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P Brooks

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'85 MAY 10 P3:18

May 1, 1985

NRC FIN B6985

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 March 1985

Dear Pauline:

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

Task 3 - Report - Waste Package Codes

During March, a first draft of the final Waste Package benchmark problem report was typed. We have not yet received the NRC's formal comments on this report. Once these comments are received, the report will be revised and resubmitted.

Tasks 4 & 5 - Siting Codes

During the month there was no significant activity on this task. A meeting with NRC Contracts is required before work on this task can be continued.

Tasks 4 & 5 - Repository Design Codes

No new codes were installed at Brookhaven this month. Once again there have been no developments on the installation of the ADINA and ADINAT codes on the Brookhaven system, which were received by the NRC almost four months ago, as stated in a letter dated December 4, 1984, from the NRC to CorSTAR. This installation delay has caused us to fall considerably behind schedule. During the month, additional computer runs were made using the computer codes COYOTE, DOT and MATLOC. Results from these runs are discussed in the technical status summary report.

Tasks 4 & 5 - Radiological Assessment Codes

During the month, the Benchmark Analysis Report was edited and we started typing a draft report.

8506050413 850501
PDR WMRES EECCORS
B-6985 PDR

CORPORATE SYSTEMS, TECHNOLOGIES, AND RESOURCES
2121 ALLSTON WAY • BERKELEY, CALIFORNIA 94704 • (415) 548-4100

BERKELEY WASHINGTON, D.C. INCLINE VILLAGE

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General

Our estimate of costs through the end of March (through March 31, 1985 for CorSTAR) is:

Actual costs this month:	31.5 K
Actual costs this fiscal year:	260.8 K
Actual costs to date:	3035 K
Planned costs this month:	12 K
Planned costs this fiscal year:	184 K

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

Sincerely,

Douglas K. Vogt

Douglas K. Vogt
Project Manager

cc: D. Fehringer

See BU 485 5/1/85
TO Brooks From Vogt

TECHNICAL STATUS SUMMARY

8506050413 850501

TECHNICAL STATUS REPORT ATTACHMENT
TO PROGRESS REPORT FOR MARCH 1985

Repository Design Codes

Task 4 - Code Procurement

The NRC letter to CorSTAR dated December 4, 1984, stated that the source tapes for ADINA, ADINAT, ADINA-IN, and ADINA-PLOT were received from ADINA Engineering. With the addition of these codes, all applicable codes have been procured.

Code Installation

No new codes have been installed this month. Once again, there have been no developments on the installation of the ADINA and ADINAT codes on the Brookhaven computer system. The delay caused by the unavailability of these codes has caused us to fall considerably behind schedule in meeting the proposed deadline date of March 15, 1985.

Run Benchmark Problems

The results for Problem 5.2 - Salt using COYOTE have been summarized this month. The temperature contour results for times of 10, 30 and 100 years are included later in the report. A comparison of these results with those of other codes is not completed but will be included in Section 2 of the Draft Task Summary Report.

Problem 5.2 (Salt and Basalt) using DOT were rerun using the same defined canister heat output decay curve as used for the COYOTE Problem 5.2 - Salt run, so that the results from these two computer codes could be more easily compared. The values of the decay curve used are given below:

Time (years)	Time (sec)	Function Value
0	0	20.000 W/m^2
10	3.156×10^8	15.068
20	6.312×10^8	11.352
30	9.468×10^8	8.552
40	1.264×10^9	6.443
50	1.578×10^9	4.854
60	1.894×10^9	3.657
70	2.209×10^9	2.755
100	3.156×10^9	1.178
150	4.734×10^9	0.286
200	6.312×10^9	0.069
300	9.468×10^9	0.004
350	1.105×10^{10}	0.001
500	1.578×10^{10}	0.0
11000	3.472×10^{11}	0.0

These revised values more closely model the exponential decay of a canister heat output. The DOT temperature results for the Salt and Basalt runs at chosen

points for the first hundred years are given later in the report. The revised DOT (Salt) results are essentially identical to those from the COYOTE (Salt) run. The COYOTE (Salt) results were included in the November 1984 Progress Report. No comparison can be made with the DOT (Basalt) run since DOT is the only code for which the Basalt data were used as input to the computer run.

The rerun of Problem 5.2 (Basalt) using DOT required the rerun of MATLOC Problem 5.2 (Basalt) because the output temperature results from the DOT run are used as input to the MATLOC run. The revised MATLOC results which will include stress and displacement contours, have not yet been summarized.

Problem 6.3 BWIP was revised and rerun using DOT. The original run (November 1984 Progress Report) resulted in computer temperatures that were greater than field measured temperatures when using the specified heater input data. Since MATLOC Problem 6.3 BWIP uses temperatures computed by DOT as input data to perform a stress analysis, the higher computer temperatures from the DOT run adversely affected the results obtained from MATLOC. The original MATLOC results for this problem were included in the January 1985 Progress Report. To better judge the performance of the MATLOC code, temperatures closer to those measured in the field are required. This temperature reduction was accomplished by using a reduced heater output. By assuming 90 percent of that used in the original field experiment, a new temperature history which closely matches the field data was obtained. The results are shown at the end of the report. These new DOT temperature results were used as input to MATLOC to perform stress and displacement calculations. The displacement results from the new MATLOC run are summarized and included at the end of the report. While the revised results show that the displacements calculated using the reduced heater output are closer to the field measured values than those calculated previously, there is still a significant difference present.

The reason for the discrepancies between the calculated and observed temperatures using the correct heater input to the DOT code is presumed to be the result of variations between assumed and actual material properties. It should be noted that this new DOT run using a reduced heater output was done only for the purpose of evaluating the MATLOC results and is not intended to be used to justify the changing of the given DOT input parameters.

In order to get a better understanding of the MATLOC code, Problem 3.2a was rerun with MATLOC using a revised finite element mesh that is twice as fine (i.e., reducing the angle between radial lines from 30° to 15°) as the one used originally. The original finite element mesh was included in the February 1985 Progress Report, while the original MATLOC run results for this problem were included in the January 1985 Progress Report. The new results comparing the computer and analytical principal stress results are included at the end of the report and show that the use of the finer mesh resulted in the computer solution being much closer to the analytical results. Thus, it can be assumed that if the finite element mesh were made fine enough, at the expense of considerably greater computer run time, the MATLOC results would duplicate the analytical results.

Problem 6.1 PSV was run this month using SALT4. Since SALT4 does not have the ability to model a temperature-dependent thermal diffusivity, two runs were made using different constant thermal diffusivity values. The temperature and displacement results for these two SALT4 runs at various points, together with the field-measured results, are included at the end of the report. The temperature results show that the use of a lower thermal diffusivity, which means that it is more difficult for heat conduction to occur, causes high temperatures to develop near the heat source and lower temperatures to develop away from the heat source when compared to using a higher thermal diffusivity. The use of the lower thermal diffusivity results in temperature solutions closer to the field-measured values. The Room 4 floor uplift results show a slight change in the computed values when the two thermal diffusivity values are used. However, the computer results are quite different from the field-measured results, especially for points in the center of the room. One reason for this difference is that, unlike the actual field condition, the SALT4 code cannot take the creep of the floor and roof into account, which would result in larger vertical displacements to occur in the room. The calculated SALT4 deflections are the result of a pure elastic analysis. Note that the field-measured floor uplift values away from the center of the room, where the effect of creep is lower and the elastic effect is dominant, match more closely to those uplift values calculated with SALT4.

During the month, an attempt was made to clarify the analytical solution for Problem 3.5 (Plane Strain Compression of an Elastic-Plastic Material) using both the Von Mises and Drucker-Prager failure criteria. Errors in some equations published in NUREG/CR-3636 were previously identified. We are still awaiting reference material regarding the Von Mises criteria to support our clarifications. The corrected equations and procedures for these two failure criteria are detailed below:

Von Mises Failure Criteria

The corrected solution equations to be used in conjunction with the benchmark problems Report (CR-3636 p. 81) are as follows:

$$P = k_M \sqrt{3} / (1-\nu+\nu^2)^{1/2} \tag{2}$$

$$\varepsilon_1^T = \frac{-1}{E}\left[-(1-2\nu)\sigma_3 + \frac{3}{4} k_M \ln\left(\frac{2k_M + P}{2k_M - P}\right) + A\right] + \varepsilon_1^{E'} \tag{3}$$

$$A = -\sqrt{3}\, k_M \left[\frac{\nu(1-2\nu)}{\sqrt{1-\nu+\nu^2}} + \frac{\sqrt{3}}{4} \ln\left(\frac{2/\sqrt{3} + 1/\sqrt{1-\nu+\nu^2}}{2/\sqrt{3} - 1/\sqrt{1-\nu+\nu^2}}\right)\right] \tag{4}$$

$$\varepsilon_1^{E'} = \frac{-k_M \sqrt{3}\,(1-\nu^2)}{E\sqrt{1-\nu+\nu^2}} \tag{5}$$

All other equations are correct as shown for the Von Mises failure criteria in the benchmark problems Report. As stated in the benchmark problems Report for loadings, P, greater than yield, σ_3 can be determined directly from an equation given in the report. These values of P and σ_3 can be input into the equations given above to determine ε_1^T. Then ε_2^T can be calculated using equation (6) in CR-3636, page 82, which is quoted below for reference:

$$\varepsilon_2^T = \frac{1}{3K}(-P+\sigma_3) - \varepsilon_1^T \qquad (6)$$

Drucker-Prager Failure Criteria

The revised solution equations to be used in conjunction with the benchmark problems Report (CR-3636, page 82) are as follows:

$$P = k_{DP} / \left[-\alpha(1+\nu) + \sqrt{(1-\nu+\nu^2)/3} \right] \qquad (9)$$

$$\dot{\sigma}_1 = D_{11}\,\dot{\varepsilon}_1^T + D_{12}\,\dot{\varepsilon}_2^T \qquad (10a)$$

$$\dot{\sigma}_2 = D_{21}\,\dot{\varepsilon}_1^T + D_{22}\,\dot{\varepsilon}_2^T \qquad (10b)$$

$$D_{12} = D_{21} = -2G\left[h_2 - h_1 P\right] \qquad (12a)$$

$$D_{22} = 2G\left[1-h_2\right] \qquad (12b)$$

Where $\dot{\sigma}$ and $\dot{\varepsilon}$ are stress and strain rates respectively.

