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January 15, 1985

NRC FIN 6985

WM-RES
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CorSTAR

WM Project 10,11,16
Docket No. ✓
PDR ✓
LPDR ✓(B,N,S)

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Ms. Pauline Brooks, Project Officer
Division of Waste Management
MS 623 SS
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

Subject: Contract No. NRC-02-81-026
Benchmarking of Computer Codes and Licensing Assistance
Monthly Letter Progress Report for December 1984

Dear Pauline:

This letter contains a management level summary of progress during the month of December. Attached to the report is a copy of the technical status summary with further discussion of work performed during this period. We are submitting a cost summary under separate cover.

Task 1- Literature Search - Waste Package Codes

We are still waiting to obtain permission to use certain tables and figures in the final data set report. When permission is obtained from all publishers we will forward a final camera-ready copy to you.

Task 3 - Benchmark Problem Report - Waste Package Codes

As of the date of the monthly progress report we are awaiting receipt of the NRC's comments on this report. Upon receipt of the NRC's comments, appropriate changes in the report will be made and reviewed with you. The report will then be prepared in final form and submitted for publication. We estimate that six to ten weeks will be required to prepare the report in final form after receipt of the NRC's comments.

Tasks 4 & 5 - Siting Codes

During December no significant activities were conducted on this task. In January we will begin efforts to revise the final report covering Tasks 4&5 of the Siting Codes.

CORPORATE SYSTEMS, TECHNOLOGIES, AND RESOURCES
7315 WISCONSIN, NORTH TOWER #702 • BETHESDA, MARYLAND 20814 • (301) 654-8096
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Tasks 4&5 - Radiological Assessment Codes

In early January we resolved the problem in running the code ORIGEN at ORNL for problems with more than 10,000 lines of printed output. As of the date of the monthly progress report, all of the ORIGEN runs have been submitted. The section of the radiological assessment code report dealing with ORIGEN has been approximately 30 percent written as of the date of the progress report.

Tasks 4&5 - Repository Design Codes

During the month of December work continued on Task 4. No new codes were installed at Brookhaven this month. We are waiting notification from the NRC that the codes ADINA and ADINAT have been installed in the Brookhaven system. We have received a response from the NRC in a letter dated December 21, 1984 authorizing changes in the scope of work brought about by the unavailability of the SPECTROM codes. These changes are reflected in the project's status table included in the technical status summary report. The scope changes will not result in changes to cost or delivery of contract products.

During the month, Problem 3.2A was analyzed with MATLOC. The results of this run are included at the end of this report. Problems 5.2-BASALT and Problem 6.3 have been run with MATLOC. Results of these problems have not yet been summarized.

By letter dated December 4, 1984, the NRC commented on certain aspects of the benchmark results for the code DOT. A copy of the NRC letter and comments along with our response is included with the Technical Status Summary Report.

General

Our estimate of costs through the end of December (through December 8, 1984 for CorSTAR) is:

Actual costs this month:	25K
Actual costs this fiscal year:	133K
Actual costs to date:	2907K
Planned costs this month:	36K
Planned costs this fiscal year:	136K

These estimated costs include labor, labor additive, overhead, subcontractor costs, other direct costs, G&A and fee. These cost estimates have not been confirmed by our accouting department.

Sincerely,

Doug

Douglas K. Vogt
Project Manager

cc: D. Fehringer

TECHNICAL STATUS SUMMARY

TECHNICAL STATUS REPORT ATTACHMENT
TO PROGRESS REPORT FOR DECEMBER 1984

Repository Design Codes

Task 4 - Code Procurement

NRC letter to CorSTAR dated December 4, 1984 and included in this report, states that the source tapes for ADINA, ADINAT, ADINA-IN, and ADINA-PLOT have been received from ADINA Engineering. We are awaiting word of the installation of these codes on the Brookhaven system.

Scope changes, brought upon by the unavailability of the SPECTROM codes, were authorized by the NRC in their letter dated December 21, 1984. These scope changes are reflected in the Project Status table included at the end of this report. They do not result in changes to costs or delivery of contract products.

Code Installation

No new codes have been installed this month. We are awaiting notice of the installation of the ADINA and ADINAT codes at Brookhaven.

Run Benchmark Problems

Problems 3.2a, 5.2 - Basalt, and 6.3 have been run using MATLOC. Only the results of Problem 3.2a have been summarized to date. These results, which are included later in this report, agree well with the analytical solution of this problem.

Write-up Results

The NRC response to the Monthly Progress Report for October, 1984 (letter dated December 4, 1984) to CoSTAR included comments and questions regarding the draft write-up of the DOT report. A copy of the NRC letter is attached to this report for ease of reference.

Many of the comments were somewhat unexpected since they appear to question the use of values for certain parameters even though the values were given in the earlier report NUREG/CR-3636 - Benchmark Problems for Repository Design Models. This report was reviewed by NRC and formed the basis for the problems now being tested by the various codes being benchmarked. Although in most cases the problems could be rerun with different values for parameters, this would involve additional costs and schedule changes. For the analytical problems it is of course necessary to use the same parameter values as used in the original analytical solution and such problems were never intended to simulate actual repository site materials.

Detailed responses to the various comments are as follows:

1. Section 6-2, Problem 2.6

   While the use of temperature dependent material properties creates a more realistic problem, this was not the way the input data was given in "Benchmark Problems for Repository Design Models" (NUREG/CR-3636). This problem is meant to be only a comparison between a proven analytical solution and computer code results. As long as both methods use the same input parameters, a comparison between the two methods can be made. Additionally, incorporating temperature dependent variables into the analytical solution method could prove to be difficult.

