See Pocket for ON

CorSTAR

A TEKNEKRON INDUSTRIES AFFILIATE

WM DOCKET CONTROL CENTER

'84 NOV 16 A11:26

NRC FIN B6985

November 15, 1984

WM-RES
WM Record File
B-6985
CORSTAR

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

Distribution:
x Brooks
x Ditto
(Return to WM, 623-SS)

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 October 1984

Dear Pauline:

This letter contains a management level summary of progress during the month of October. 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 report under separate cover.

Task 1 - Literature Search - Waste Package Codes

We are still obtaining permission to use tables and figures in the final data set report for the waste package codes. As of the date of this progress report, we have obtained permission from two out of a total of five publishers to use figures and tables. Once permission is obtained from all publishers, we will forward a final camera ready copy to you for publication.

Task 3- Benchmark Problem Report - Waste Package Codes

This report was submitted for NRC review by letter dated September 21, 1984. Concurrently the report was submitted for external QA review. Copies of the external QA review comments on the report are being sent to you under separate cover. We would appreciate receiving the NRC's comments on this report within the next three weeks.

Tasks 4&5 - Siting Codes

During October no significant activities were conducted on this task.

8412050231 841115
PDR WMRES EECCORS
B-6985 PDR

CORPORATE SYSTEMS, TECHNOLOGIES, AND RESOURCES
7315 WISCONSIN, NORTH TOWER #702 • BETHESDA, MARYLAND 20814 • (301) 654-8096
BERKELEY WASHINGTON, D.C. INCLINE VILLAGE

1654

Tasks 4&5 - Radiological Assessment Codes

During October, work on the benchmarking of the Radiological Assessment Codes dealing with Environmental Transport and Dose to Man was completed and the results documented. Benchmarking of the code ORIGEN is nearing completion. Conclusions reached during the Environmental Transport and Dose to Man code benchmarking include the following:

- The separation of the radionuclide transport and food chain calculations from the dose-to-man calculation can facilitate the use of alternate dosimetry systems. The codes BIODOSE and PABLM will have to be substantially modified to accept a new system of dose factors since the dose factor calculation is performed within these codes.

- The environmental compartment approach with solid and liquid components, as used in PATH1 and CELLTRANS, appears to be the best general framework for handling environmental transport problems. From the users point of view it also seems to be the least confusing. Furthermore, with the eigenvector method used in CELLTRANS, these problems can be run on microcomputers.

- The preparation of input data for these codes could be facilitated by use of input preprocessor programs. This approach would require no change to a code itself, which would still be run in a batch mode.

- The PABLM and LADTAP codes have poor internal documentation. This not only makes future improvements to the codes more difficult, but makes it more probable that these modifications will introduce errors in the code.

- The codes PATH1/DOSHEM and BIODOSE are parts of larger systems. In these systems data is generally passed from one component to another in the form of disk files. When run in a stand-alone mode, these codes require that this data be manually entered in a rather cumbersome or confusing format. For example, DOSHEM input had to be prepared manually from PATH1 output since only the steady-state version of PATH1 will generate a file for direct input to DOSHEM. The code developers never bothered to link the time-dependent version of PATH1 with DOSHEM since the overall system was only used to model steady-state conditions. When run in a stand-alone mode, the code BIODOSE does not allow the user to specify radionuclide inputs in conventional units such as Ci/yr. Instead,

BIODOSE requires an inventory value for each radionuclide in units of Ci/MWe-yr. By consulting the documentation for the NUTRAN system, of which BIODOSE is a part, one finds that the BIODOSE calculated dose reported in Rem must be multiplied by the spent fuel stored (MWe-yr) and the transport rate from the repository to the surface environment (yr^{-1}).

- The doses calculated by PATH1/DOSHEM and CELLTRANS are virtually identical. The results from the two codes at other times also show this close agreement. This result constitutes a verification of the compartmental equation solving methods used in the two codes.

- Contrary to the documentation, the PATH1/DOSHEM code does not calculate an external dose to the skin. Only the external total body dose is calculated. Also, contrary to the documentation, the DOSHEM binary format dose factor library contains an external dose factor for ^{222}Rn.