All other equations are correct as shown for the Drucker-Prager failure criteria in the benchmark problems Report. Knowing that $\sigma 2=0$ and thus $\dot{\sigma}2=0$, equation (10b) can be rewritten as such:

$$\dot{\varepsilon}_2^T = \frac{-D_{21}}{D_{22}}\,\dot{\varepsilon}_1^T \qquad (A)$$

Substituting into equation (10a) gives:

$$\dot{\sigma}_1 = D_{11}\,\dot{\varepsilon}_1^T + D_{12}\left(\frac{-D_{21}}{D_{22}}\right)\dot{\varepsilon}_1^T \quad \text{or} \quad \frac{\dot{\sigma}_1}{\dot{\varepsilon}_1^T} = D_{11} - \frac{(D_{12})^2}{D_{22}} \qquad (B)$$

Also knowing that $\dfrac{\dot{\sigma}_1}{\dot{\varepsilon}_1^T} = \dfrac{d\sigma_1}{d\varepsilon_1^T} = \dfrac{\Delta\sigma_1}{\Delta\varepsilon_1^T}$, equation (B) becomes:

$$\Delta\varepsilon 1^{T} = \Delta\sigma 1 \Big/ \left[D_{11} - \frac{(D_{12})^2}{D_{22}^{T}} \right] \qquad \text{(C)}$$

By selecting a small $\Delta\sigma 1$, $\Delta\varepsilon 1$, can be determined from equation (C) and then $\Delta\varepsilon 2$ from equation (A). Using the secant method, differentials are found at the midpoint of the interval chosen. Total strains can now be calculated from the equations below:

$$\varepsilon_1^{T} = \varepsilon 1 \text{ @ yield } + \sum \Delta\varepsilon_1^{T} \qquad \text{(D)}$$

$$\varepsilon_2^{T} = \varepsilon 2 \text{ @ yield } + \sum \Delta\varepsilon_2^{T} \qquad \text{(E)}$$

Problem 3.5 was attempted with VISCOT for both failure criteria. However, a valid solution from VISCOT has not yet been obtained.

JAB
4/4/85
P6678.250

PROJECT STATUS

TABLE 3

MATRIX OF CODE/PROBLEM COMBINATIONS*
(Revised 2/21/85)

Legend:

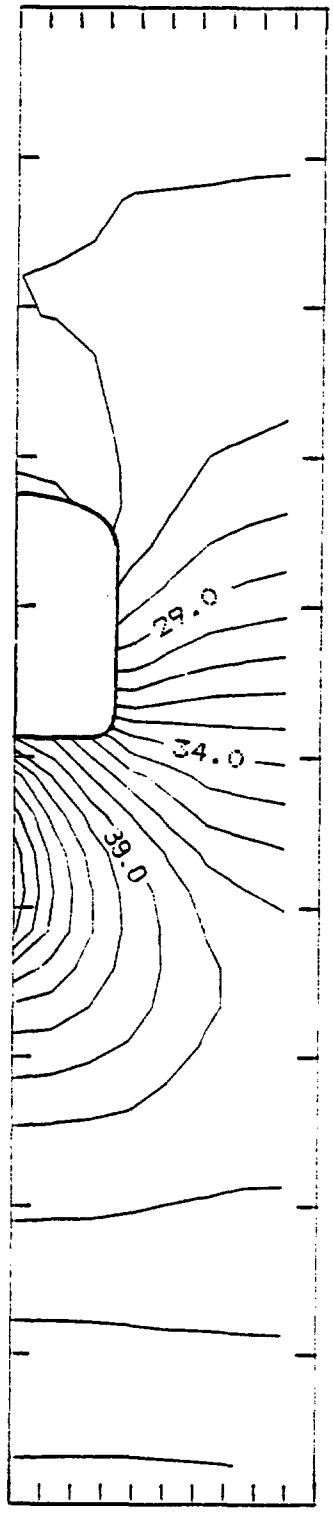
x Benchmark Problems by Acres.
0 Benchmark Problems by Teknekron.
(1) Requires 2 runs, one for MATLOC and one for VISCOT.
(2) Two-Dimensional Analysis.
(3) Requires 3 runs, one for MATLOC and two for VISCOT.
(4) Requires 2 runs, one for Salt and one for Basalt.
S - Problems run for Salt.
B - Problems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

	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		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)									0
6.3 In Situ Heater Test-Basalt Waste Isolation Project	(2)	(2)						x			0

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

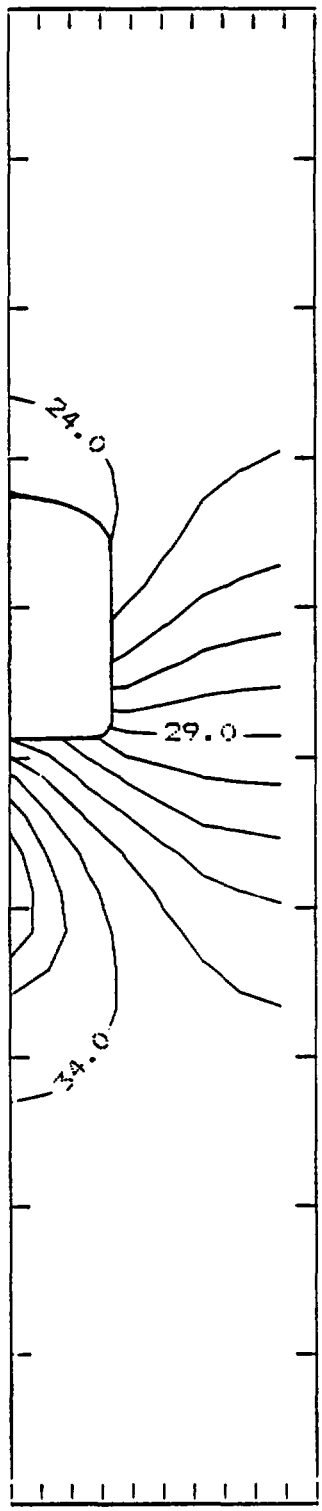
Problems completed

Problems attempted, results not analyzed



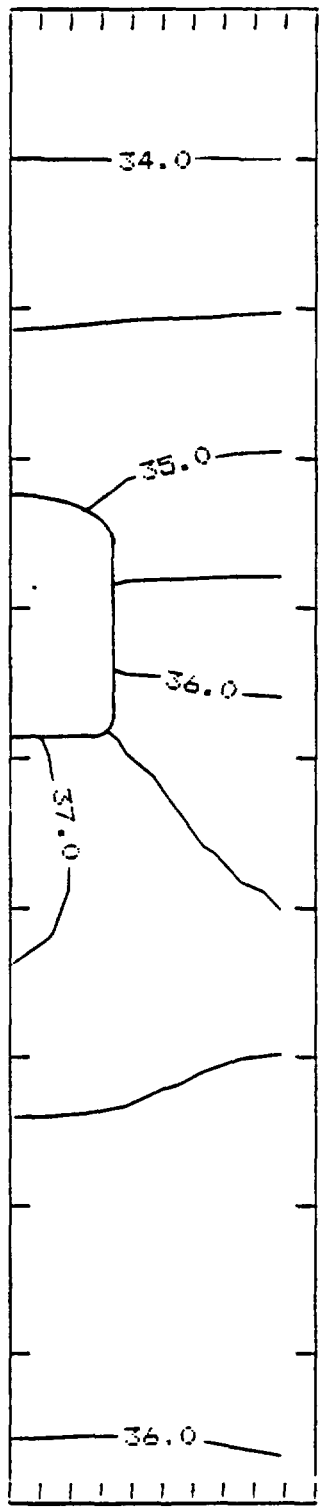
CØNTØUR FRØM 24.000 TØ 46.000 CØNTØUR INTERVAL ØF 1.0000
X INTERVAL= 0.75000 Y INTERVAL= 3.7000