2. Section 6.3, Problem 5.2B (Basalt)

   2a. The use of constant thermal conductivity and specific heat material properties was proposed in the Benchmark Problems Report (NUREG/CR-3636), which was reviewed by NRC.

   2b. The material property table in question is repeated below.

Temperature (°C)	Conductivity (W/m°C)			Specific Heat (J/kg°C)
<u>T</u>	<u>k_x</u>	<u>k_y</u>	<u>k_{xy}</u>	<u>c</u>
-100	1.1	1.1	0	835
10,000	1.1	1.1	0	835

   As shown by this table, the material properties are constant. Prior to the computer run, it was not known what upper temperature boundary could be expected. As a result, very high bounding temperature values were chosen which, because the material properties are constant, do not have any affect on the results of the computer run.

   2c. The use of 35°C as the initial temperature at a depth of 1000 m was based on an assumed temperature gradient of 2°C per 100 m. While a higher temperature gradient could be used, it would not affect the repository temperature response caused by the nuclear waste canister because the material properties are not temperature dependent in this problem. The resulting temperature difference would be due to the difference in initial temperature gradients only. As long as all codes use the same initial temperature gradients, a comparison between computer codes can be made. Since this is a hypothetical problem, it is considered that the initial temperatures need not be changed.

2d. The canister decay heat curve was given in the Benchmark Problems Report (pg. 108, NUREG/CR-3636) and is referenced from the RHO "Site Characterization Report for BWIP" (Report DOE/RL 82-3, Nov. 1982). This is a hypothetical problem and was not meant to model specific repository conditions. As long as the same heat decay curve is used for all computer codes, a comparison of results can be made.

3. Section 6.4, Problem 5.2S (Salt)

3a. Interbeds can be accommodated only if the location, size, and material properties are known. In this case, the interbeds would be incorporated into the finite element mesh as a separate material. If the location, size, or material properties of the interbeds are unknown, they cannot be accommodated by this computer code.

3b. Since material properties are constant, any bounding temperature values can be used to define the material property curve. Prior to the computer run, it was not known what material temperatures could be expected. The choice of very high bounding temperature values, while not very realistic, does not have any affect on the results of the computer run.

3c. A constant thermal conductivity was used as specified in the Benchmark Problems Report (NUREG/CR-3636). The conductivity value used is referenced in "Parameters and Variables Appearing in Repository Design Models (pp. 14-15, NUREG/CR-3586). The code does not have the capability to model pressure dependent variables.

3d. The use of a constant specific heat variable is specified in the Benchmark Problems Report (NUREG/CR-3636). The specific heat value used is referenced from Figure 2.1.2-3 of the Parameters Report (pg. 29, NUREG/CR-3586). The purpose of this problem is to benchmark specified computer codes. Determining the sensitivity of the model to variations of specific heat would require additional computer runs and is not included in the present scope of work.

4. Section 6.5, Problem 6.1 (SALT)

4a. The temperature dependent conductivity values were given in the Benchmark Problems Report (pg. 147, NUREG/CR-3636) and was referenced from "Project Salt Vault: A Demonstration of the Disposal of High-Activity Solidified Wastes in Underground Salt Mines" (pg. 3, ORNL-4555, April 1971).

4b. The approved Benchmark Problems Report (pg. 147, NUREG/CR-3636) specified the use of a constant specific heat value.

5. Section 6.6, Problem 6.3

5a. The thermal conductivity relationship is given in the Benchmark Problems Report (pg. 164, NUREG/CR-3636). This variable relationship is referenced from "Supporting Document Preliminary Results for Full-Scale Heater Tests #1 and #2" (pg. 39, RSD-BWI-TI-061, Vol. I). This reference shows thermal conductivity increasing with temperature.

5b. An error has been found in the reference equation for specific heat and has been corrected. The reference equation was taken from "Supporting Document ...", (pg. 39, RSD-BWI-TI-061, Vol. I) and should read as follows:

$$cp = 1.28\times10^{3} - 0.108T - 4.8\times10^{7}/T^{2} \quad (J/kg°K)$$

The revised specific heat values used for DOT are shown below.

Temperature (°C) T	Specific Heat (J/kg°C) cp
0	606.5
100	894.7
200	1014.4
500	1116.2
700	1124.2
1,000	1112.9
2,000	1025.2
10,000*	170.1*

*(Values for 10,000°C are present to prevent temperatures from possibly going out of range.)

This tabulation indicates specific heat increasing with temperature to a maximum value in the region of 600 to 800°C, then decreasing at a slow rate.

5c. Using the revised specific heat values while keeping the thermal conductivity the same as before yields results that agree well with field measurements. These revised results were included with the November Progress Report. Since the input data used was specifically created for this problem (see pg. 39, RSD-BWI-TI-061), the fact that the output results agree well with the field measured results (see App. II, RSD-BWI-TI-061 and "Status Report ...", RHO-BW-SA-231A P) should not be unexpected.

5d. The vertical orientation of the heat source was specified in the Benchmark Problems Report (pg. 163, NUREG/CR-3636) and "Supporting Document ..." (RSD-BWI-TI-061). While a horizontal orientation is possible to model, it would constitute a new problem which is not included in our current scope of work.