- There is good agreement between BIODOSE and PATH1/DOSHEM-CELLTRANS with the following exceptions:

  - The ^{210}Pb doses are underpredicted by BIODOSE because the code does not account for the ingrowth of ^{210}Pb due to chain decay from ^{226}Ra. The ^{226}Ra skin dose for Benchmark Problem BMP3.0B is underpredicted since BIODOSE does not account for ^{226}Ra in growth due to ^{230}Th decay.

  - Since BIODOSE does not explicitly account for chain decay, only ^{242}Pu doses are calculated for Benchmark Problem BMP 3.1B.

  - The ^{129}I skin dose calculated by BIODOSE is 15 percent greater than that calculated by CELLTRANS since BIODOSE is not able to account for the low ^{129}I Kd value for the soil.

- PABLM dose calculations show good agreement with those from PATH1/DOSHEM and CELLTRANS only when the soil concentration is not an important factor in the dose calculation.

- Even if PABLM could simulate the transport of radionuclides beyond the dose commitment time, there would still be a problem since the radionuclide library in PABLM does not account for the full decay chain.

- The ^{14}C uptake model used in PABLM gives ^{14}C doses which are a factor of 75 higher than those calculated by PATH1/DOSHEM, CELLTRANS and BIODOSE, all of which use the concentration factor method for calculation of ^{14}C uptake.

- The LADTAP code gave doses which were generally within a factor of two to three of those calculated with PATH1/DOSHEM and CELLTRANS.

Tasks 4&5 - Repository Design Codes

No new codes were obtained during the month. An agreement was signed by the NRC and Acres with Adina Engineering to obtain the codes ADINA and ADINAT. A letter outlining proposed scope changes due to the unavailability of the SPECTROM codes was submitted to the NRC during October. On November 9, we received verbal authorization to proceed with this code substitution.

During October, the large core memory version of VISCOT was successfully compiled at Brookhaven National Laboratory. The code SALT4 was also compiled and successfully run. During the month problems 3.2b and 3.2c were run with VISCOT. Problem 5.2 was set up with the code VISCOTLCM. Problem 5.2 was run with the code SALT4 and problem 5.3 is being prepared. During the month the results of the DOT benchmarking were documented. A draft copy of these results is included with the technical status summary report.

General

The following items were identified earlier as having the potential to impact project schedule and budget. Their status is updated below:

- We have met with the NRC to review the approach for responding to comments on the Tasks 4&5 report for the siting codes.

- The NRC will obtain the codes ADINA and ADINAT directly from Adina Engineering for use on this project. We are still awaiting receipt of the codes by the NRC.

- We received verbal authorization to substitute problems for the SPECTROM codes.

- A charge number was obtained to use the code STEALTH at the INEL computer facility.

Our estimate of costs through the end of October (through November 10 for CorSTAR) is:

Actual costs this month:	53K
Actual costs this fiscal year:	53K
Actual costs to date:	2,827K
Planned costs this month:	50K
Planned costs this fiscal year:	50K

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 accounting department.

Sincerely,

Michael T. Mills
for
Douglas K. Vogt
Project Manager

cc: D. Fehringer

See folder for Mr. Bo
P Brooks from Vogt 11-15-84

TECHNICAL STATUS SUMMARY

CorSTAR

TECHNICAL STATUS REPORT ATTACHMENT
TO PROGRESS REPORT FOR OCTOBER 1984

Repository Design Codes

Task 4 - Code Procurement

For the procurement of the ADINA and ADINAT codes, a signed lease agreement was sent to ADINA Engineering on October 19, 1984. A response to this lease agreement is awaited. Additionally, proposed scope changes, brought on by the unavailability of the SPECTROM codes, have been sent to the NRC in a letter included with the September Progress Report. A decision from the NRC on these proposed scope changes has yet to be received.

Code Installation

The installation of SALT4 (QA version identifier 420--06C-02) was completed this month.

A Large Core Memory (LCM) version of VISCOT (QA version identifier 420-11C-02) has been compiled. The original VISCOT required downsizing of the real storage array to allow compilation within the small core memory. The large core version, VISCOTLCM, is necessary to run the large hypothetical and field validation problems.

Run Benchmark Problems

Problems 3.2b and 3.3c were run this month using using VISCOT. Problem 5.2 is currently being set up for use with VISCOTLCM.

Problem 5.2 was run using SALT4 while Problem 5.3 is being set up for SALT4. The results have not yet been analyzed.

PROJECT STATUS

TABLE 3

MATRIX OF CODE/PROBLEM COMBINATIONS*
(Revised 5/21/84)

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.