Figure 10.5-6a COYOTE Problem 5.2 - Salt Temperature Contours at 10 years



CØNTØUR FRØM 22.000 TØ 38.000 CØNTØUR INTERVAL ØF 1.0000
X INTERVAL = 0.75000 Y INTERVAL = 3.7000

Figure 10.5-6b COYOTE Problem 5.2 - Salt Temperature Contours at 30 years



CØNTØUR FRØM 33.000 TØ 38.000 CØNTØUR INTERVAL ØF 0.50000
X INTERVAL = 0.75000 Y INTERVAL = 3.7000

Figure 10.5-6c COYOTE Problem 5.2 - Salt Temperature Contours at 100 years

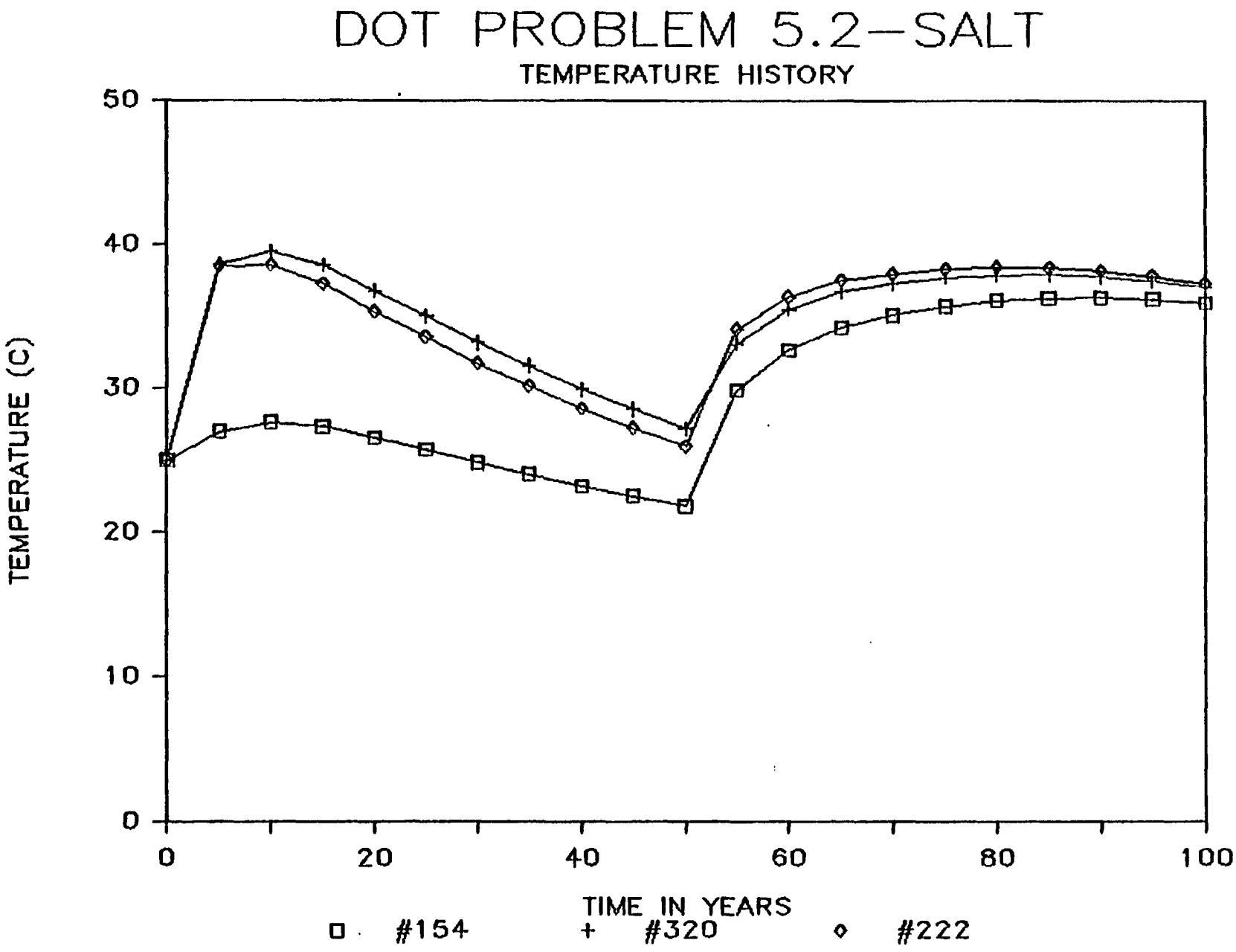


Figure 6.4-1R1 DOT Problem 5.2 - Salt
Temperature History 0-100 Years

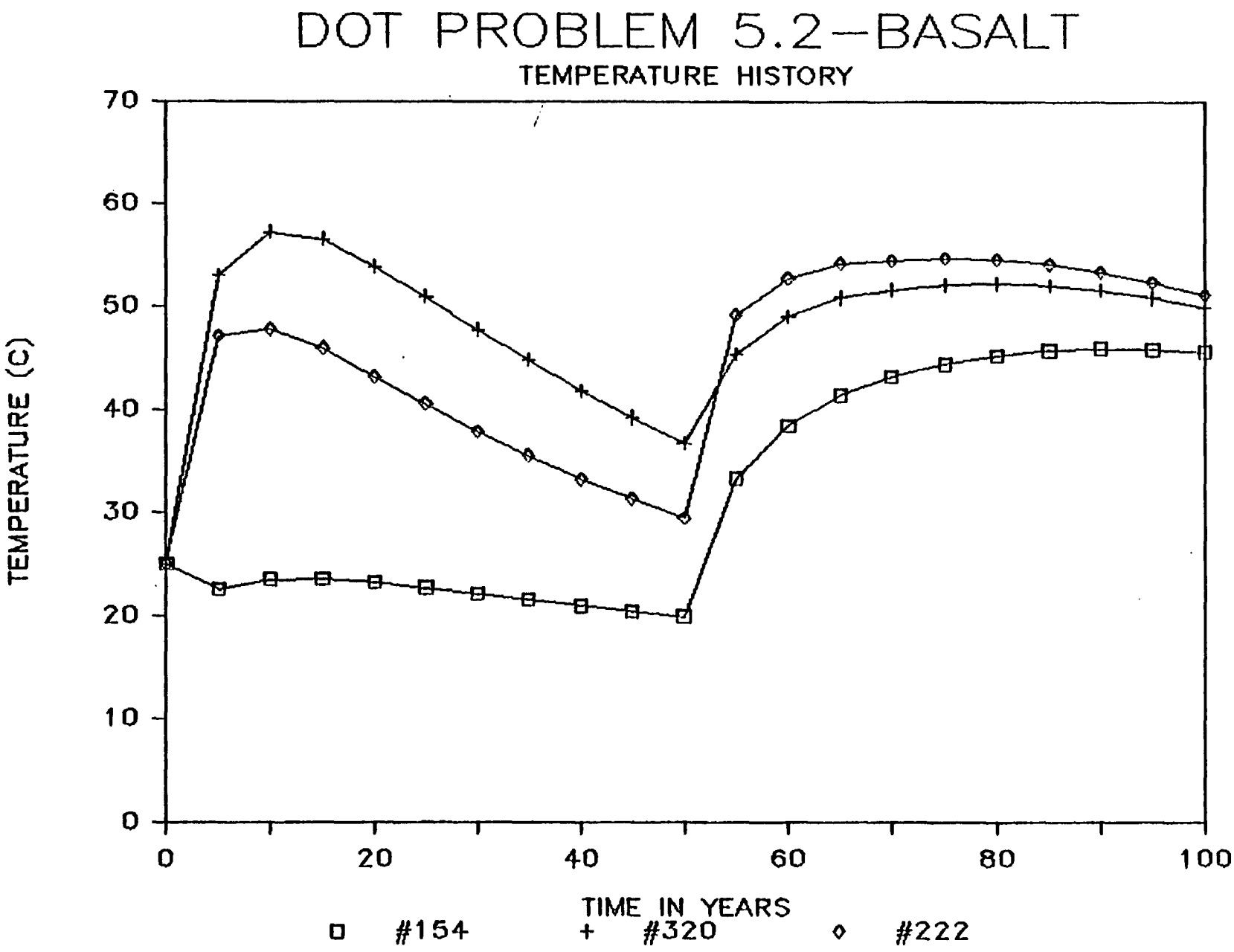


Figure 6.3-2R1 DOT Problem 5.2 - Basalt
Temperature History 0-100 Years

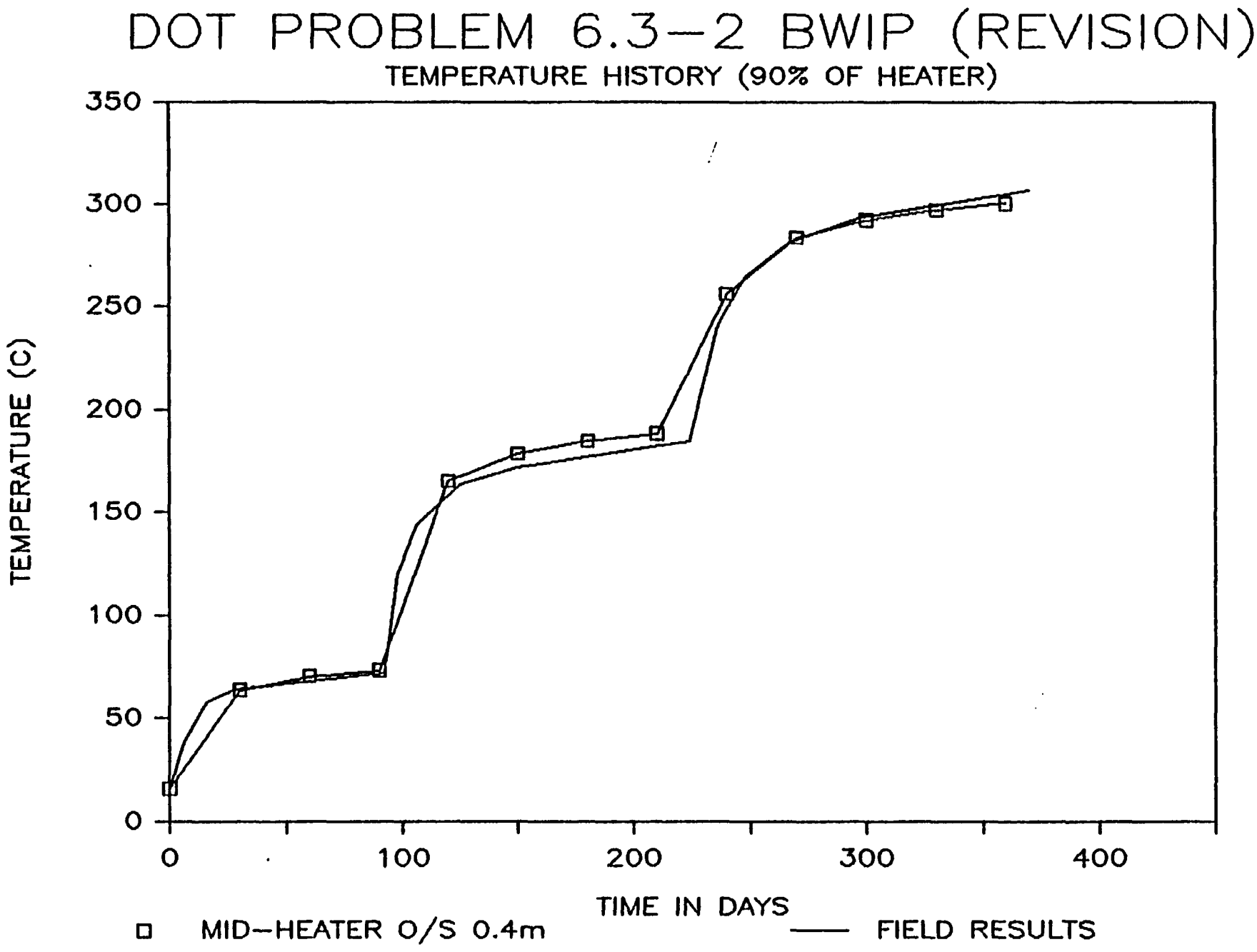


Figure 6.6-2R1 DOT Problem 6.3 BWIP (Run #2)
Temperature History using
90% of the Specified Heater Output

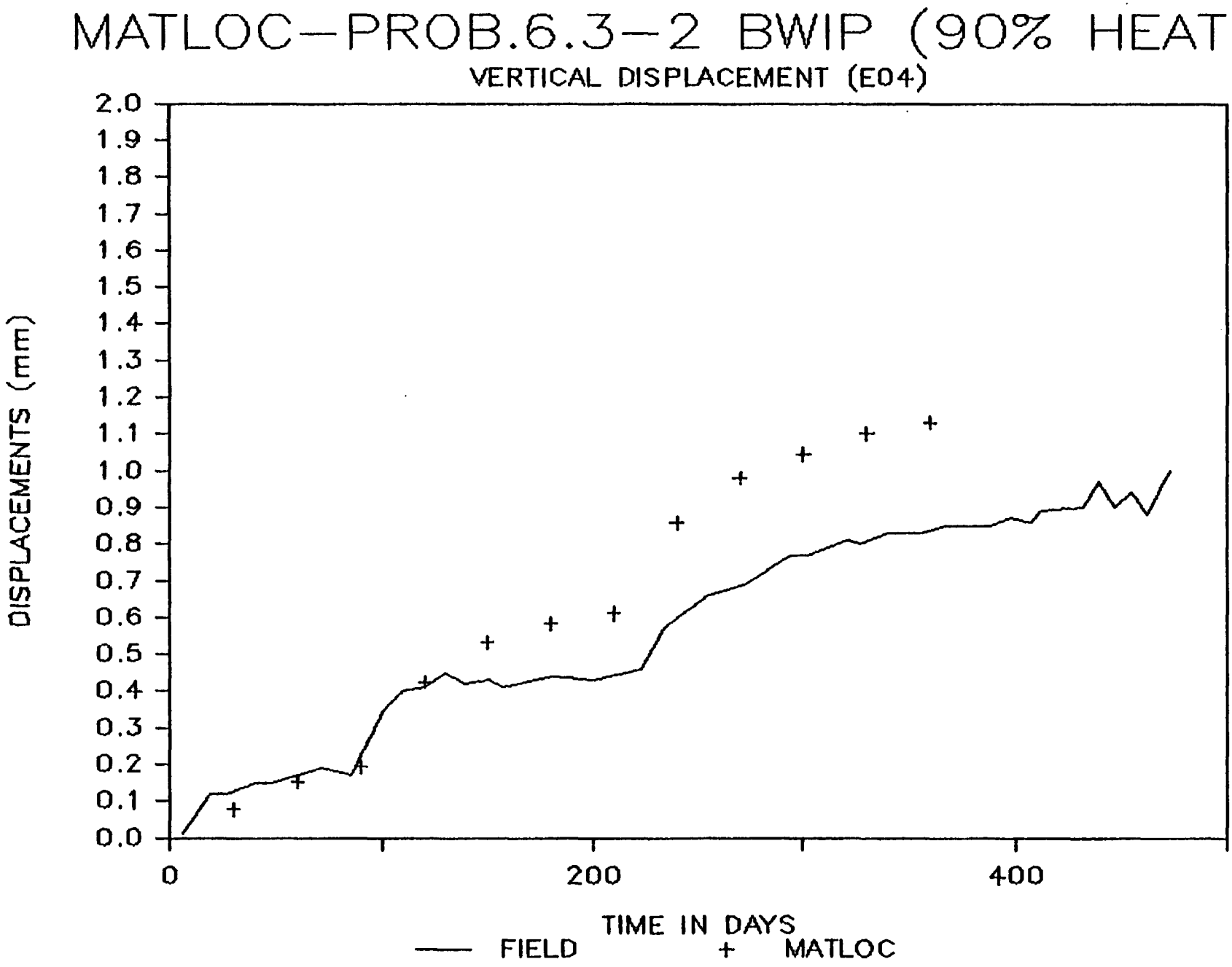


Figure 7.4-2R1 MATLOC Problem 6.3 BWIP (Run #2)
Vertical Displacements at Point EØ4 using
90% of the Specified Heater Output in DOT