6a. The hypothetical problems were not meant to model specific repository conditions. They are to be used only as a general model for which computer code comparisons can be made. The DOT computer code, as with most of the codes, can effectively model temperature-dependent thermal conductivity and specific heat variables but cannot model temperature-dependent density parameters. Pressure-dependent variables cannot effectively be modeled by this code.

6b. Interbeds and impurities can be modeled only if their location, size, and properties are known. The interbeds could then be incorporated into the finite element mesh as a separate material. If the location of the interbeds is unknown, they cannot be effectively modeled.

DWL/JAB:paf
P6678.250
1/9/85

PROJECT STATUS

TABLE 3

MATRIX OF CODE/PROBLEM COMBINATIONS*
(Revised 1/4/85)

Legend:

x Benchmark Problems by Acres.
0 Benchmark Problems by Teknekron.
(1) Requires 2 runs.
(2) Two-Dimensional Analysis.
(3) Requires 3 runs, one for MATLOC and two for VISCOT.

	CODES										
	ADINA - 3D	ADINAT - 3D	DOT	HEATING	MATLOC	SPECTROM 11	SPECTROM 41	VISCOT	COYOTE	SALT 4	STEALTH
2.0 THERMAL ANALYSIS CASE PROBLEMS											
2.6 Transient Temperature Analysis of an Infinite Rectangular Bar With Anisotropic Conductivity (Schneider, 1955, pp. 261)		(2)	▩	0					▩		0
2.8 Transient Temperature Response to the Quench of an Infinite Slab With a Temperature-Dependent Convection Coefficient (Kreith, 1958, pp. 161)		(2)		0					▩		0
2.10 Steady Radiation Analysis of a Infinite Rectangular Opening (Rohsenow and Hartnett, 1973, pp. 15-32)		x		0					x		0
3.0 GEOMECHANICAL ANALYTICAL PROBLEMS											
3.2 Circular Tunnel (Long Cylindrical Hole in An Infinite Medium) a) Unlined in elastic medium - biaxial stress field b) Unlined in plastic medium (Tresca) von Mises	(2)				▩			⊗			0
3.3 Thick-Walled Cylinder Subjected to Internal and/or External Pressure c) Plane strain - creep	(2)							⊗			
3.5 Plane Strain Compression of an Elastic-Plastic Material von Mises; Drucker, Prager	(2)										0
5.0 HYPOTHETICAL REPOSITORY DESIGN PROBLEMS											
5.1 Hypothetical Very Near Field Problem	x	x		0							
5.2 Hypothetical Near Field Problem			S,B ▩(3)		B ⊗			S,B ⊗	S ▩	S ⊗	0
5.3 Hypothetical Far Field Problem	(2)	(2)								x	0
6.0 FIELD VALIDATION PROBLEMS											
6.1 Project Salt Vault-Thermomechanical Response Simulation Problem	(2)	(2)	▩					x		x	0
6.3 In Situ Heater Test-Basalt Waste Isolation Project	(2)	(2)	▩		⊗				▩		0

* From NUREG/CR-3636, Benchmark Problems for Repository Design Models, February 1984.