	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)		x		0			x				0
2.8 Transient Temperature Response to the Quench of an Infinite Slab With a Temperature-Dependent Convection Coefficient (Kreith, 1958, pp. 161)		x		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	x					x					0
3.3 Thick-Walled Cylinder Subjected to Internal and/or External Pressure c) Plane strain - creep	x										
3.5 Plane Strain Compression of an Elastic-Plastic Material von Mises; Drucker, Prager	x					x					0
5.0 HYPOTHETICAL REPOSITORY DESIGN PROBLEMS											
5.1 Hypothetical Very Near Field Problem	x	x	(1)	0							
5.2 Hypothetical Near Field Problem						x	x				0
5.3 Hypothetical Far Field Problem	(2)	(2)				x	x			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)				x	x				0

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

Problems Completed

Problems Run, Results Not Analyzed

6 - BENCHMARKING OF DOT

6.1 - Code Background and Capabilities

DOT, an acronym of Determination of Temperature, is a two-dimensional finite element heat transfer computer program developed by R.M. Polivka and E.L. Wilson[1] at the University of California - Berkeley. The program and the documentation[2] was obtained from the Office of Nuclear Waste Isolation (ONWI). DOT is one of the codes documented as part of the SPECTER technology package. The QA identification number for this version is 420--05C-02$_b$ (b=blank).

The DOT program can be used for the solution of both linear and non-linear two-dimensional planar and axisymmetric heat transfer problems. The code incorporates anisotropic conductivity. Temperature-dependent thermal properties may be modeled by inputting conductivity and specific heat at various temperatures. The code performs a piecewise linear interpolation from these tabulated values. Boundary conditions may be:

1. Time-dependent temperature and heat flux functions;

2. Convection with time-dependent environmental temperature and convection coefficient; or

3. External radiation (i.e., radiation to a constant temperature).

The DOT program contains cooling pipe elements which may be used to create a heat sink at a node. These are directly applicable to cooling of mass concrete but may be useful in some repository problems.

The SCEPTER version of DOT incorporates a subroutine which automatically prepares tape files which can be used as temperature input for the MATLOC, VISCOT, and UTAH2 geomechanical analysis codes. Also

prepared is a tape file which can be used in restarting the DOT analysis. Restart of DOT actually involves editing the final temperatures on the restart tape into a new input data deck as the initial temperatures of a new DOT run. Thus, from a computation point of view it is not really a restart as opposed to a true restart in which intermediate variables are saved and used to actually restart the analysis.

A total of five problems were run using DOT. These included:

1. Problem 2.6 - Transient Temperature Analysis of an Infinite Rectangular Bar with Anisotropic Conductivity;

2. Problem 5.2B - Hypothetical Near Field Problem - Basalt;

3. Problem 5.2S - Hypothetical Near Field Problem - Salt;

4. Problem 6.1 - Project Salt Vault - Thermomechanical Response Simulation Problem; and

5. Problem 6.3 - In Situ Heater Test - Basalt Waste Isolation Project.

These problems are defined in detail in Section 3 of this report and in the benchmark problems Report (5). Table 6.1 shows the capabilities tested or utilized by each of these problems.

6.2 - Problem 2.6 - Transient Temperature Analysis of an Infinite Rectangular Bar with Anisotropic Conductivity

Input Data

One-quarter of the bar cross-section was modeled using two-dimensional planar 8-noded conduction elements and 2-noded surface convection elements. The finite element mesh utilized for this problem is shown in Figure 6.2-1. It should be noted that for compatability of shape functions, three-noded convection elements should be used against a three-noded side. However, only two-noded convection elements are available

Table 6.1

DOT Capabilities Tested or Utilized

	Problem				
	2.6	5.2B	5.2S	6.1	6.3
Problem Type					
- Planar	T	U	U	U	
- Axisymmetric			U	U	
Equation Solution	T	U	U	U	U
Conductivity					
- Linear	T				
- Nonlinear					
- Anisotropic	T				
Convection					
- Linear	T	U	U	U	U
- Temperature Dependent Coefficient					
- Time Dependent Environmental Temperature					
Radiation					
- External Source/Sink					
Cooling Pipes					

T = Tested by comparison with Analytical Solution.
U = Utilized and results of analysis compared with other code results.

in DOT. For this problem, this substitution did not significantly affect the results.