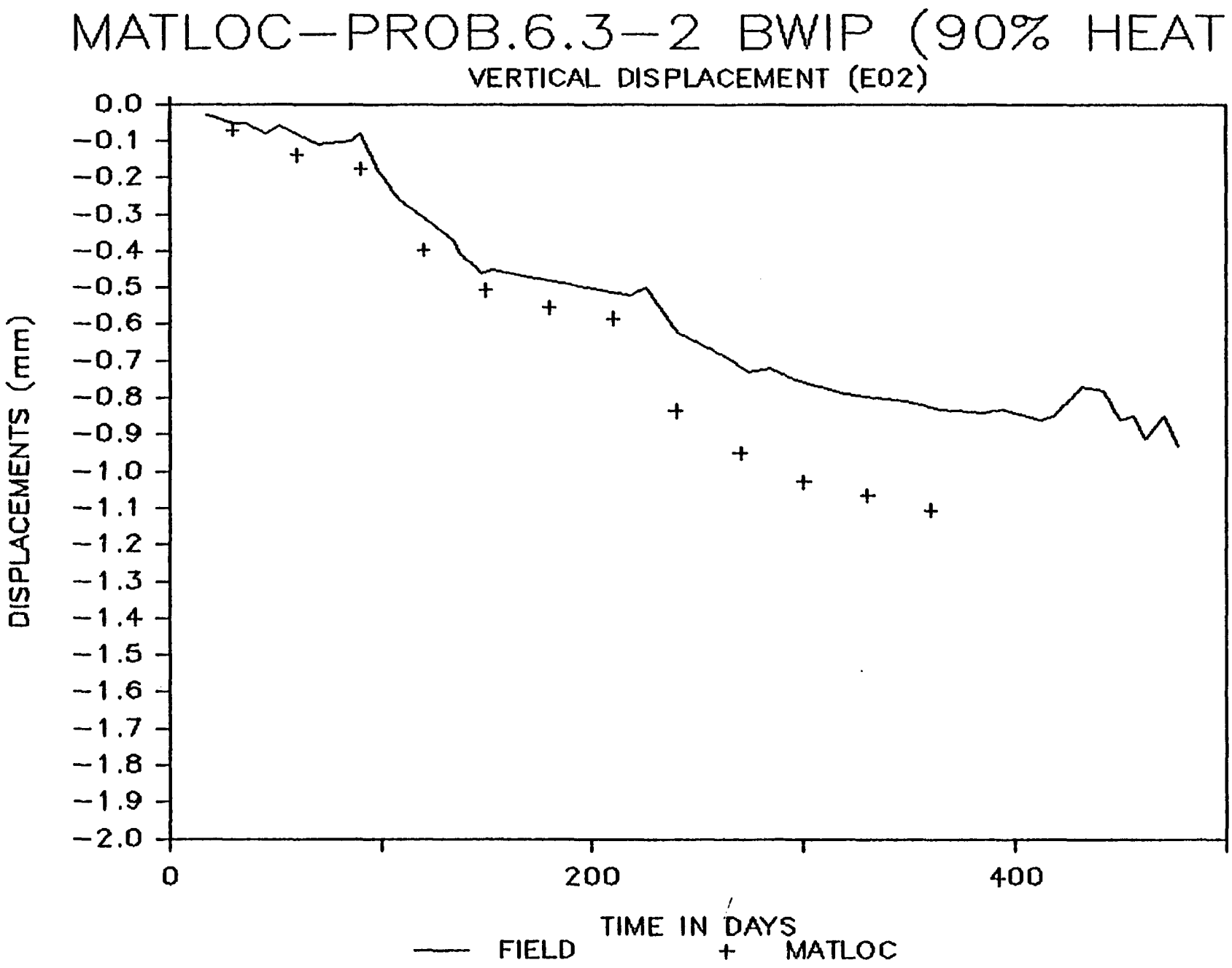


Figure 7.4-3R1 MATLOC Problem 6.3 BWIP (Run#2)
Vertical Displacements at Point EØ2 using
90% of the Specified Heater Output in DOT

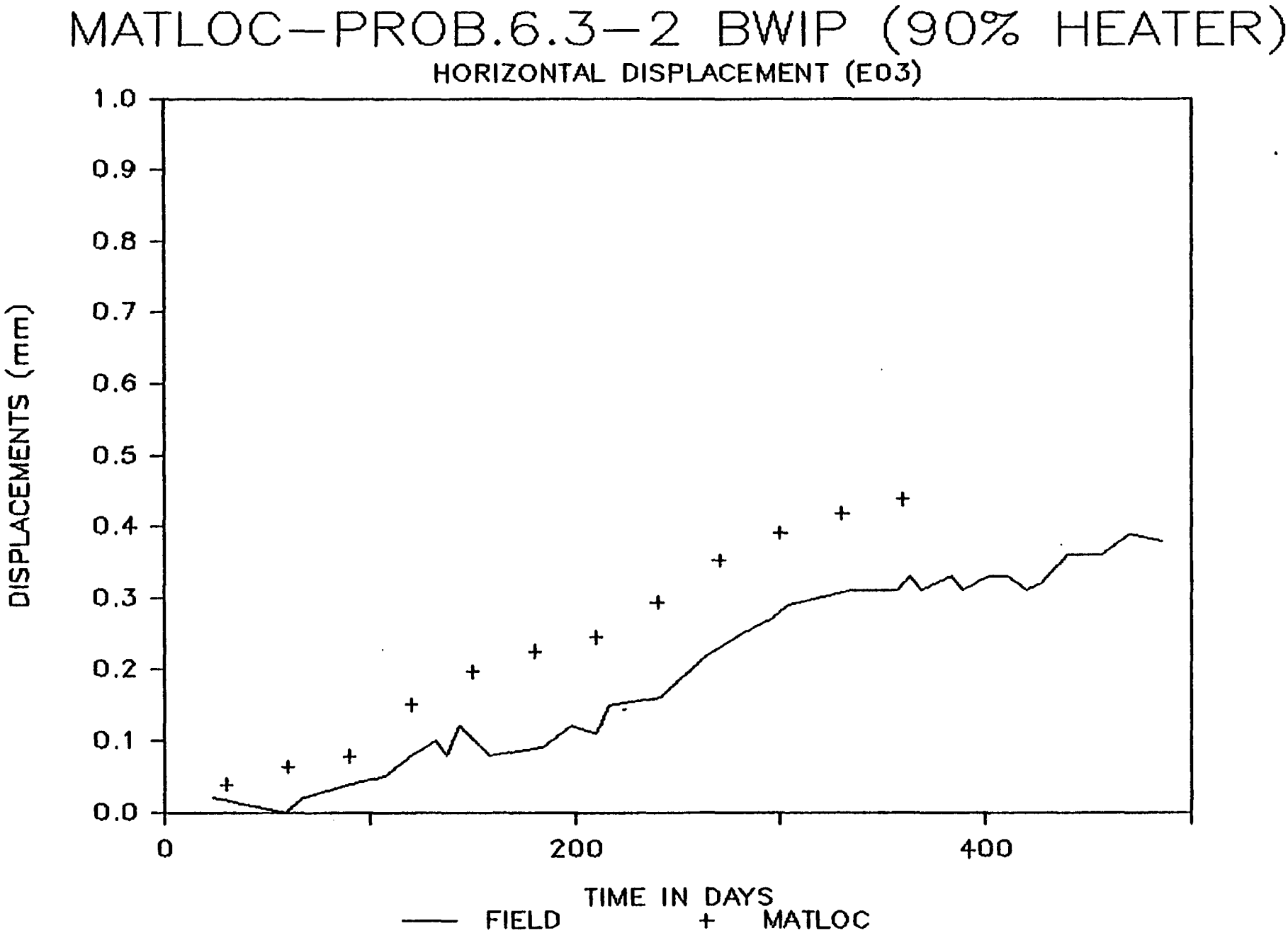


Figure 7.4-4R1 MATLOC Problem 6.3 BWIP (Run #2)
Horizontal Displacements at Point EØ3 using
90% of the Specified Heater Output in DOT

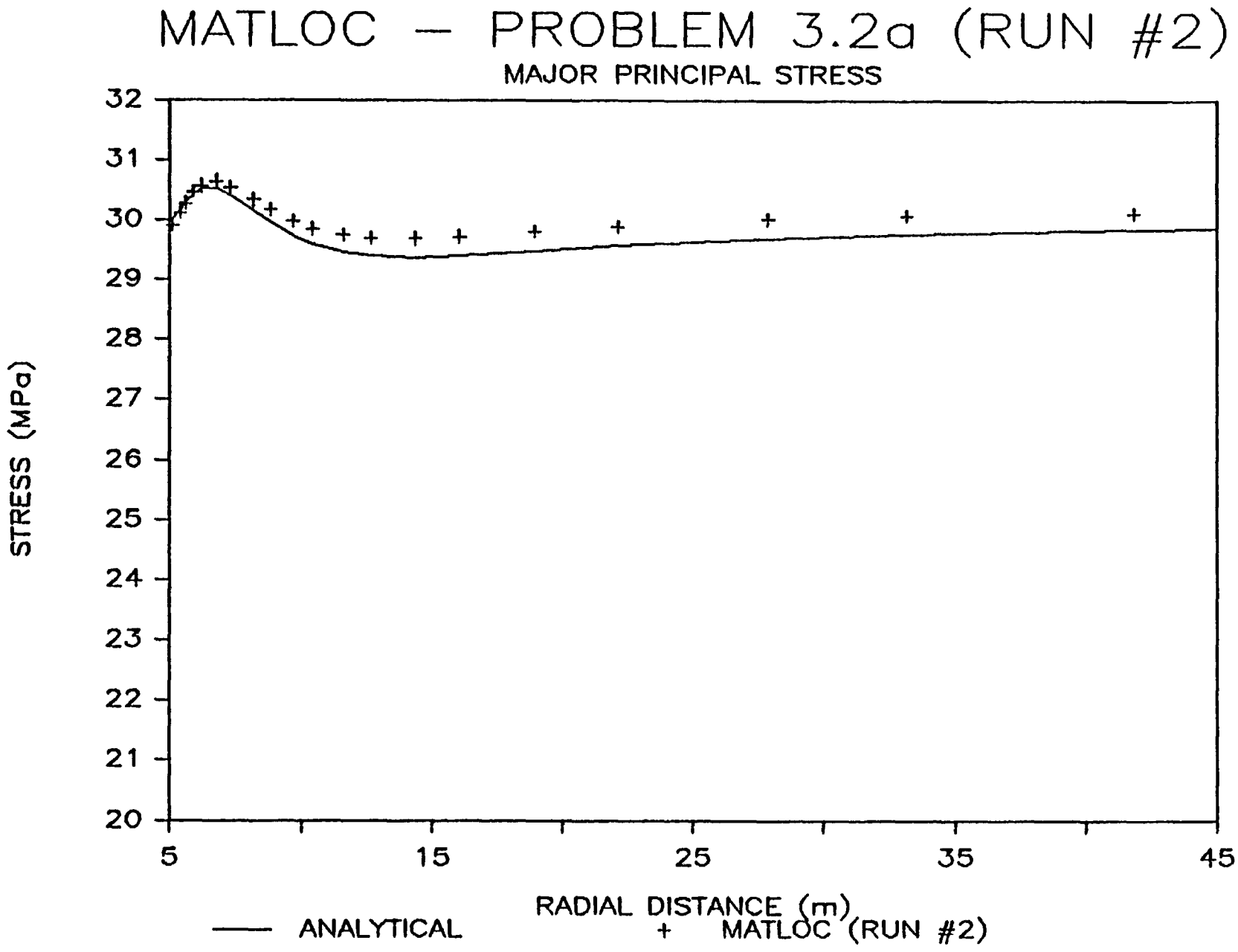


Figure 7.2-2R1 MATLOC Problem 3.2a - Finer Mesh Results
Major Principal Stresses along a Line
30 Degrees from Horizontal