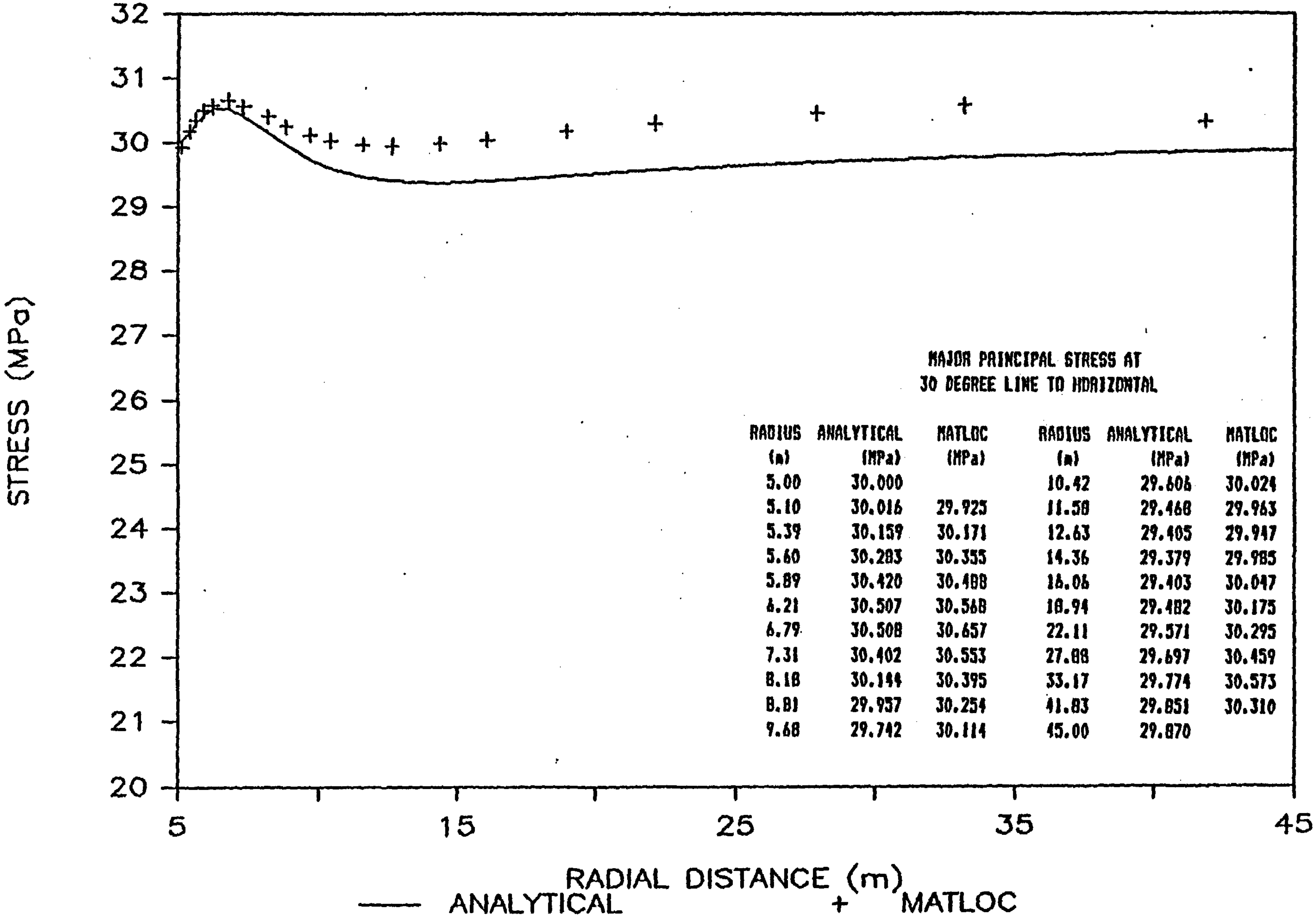
▩ Problems Completed

⊗ Problems Run, Results Not Analyzed

S - Salt
B - Basalt

MATLOC – PROBLEM 3.2a

MAJOR PRINCIPAL STRESS

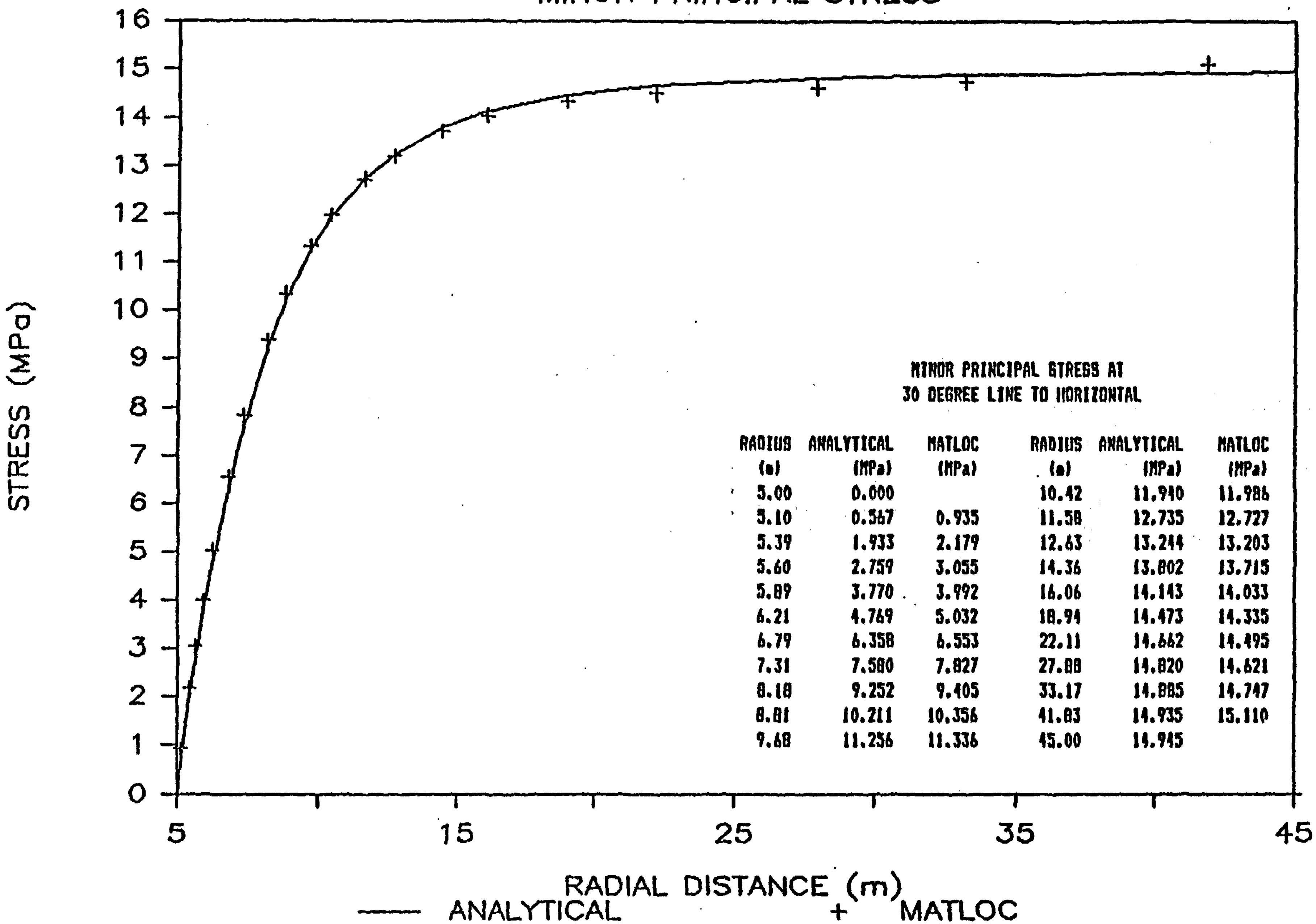


MAJOR PRINCIPAL STRESS AT
30 DEGREE LINE TO HORIZONTAL

RADIUS (m)	ANALYTICAL (MPa)	MATLOC (MPa)	RADIUS (m)	ANALYTICAL (MPa)	MATLOC (MPa)
5.00	30.000		10.42	29.606	30.024
5.10	30.016	29.925	11.58	29.468	29.963
5.39	30.159	30.171	12.63	29.405	29.947
5.60	30.283	30.355	14.36	29.379	29.985
5.89	30.420	30.488	16.06	29.403	30.047
6.21	30.507	30.568	18.94	29.482	30.175
6.79	30.508	30.657	22.11	29.571	30.295
7.31	30.402	30.553	27.88	29.697	30.459
8.18	30.144	30.395	33.17	29.774	30.573
