or myself (505-844-5303).

I am looking forward to seeing you at the workshop.

Sincerely,

E. J. Bonano
Waste Management Systems
Division 6431

EJB:6431:cv

FROM	DATE OF DOCUMENT	DATE RECEIVED	NO
SNL	11/15/85	/21/85	WM-51034

LTR	MEMO	REPORT	OTHER
XX			

TO	ORIG.	CC	OTHER
MNataraja		XX	

ACTION NECESSARY	[X]	CONCURRENCE	[ ]	DATE ANSWERED
NO ACTION NECESSARY	[ ]	COMMENT	[ ]	BY 12/5

CLASSIF	POST OFFICE	REG. NO.	FILE CODE:
			426.1

DESCRIPTION (Must Be Unclassified)

Oct 85 Report for FIN A1755

ENCLOSURES

REFERRED TO	DATE	RECEIVED BY	DATE
MGreeves	11/21		
MNataraja			

REMARKS

Closed 12/4 –
Memo to Cranwell

U. S. NUCLEAR REGULATORY COMMISSION

MAIL CONTROL FORM

FORM NRC 326 (1-75)