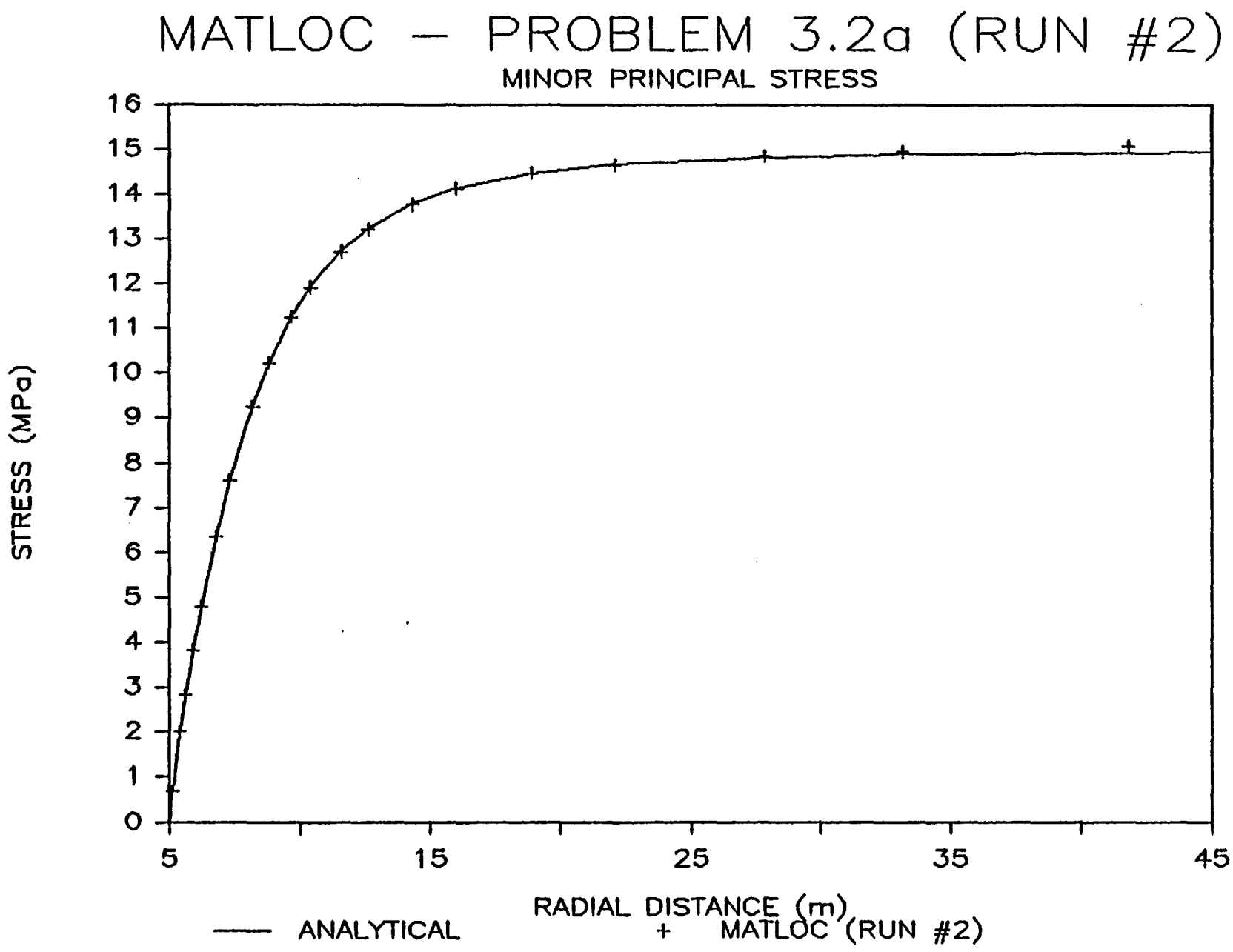


Figure 7.2-3R1 MATLOC Problem 3.2a - Finer Mesh Results
Minor Principal Stresses along a Line
30 Degrees from Horizontal

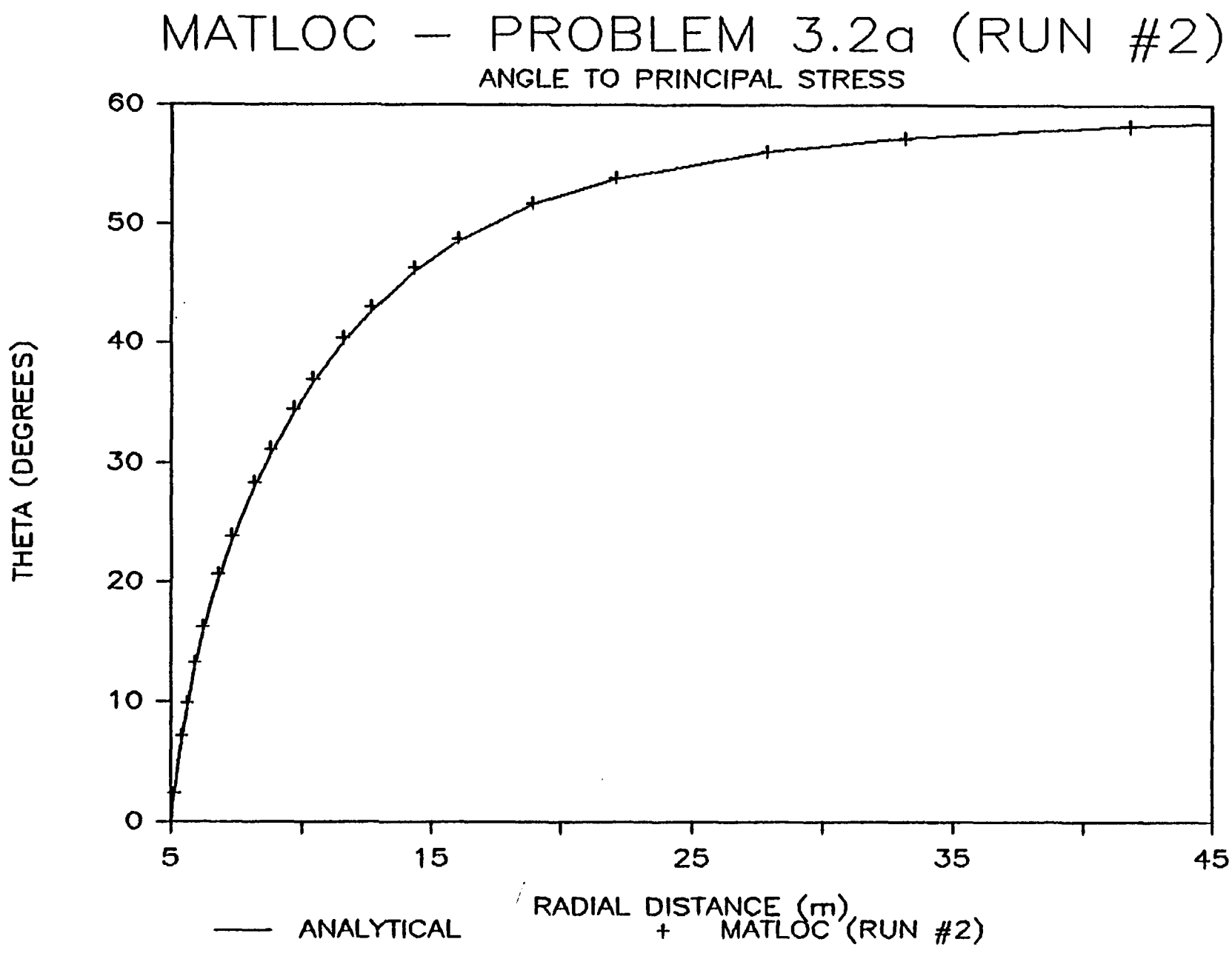
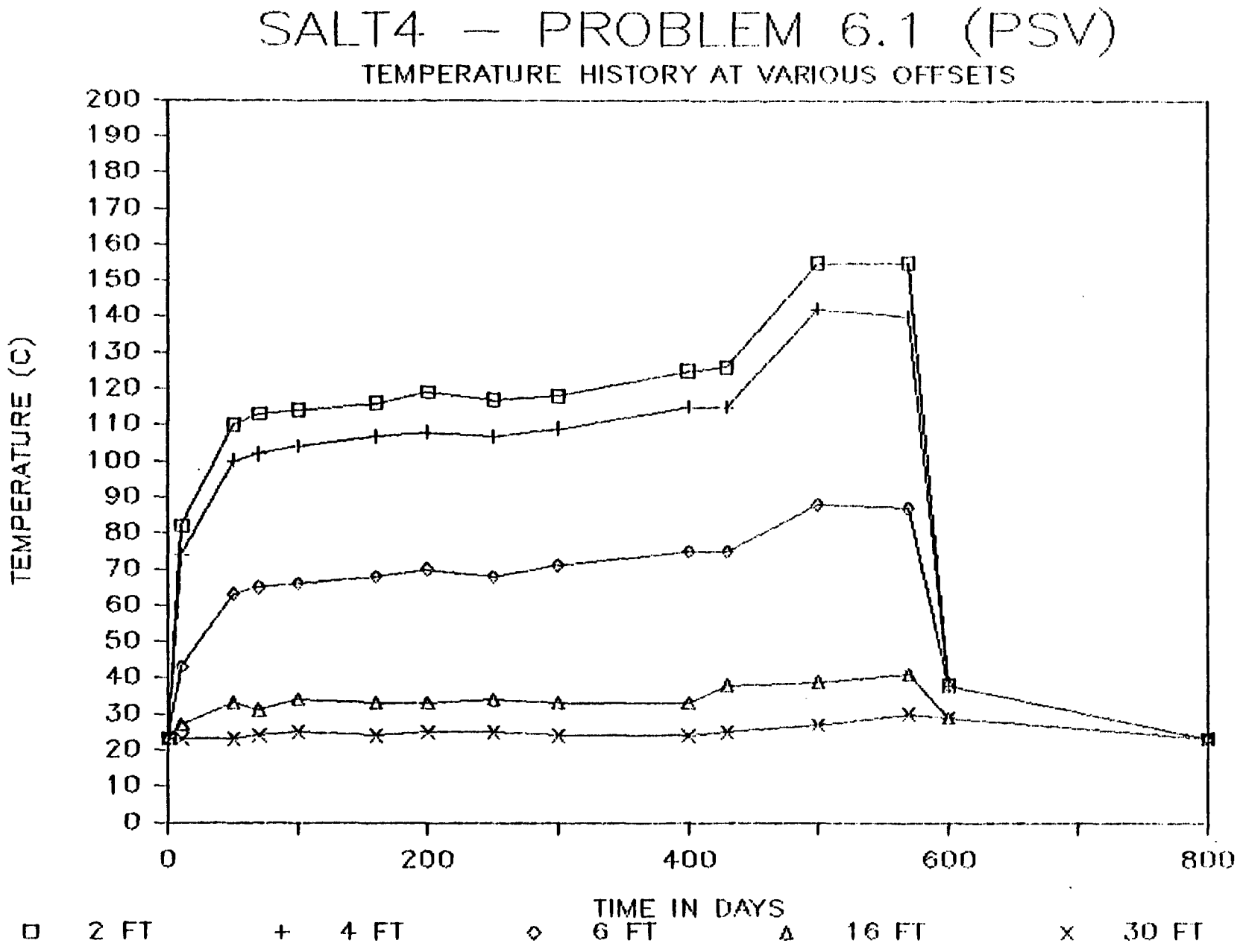
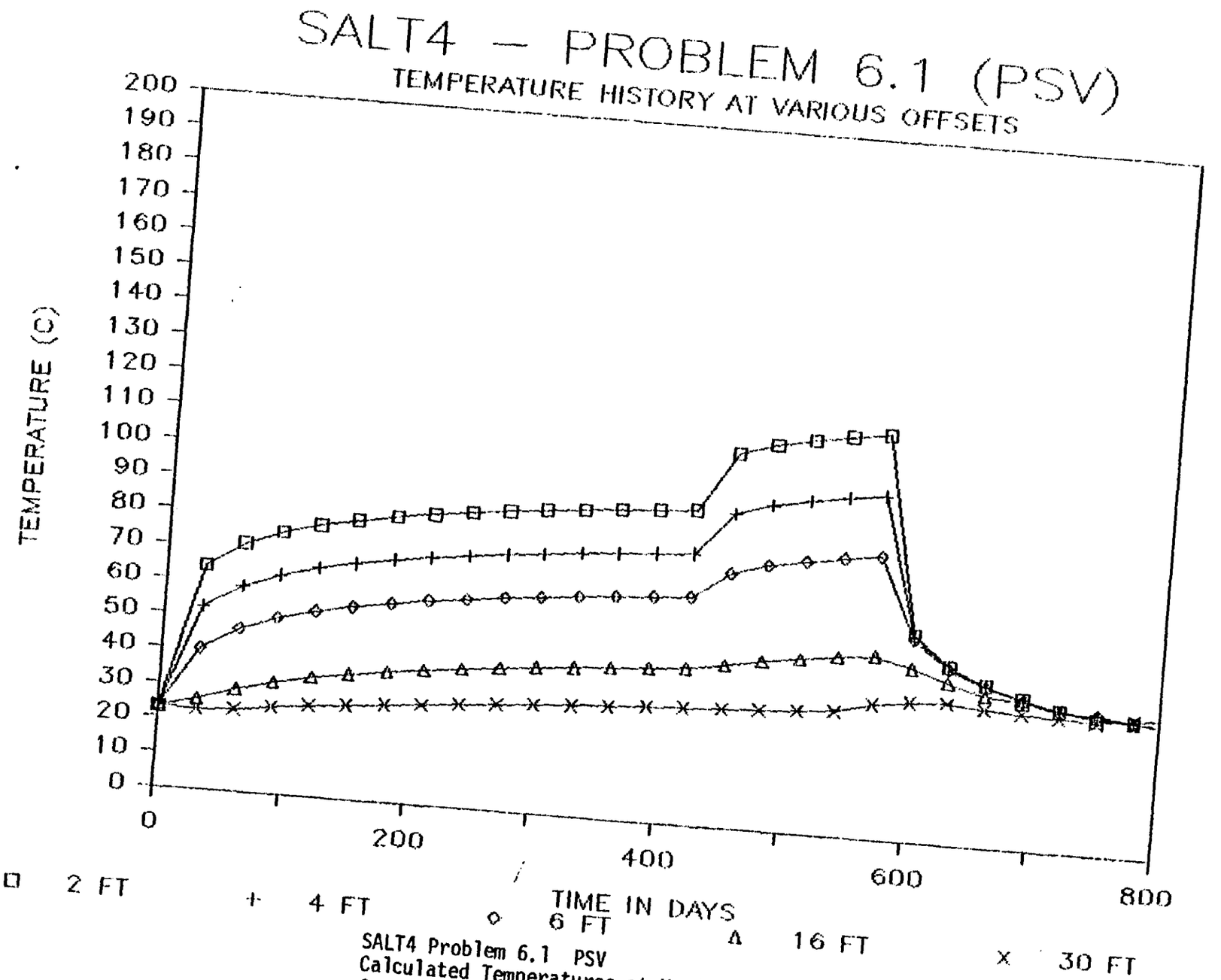