8.81	29.957	30.254	41.83	29.851	30.310
9.68	29.742	30.114	45.00	29.870	

MATLOC – PROBLEM 3.2a

MINOR PRINCIPAL STRESS

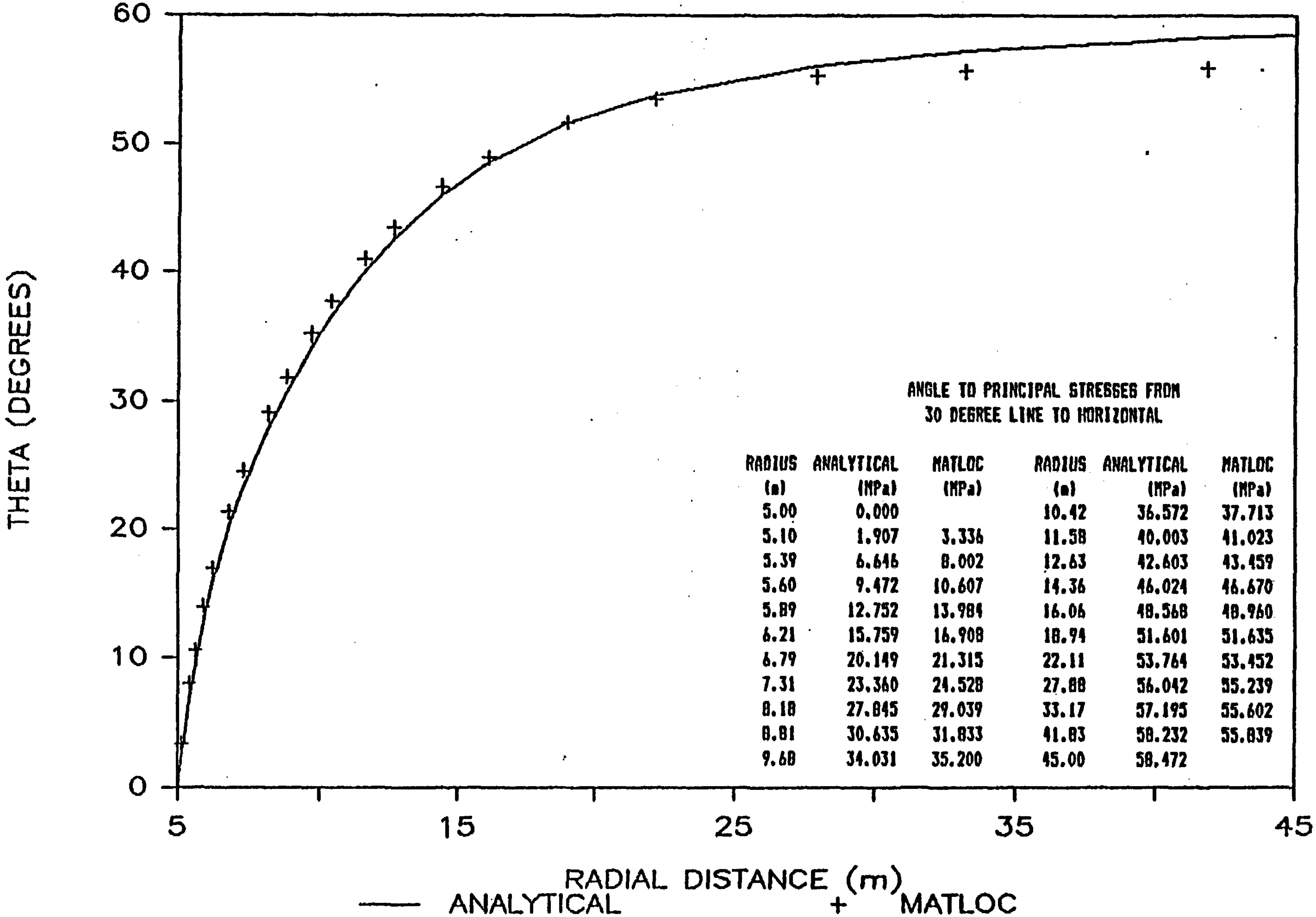


MINOR PRINCIPAL STRESS AT
30 DEGREE LINE TO HORIZONTAL

RADIUS (m)	ANALYTICAL (MPa)	MATLOC (MPa)	RADIUS (m)	ANALYTICAL (MPa)	MATLOC (MPa)
5.00	0.000		10.42	11.940	11.986
5.10	0.567	0.935	11.58	12.735	12.727
5.39	1.933	2.179	12.63	13.244	13.203
5.60	2.759	3.055	14.36	13.802	13.715
5.89	3.770	3.992	16.06	14.143	14.033
6.21	4.769	5.032	18.94	14.473	14.335
6.79	6.358	6.553	22.11	14.662	14.495
7.31	7.580	7.827	27.88	14.820	14.621
8.18	9.252	9.405	33.17	14.885	14.747
8.81	10.211	10.356	41.83	14.935	15.110
9.68	11.256	11.336	45.00	14.945	

MATLOC – PROBLEM 3.2a

ANGLE TO PRINCIPAL STRESS

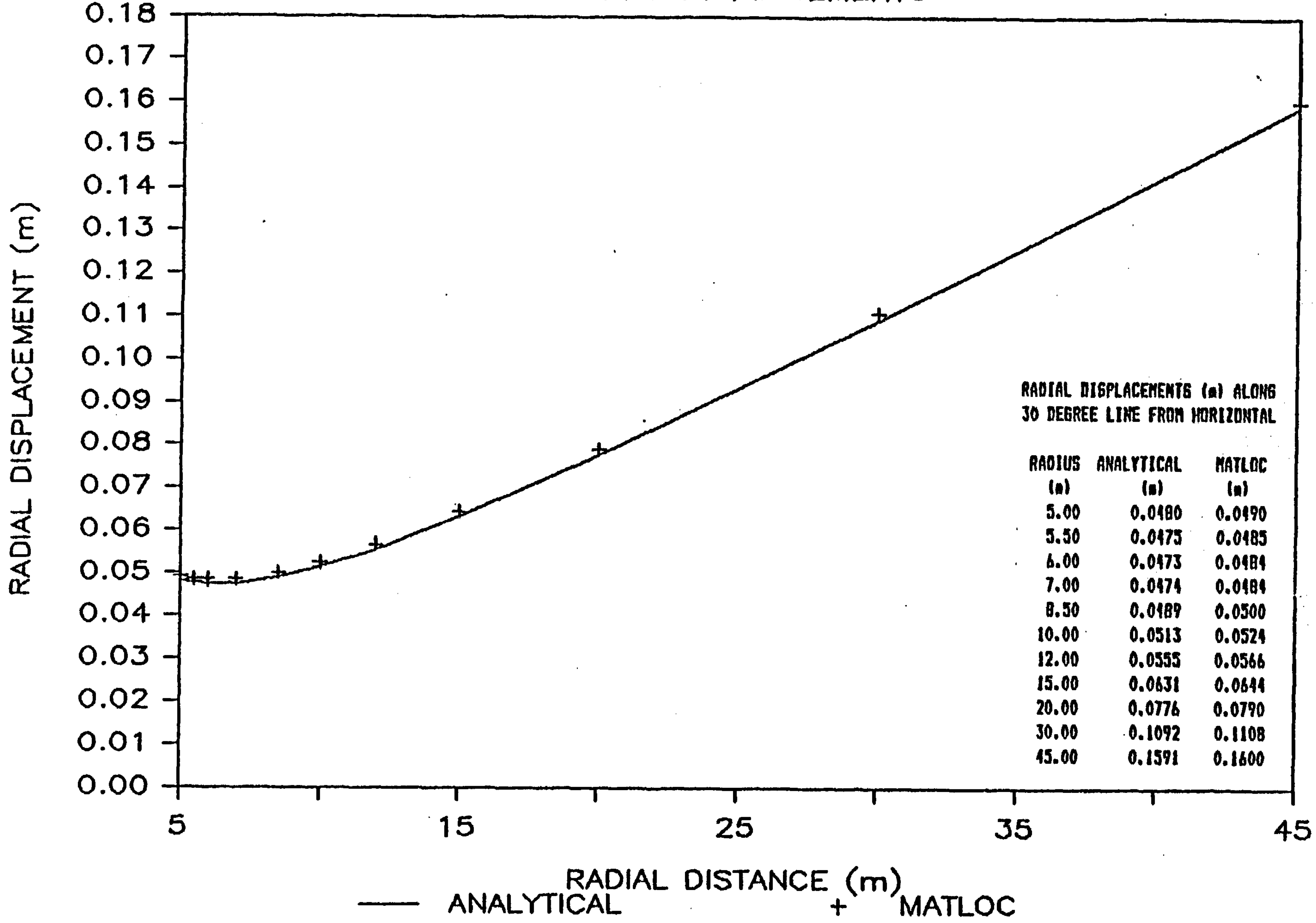


ANGLE TO PRINCIPAL STRESSES FROM 30 DEGREE LINE TO HORIZONTAL

RADIUS (m)	ANALYTICAL (MPa)	MATLOC (MPa)	RADIUS (m)	ANALYTICAL (MPa)	MATLOC (MPa)
5.00	0.000		10.42	36.572	37.713
5.10	1.907	3.336	11.58	40.003	41.023
5.39	6.646	8.002	12.63	42.603	43.459
5.60	9.472	10.607	14.36	46.024	46.670
5.89	12.752	13.984	16.06	48.568	48.960
6.21	15.759	16.908	18.94	51.601	51.635
6.79	20.149	21.315	22.11	53.764	53.452
7.31	23.360	24.528	27.88	56.042	55.239
8.18	27.845	29.039	33.17	57.195	55.602
8.81	30.635	31.833	41.83	58.232	55.839
9.68	34.031	35.200	45.00	58.472	