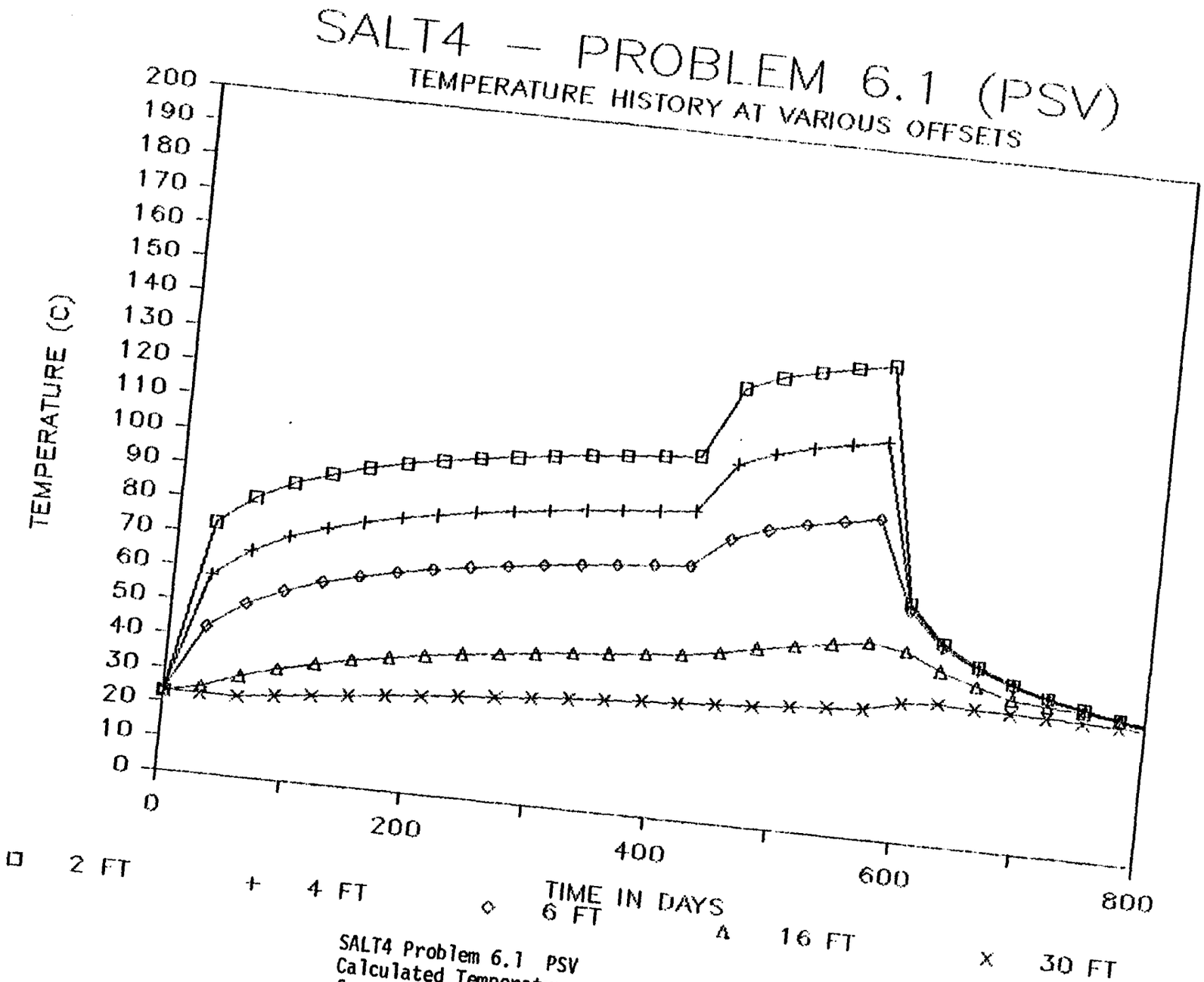
Figure 7.2-4R1 MATLOC Problem 3.2a - Finer Mesh Results
Angle to Principal Stresses Measured to a
Line 30 Degrees from Horizontal