MATLOC PROBLEM 3.2a

RADIAL DISPLACEMENTS

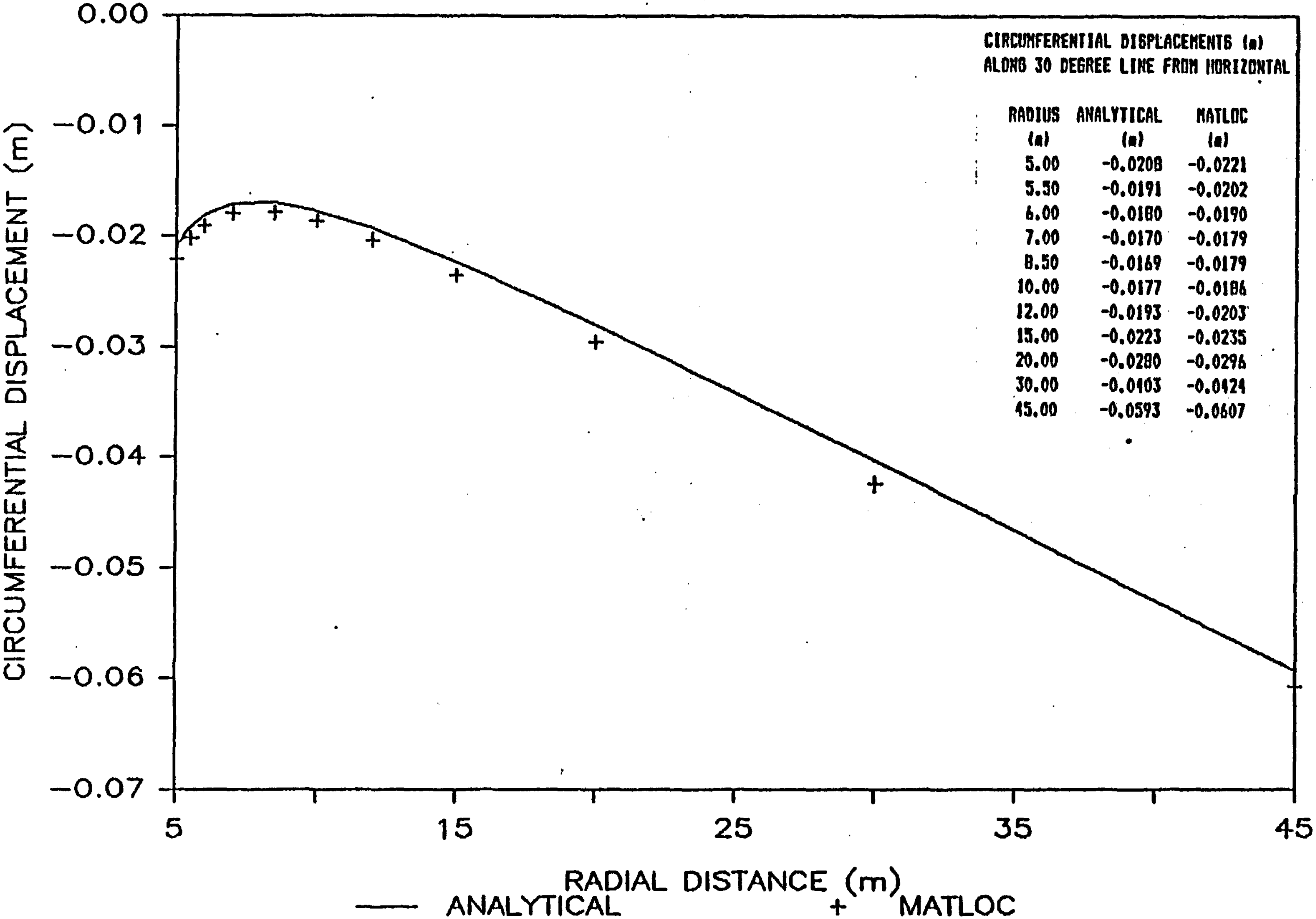


RADIAL DISPLACEMENTS (m) ALONG
30 DEGREE LINE FROM HORIZONTAL

RADIUS (m)	ANALYTICAL (m)	MATLOC (m)
5.00	0.0480	0.0490
5.50	0.0475	0.0485
6.00	0.0473	0.0484
7.00	0.0474	0.0484
8.50	0.0489	0.0500
10.00	0.0513	0.0524
12.00	0.0555	0.0566
15.00	0.0631	0.0644
20.00	0.0776	0.0790
30.00	0.1092	0.1108
45.00	0.1591	0.1600

MATLOC PROBLEM 3.2a

CIRCUMFERENTIAL DISPLACEMENTS



CIRCUMFERENTIAL DISPLACEMENTS (m)
ALONG 30 DEGREE LINE FROM HORIZONTAL

RADIUS (m)	ANALYTICAL (m)	MATLOC (m)
5.00	-0.0208	-0.0221
5.50	-0.0191	-0.0202
6.00	-0.0180	-0.0190
7.00	-0.0170	-0.0179
8.50	-0.0169	-0.0179
10.00	-0.0177	-0.0186
12.00	-0.0193	-0.0203
15.00	-0.0223	-0.0235
20.00	-0.0280	-0.0296
30.00	-0.0403	-0.0424
45.00	-0.0593	-0.0607

UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, D. C. 20555

F.202
76678.220.20
~~Dist Sul~~
c.c. JAB - please
JLD (file)

DEC 4 1984

Douglas K. Vogt
CorSTAR
7315 Wisconsin Avenue
North Tower, Suite 702
Bethesda, MD 20814

SUBJECT: RESPONSE TO MONTHLY PROGRESS REPORT FOR OCTOBER 1984 (NRC-02-81-026/FIN-B6985)

Dear Mr. Vogt:

We have reviewed your monthly progress report for October 1984. For Task 3, Waste Package Codes, the draft report has been reviewed by NRC staff and draft comments have been prepared. It is my understanding from our telephone conversations that plans to revise the benchmarking report (Tasks 4 & 5, Siting Codes) in accordance with review comments are underway. Conclusions as reported here and at our mid-October meeting from the benchmarking of the Radiological Assessment Codes (Tasks 4 & 5, Radiological Assessment Codes) appear to be quite useful. When the conclusions are incorporated into the report, they should be stated as objectively as possible.

For Tasks 4 & 5, Repository Design Codes, the source tapes for ADINA, ADINAT, ADINA-IN, and ADINA-PLOT have arrived from Adina Engineering and plans to install them at the Brookhaven Computing facility are underway. Comments and questions arising from review of the benchmarking of the program, DOT, are enclosed. These comments reflect two kinds of inconsistencies: (a) between input data for hypothetical problems and expected repository conditions, and (b) in the benchmark problem statements. Please consider these comments in preparing your draft.

The action taken by this letter is considered to be within the scope of current contract NRC-02-81-026. No changes to cost or delivery of contracted products are authorized. Please notify me immediately if you believe this letter would result in changes to costs or delivery of contract products.

Sincerely,

Pauline P. Brooks

Pauline P. Brooks
Repository Projects Branch
Division of Waste Management
Office of Nuclear Material Safety
and Safeguards

cc: P. Cukor
S. Wollett

ENCLOSURE
(see letter dated
December 4, 1984)

Comments and Questions
on the
Benchmarking of DOT

Section 6-2 Problem 2.6

Material properties input parameters show the thermal conductivity and specific heat as constant rather than temperature dependent.

2. Section 6.3 Problem 5.2B (BASALT)

a. - Thermal conductivity and specific heat should be represented as temperature dependent rather than constant. Input parameter values can be obtained from the "Repository Horizon Identification Report," Draft, RHO-BW-ST-28-P, October 1983.

b. - Bounding temperature values should be narrowed from the -100°C - +10,000°C stated as input values to about 50°C - 700°C. Is the broader temperature range required by the model?

c. - Initial temperatures and associated depths should reflect temperatures of about 50°C at depths around 1000 - 1100 meters.

d. - Heat flux values should reflect information given in ONWI-423, Engineered Waste Package System, May 1983.

3. Section 6.4 Problem 5.2S (SALT)

a. - The material density value used (2150 Kg/m^3) is for pure halite. What about the interbeds? Can interbeds be accommodated?

b. - The temperature range should reflect a more realistic range such as 30°C - 500°C.

c. - Conductivity values used do not reflect their temperature dependent nature. Conductivity values for salt samples associated with the SRP range from 2.8 to 1.7 for a temperature range of 30°C to 500°C. At temperatures above 250°C the potential effects of decrepitation must be considered. Effects of pressure on conductivity at temperatures above 200°C should also be considered.

d. - Specific heat values in the range of 900-930 J/Kg°K are more appropriate for the SRP salt samples listed to date (ONWI-522). The use of specific heat values derived from linear regression analyses of data developed from testing at temperatures below 500°C for temperatures that exceed 500°C is questionable without consideration of decrepitation effects. Consideration should also be given to determining the sensitivity of the model to variation of specific heat in the order of 1.2 - 1.5 for non-pure halite salt materials.

4. <u>Section 6.5 Problem 6.1</u> (SALT)

Input data appear inappropriate for the SRP program.

a. - The range of conductivity is too high to be representative of the salt sample stated for this SRP (ONWI-522), as indicated in the comments above for Section 5.2S.

b. - The specific heat is shown as a constant 930.97 J/Kg°K. Specific heat may be temperature dependent for repository induced conditions at temperatures in the higher end of the ranges.

5. <u>Section 6.6 Problem 6.3</u> (BASALT)

Input data:

a. - Thermal conductivity is shown to be temperature dependent, but the values increase with temperature rather than decrease with increasing temperature as they should.

b. - Specific heat values are far too high and decrease with increasing temperature. (Compare Input Specifications, p. 164, NUREG/CR-3636.) Specific heat values should increase with increasing temperature.

Results:

c. - First paragraph says that the results agree very well with field measurements. If the results compare favorably with incorrect input, there may be something wrong with the model.

d. - Figures 6.3-5, 6.6-1 indicate that the heat source is located at the center of the placement room in a vertical orientation. This is not the correct orientation. The latest thinking out of BWIP is a horizontal emplacement scheme. See references:

a. SD-BWI-ES-020, Two-Phase Repository Study, July 1984.

b. PKE/PB, 1983, Conceptual Systems Design Description, Nuclear Waste Repository in Basalt, Project B-301, SD-BWI-SD-005, REV 0-0, 3 vols.

5. Summary of Major Concerns

a. Hypothetical problems do not closely resemble repository conditions. Can the models adequately handle temperature dependent thermal conductivities and specific heats that may not be constant through the required range of temperatures?

b. Input data for salt hypothetical problems includes material properties for pure halite only. Can interbeds and impurities be adequately modeled?