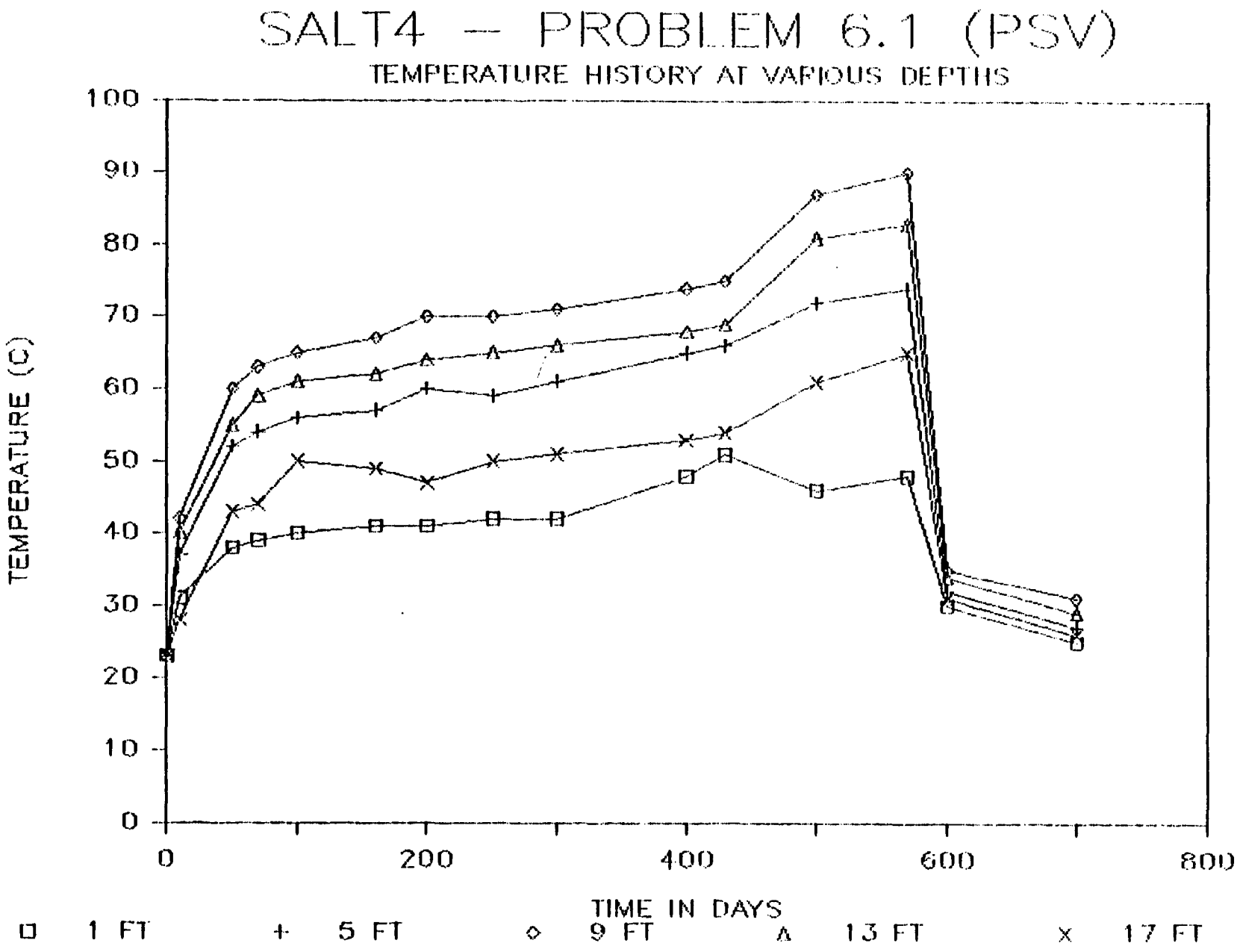
SALT4 Problem 6.1 PSV
Field Measured Temperatures at Various Offset
Locations from Center of Room 1 at
9 ft Depth Below Floor



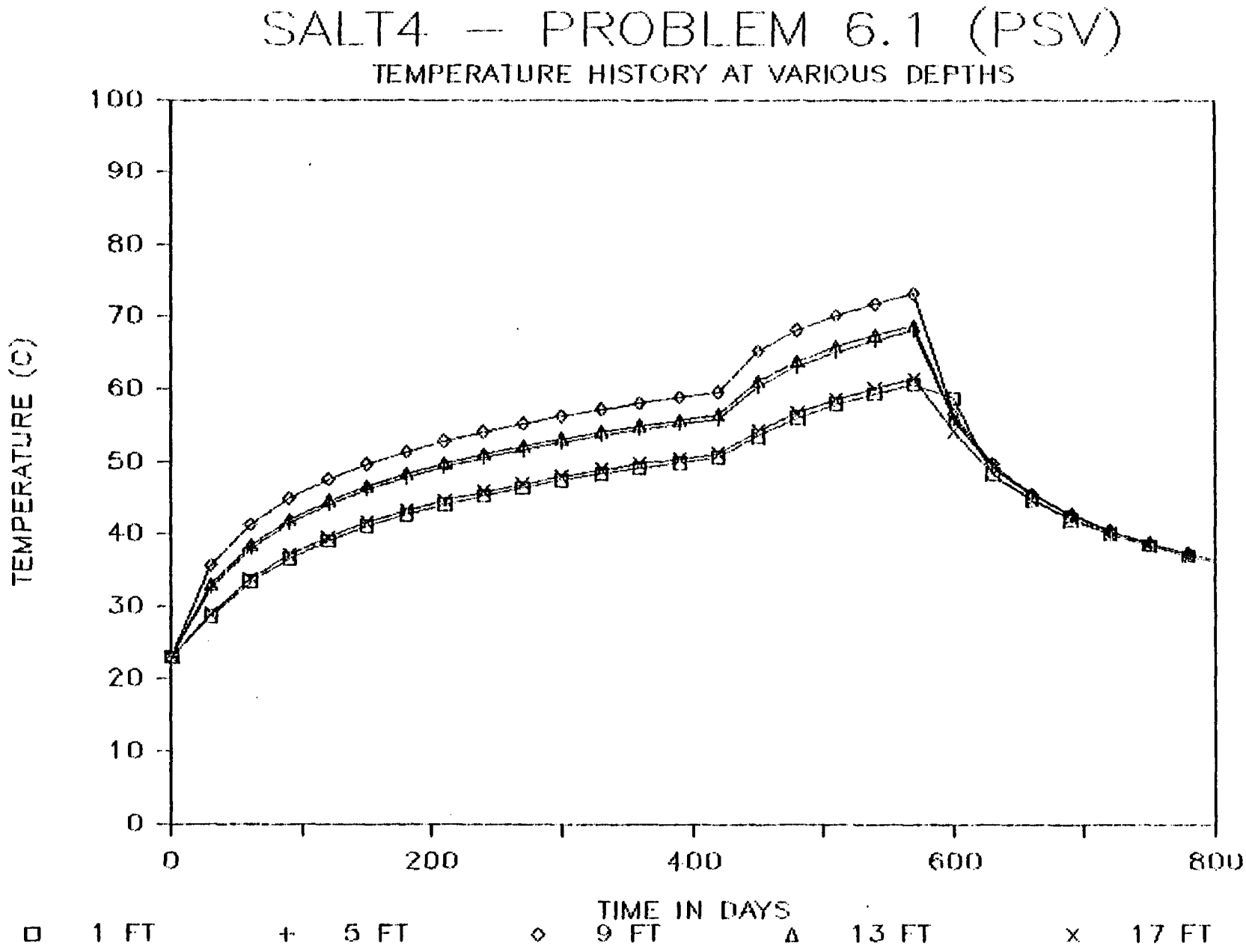
SALT4 Problem 6.1 PSV
Calculated Temperatures at Various Offset Locations
from Center of Room 1 at 9 ft Depth Below Floor
(Thermal Diffusivity = 0.090 ft^2/hr)



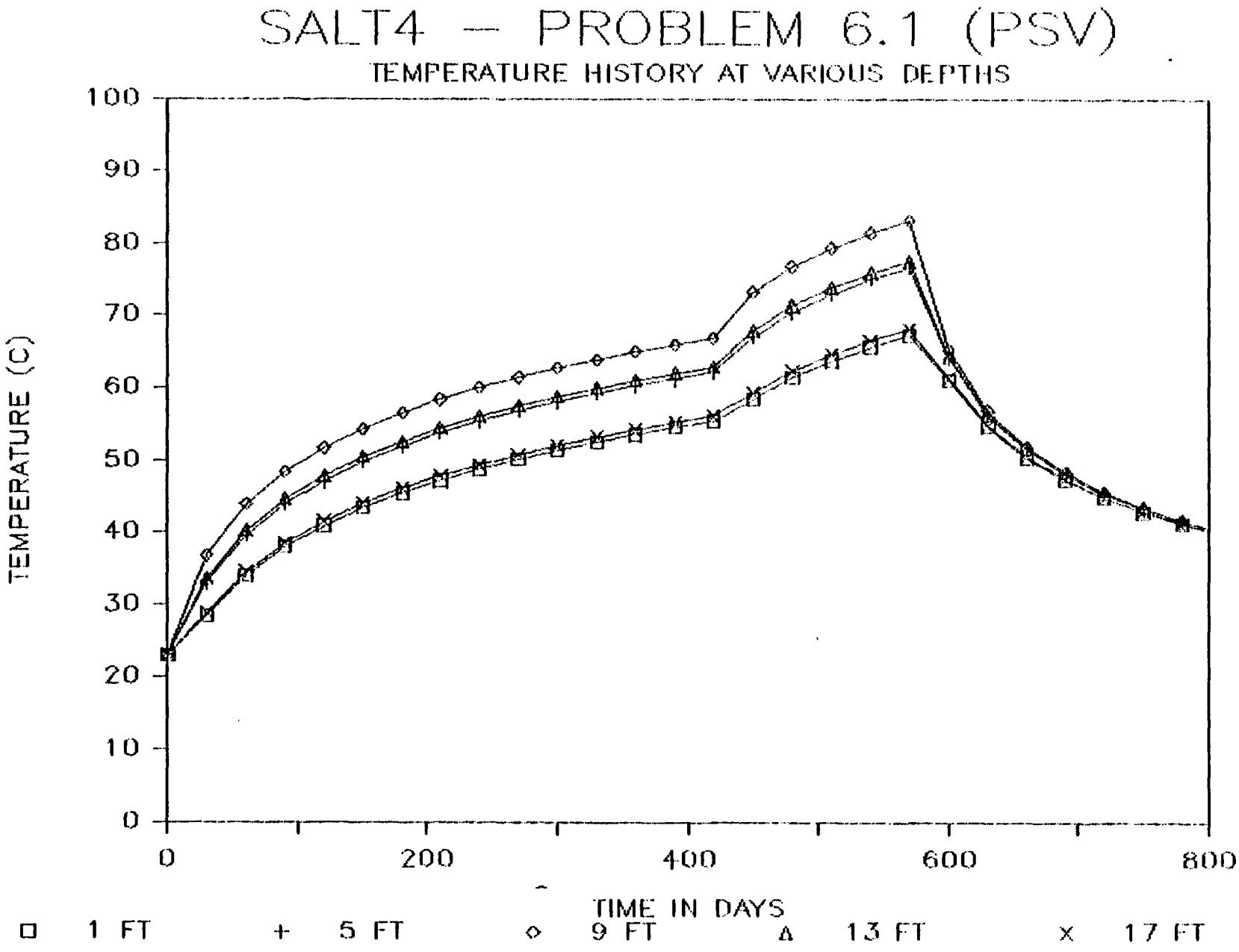
SALT4 Problem 6.1 PSV
Calculated Temperatures at Various Offset Locations
from Center of Room 1 at 9 ft Depth Below Floor
(Thermal Diffusivity = 0.070 ft^2/hr)



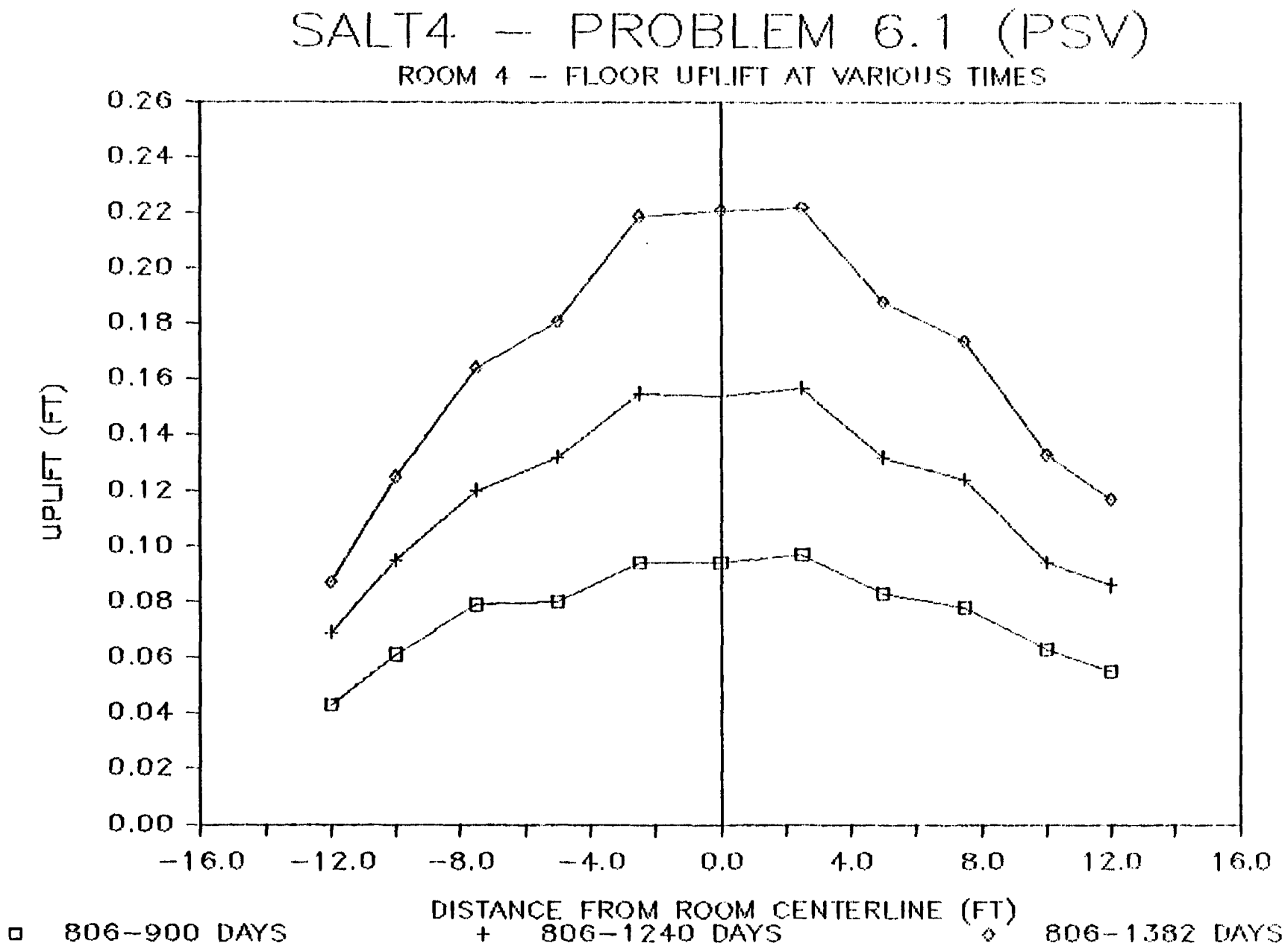
SALT4 Problem 6.1 PSV
Field Measured Temperatures at Various Depths
Below Floor of Room 4 at 8 ft Offset from
Center of Room



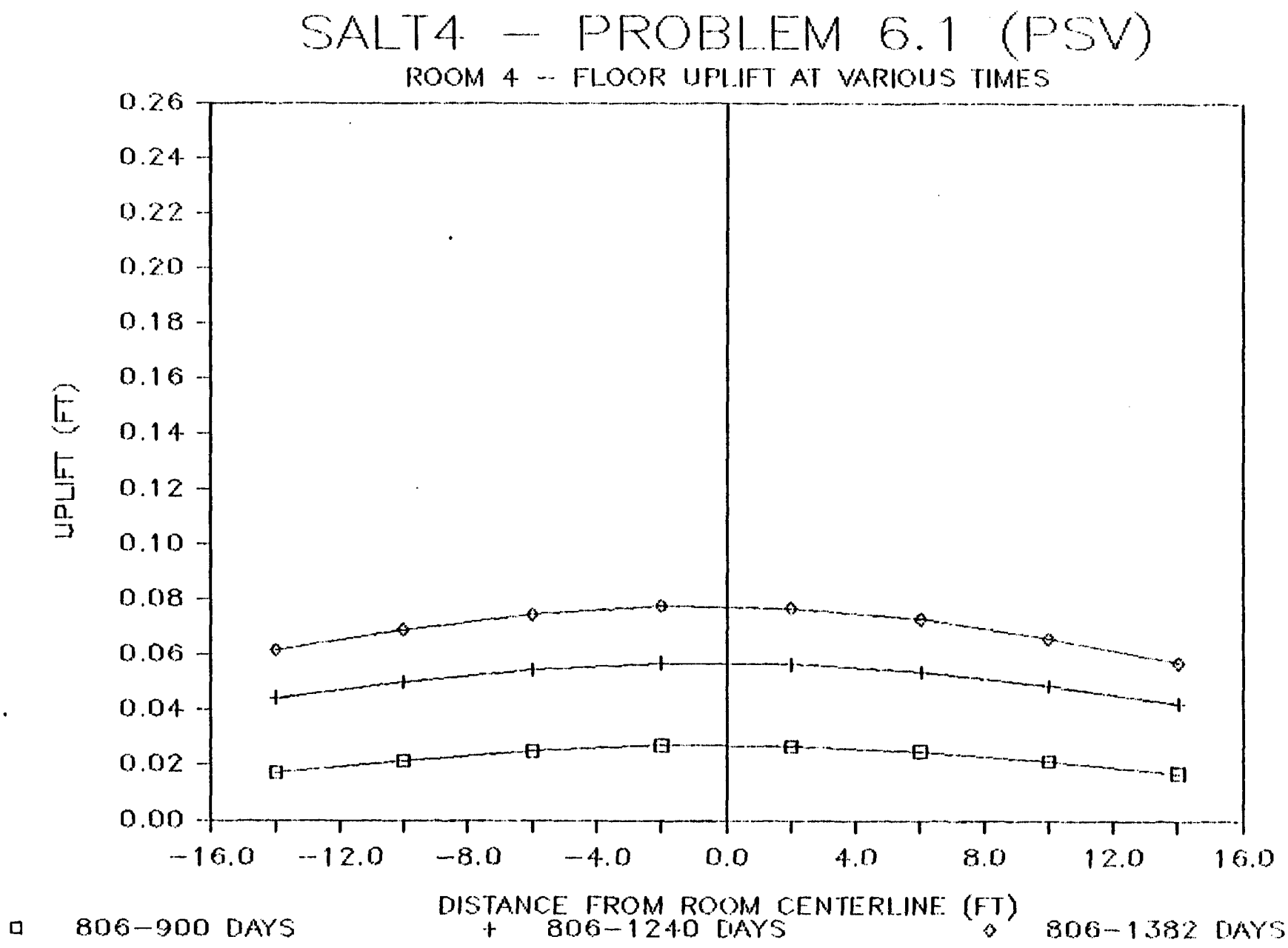
SALT4 Problem 6.1 PSV
Calculated Temperatures at Various Depths Below
Floor of Room at 8 ft Offset from Center of Room
(Thermal Diffusivity = 0.090 ft^2/hr)



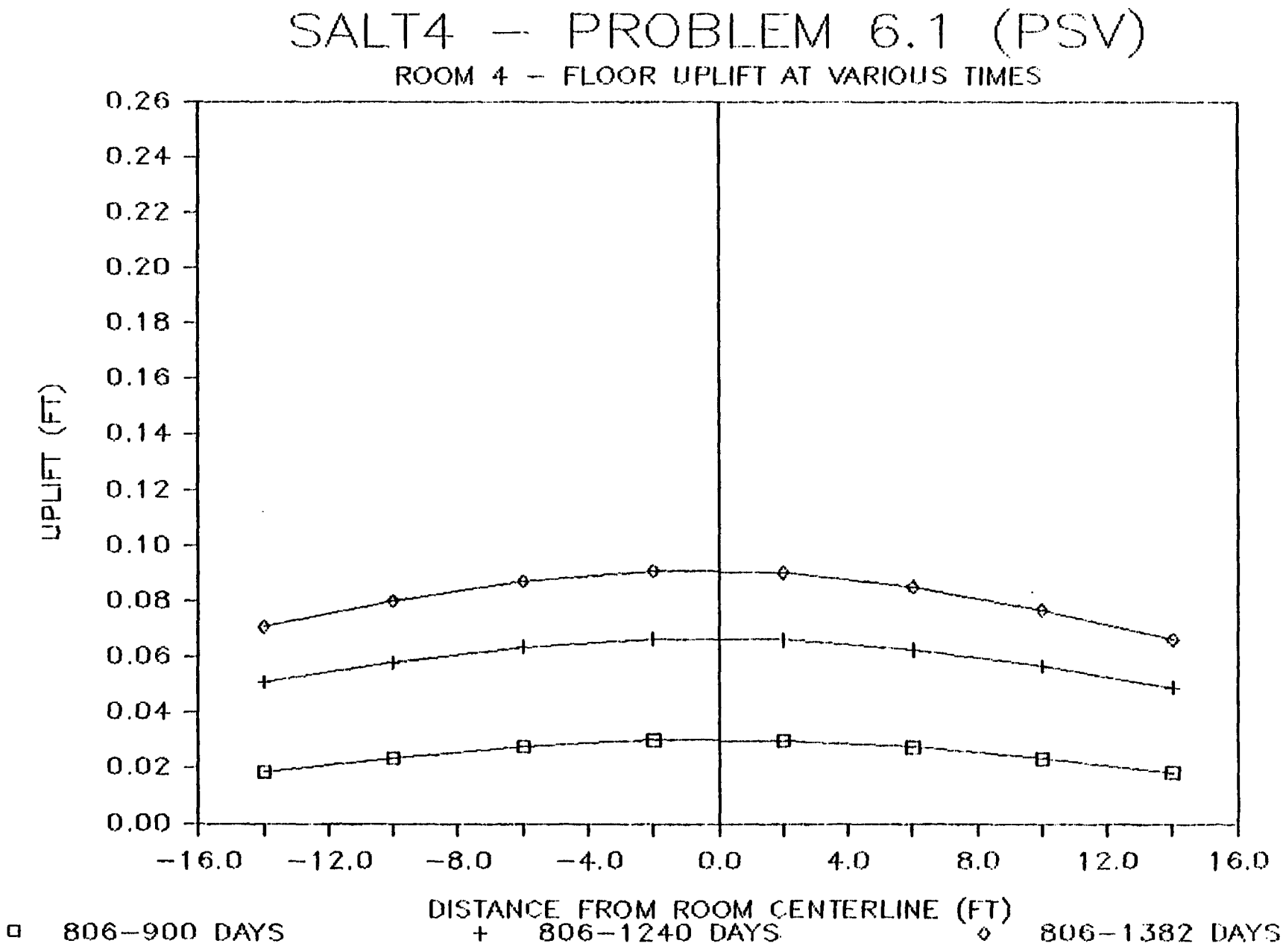
SALT4 Problem 6.1 PSV
Calculated Temperatures at Various Depths Below
Floor of Room 4 at 8 ft Offset from Center of Room
(Thermal Diffusivity = 0.070 ft^2/hr)



SALT4 Problem 6.1 PSV
Field Measured Floor Uplift in
Room 4 at Various Times



SALT4 Problem 6.1 PSV
Calculated Floor Uplift in
Room 4 at Various Times
(Thermal Diffusivity = 0.090 ft^2/hr)



SALT4 Problem 6.1 PSV
Calculated Floor Uplift in
Room 4 at Various Times
(Thermal Diffusivity = 0.070 ft^2/hr)