Input data used for the problem, included the following:

Material Properties

1. Density 2760 kg/m^3
2. Specific Heat and Conductivity Table

Temperature (°C)	Conductivity (W/m°K)			Specific Heat (J/kg°K)
T	k_x	k_y	k_{xy}	C
200°K	2.0	1.0	0.0	725
600°K	2.0	1.0	0.0	725

Time Step Data

1. Number of time steps 80 and 20
2. Time step 100,000 sec and 400,000 sec

Initial Conditions/Boundary Conditions

1. Initial Temperature 573°K
2. Environmental temperature 303°K
3. Convection Coefficient 2.0 W/m^2°K

Two separate runs were made with different time steps to check the convergence to the analytical solution.

Run Problem

This was the first problem solved using DOT and, as such, there were a number of minor difficulties encountered before a successful analysis

was completed. These were not necessarily problems with the code but rather in interpretation and application. The problems were as follows:

1. The problem as initially submitted had temperatures in °C, used a temperature shift of 273°, included the Stefan-Boltzmann constant, a shape factor of 0.0, and had an external emmissivity of 1.0. The user's manual states under the shape factor input variable that a value of zero indicates that radiation is ignored. This did not appear to be the case since the program stopped after one time step with the message "computed temperature out of range of values given in material table . . . T = -11.6°." This error was overcome by using absolute temperatures, using a temperature shift of zero, and setting all radiation parameters to zero.

2. After obtaining results using a time step of 400,000 sec., the time step size was estimated based on a procedure originally developed by Nickell and Levi and outlined by Gartling (3) in the COYOTE manual.

Results

The results of both the analysis using the steps of 100,000 sec and 400,000 sec are shown graphically and tabulated in Figures 6.2-2 through 6.2-4. In general the DOT solutions showed slightly higher temperatures throughout the analysis. Since the problem calculates decreases in temperature with time, the magnitude of the temperature change is computed to be less using DOT than the analytical solution.

Figure 6.2-2 shows the temperature of the centerline of the bar as a function of time for both the 100,000 sec time step and 400,000 sec time step analyses as compared to the analytical solution. The maximum temperature difference for the 100,000 sec analysis is 6.4°C and a maximum difference of 19.6°C was obtained with the 400,000 sec. Expressed as a percentage of the temperature change, these differences are a 4.6% and 11.1%, respectively.

Figures 6.2-3 and 6.2-4 show the temperature distribution along the x and y axes respectively at a time of 400,000 sec. At this time step the temperatures are slightly less than the analytical temperature at small x and y valves. The computed temperatures are slightly greater than the analytical temperatures when x is greater than mid-width or y is greater than mid-length. The maximum difference is 9.4°C for a 100,000 sec time step and 21.5°C for a 400,000 sec time step. These differences are 8.8% and 20.0% of the temperature change, respectively.

6.3 - Problem 5.2B - Hypothetical Near Field Problem - Basalt

Input Data

A two-dimensional section through a repository with an infinite number of rooms was modeled using 8-noded isoparametric planar elements and two-noded convection elements. Although the model extended from an depth of 3500 m to the ground surface, 124 of a total of 152 elements were located between depths of 479 m and 510 m. This region is shown in Figure 6.3-1. The remainder of the model consisted of "filler" elements with vertical dimensions of each element not exceeding 1.5 to 2.0 times the vertical dimension of the previous element. Although the aspect ratio of these "filler" elements is extreme, numerically these elements model the boundary conditions that are imposed on the repository very well.

Input data used for the problem included:

Material Properties

1. Density 2700 kg/m^3
2. Specific Heat and Conductivity Table:

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

Time Step Data

1.	Run number	1	2	3	4
2.	Number of Time Steps	10	10	9	9
3.	Time Step Increment(s) ($\times 10^8$ sec)	1.577	1.577	31.54	315.4
4.	Time Step Increment (years)	5	5	100	1000

Initial Conditions/Boundary Conditions

1. Initial Temperatures
   a) between depths of 479 m and 510 m — 25°C
   b) other depths — T = 15°C + 0.02 x Depth
2. Environmental Temperature in Room (run 1 only) — 15°C
3. Convection Coefficient (Run 1 only) — 0.40 W/m^2°C
4. Constant Ground Surface Temperature — 15°C
5. Constant Temperature at Depth = 3500 m — 85°C
6. Externally Supplied Heat Flux:

Time (sec)	Function Value
0	20 W/m^2
3.16×10^8	13.3
6.31×10^8	10.3
9.47×10^8	8.0
1.26×10^9	6.33
2.52×10^9	3.33
5.68×10^9	0.33
8.83×10^9	0.03
1.58×10^{10}	0.0
2.47×10^{11}	0.0

The function value of the externally supplied heat flux is multiplied by the following contributing areas for each of the nodes:

Nodes	Contributory Area
248	0.0833
265	0.3333
274	0.2500
291	0.6667
300	0.3333
317	0.6667
326	0.3333
343	0.6667
352	0.3333
369	0.6667
378	0.2500
395	0.3333
404	0.0833

Ideally, the heat transfer across the room after repository sealing should be modeled. This transfer would occur by a combination of natural convection, radiation, and conduction through the air mass. The DOT model does not allow radiation or convection between surfaces and thus these effects were not modeled. In an actual problem, it may be possible to approximate these effects with conduction elements by making assumptions to approximate an artificial conductivity. However, this was not the intent of the benchmarking process and was not performed.

Run Problem

The analysis of this problem requires four separate finite element runs. This is due to the fact that, for DOT, the time steps must be constant within each analysis. The first run included boundary convection elements to model the cooling effects of forced repository ventilation. These elements were eliminated during the second through fourth runs (i.e., time >50 years).

The DOT code is used to compute temperature distributions for use as input to geomechanical codes. Although DOT allows the use of variable

noded elements, MATLOC does not. This caused some wasted effort in that the problem was set up using the DOT manual and it was later determined that the problem had to be rerun for compatability with MATLOC using either 4-noded or 8-noded elements. This could be avoided by noting this requirement within the DOT manual.

The actual restart of the problems requires editing final temperatures out of an output tape file and merging these temperatures as initial conditions into a new input data deck. Thus the restart is really a completely new analysis with initial conditions equal to the final conditions of the previous analysis.

Results

The temperature as a function of time from emplacement for three points, 1) cavern mid-wall (Node 154), 2) cavern mid-floor (Node 222), and 3) mid-heater offset 2.5 m (Node 320), are shown in Figures 6.3-2 through 6.3-4. Temperature contours over the modeled region between elevations of -479 and -510 m are shown at time of 10, 30, and 100 years are shown in Figure 6.3-5 and vertical temperature profiles along the centerline of the pillar are shown in Figure 6.3-6 for time of 100, 300 and 1000 years.

A comparison of these results with results of other codes is included in Section 2 of this report.

6.4 - Problem 5.2S - Hypothetical Near Field Problem - Salt

Input Data

The geometry and finite element mesh used for this problem is the same as that used for problem 5.2B (See Section 6.3). Input data specific to the salt problem is as follows:

Material Properties

1. Density 2150 kg/m^2
2. Conductivity and Specific Heat Table

Temperature (°C)	Conductivity (W/m°K)			Specific Heat (J/kg°K)
T	k_x	k_y	k_{xy}	C
-100	4.5	4.5	0	830
+10,000	4.5	4.5	0	830

Time Step Data

Same as Problem 5.2B (See Section 6.3).

Initial Conditions/Boundary Conditions

Same as Problem 5.2B (see Section 6.3).

Run Problem

The actual running of Problem 5.2S was the same as for Problem 5.2B as outlined in Section 6.3. VISCOT is similar to MATLOC in that elements must be 4-noded or 8-noded (or 9-noded). An additional problem was encountered in running VISCOT in that triangular elments cannot be accommodated in VISCOT by using repetitive nodes in the same element. This was overcome within the VISCOT analysis and is described more fully in Section 8.

Results

The temperature as a function of time from emplacement is plotted for three points in Figures 6.4-1 to 6.4-3. Temperatures are given at: 1) mid-cavern wall (Node'154), 2) mid-cavern floor (Node 222), and 3) mid-heater level offset 2.5 m from the centerline of the heater (Node 320). Temperature contours over the modeled region between elevations -479 m and -510 m are shown at times of 10, 30 and 100 years in Figures 6.4-4. The vertical temperature profile along the pillar centerline is shown in Figure 6.4-5 for times of 100, 300 and 1000 years.

6.5 - Problem 6.1 - Project Salt Vault - Thermomechanical Response Simulation Problem

Input Data

Problem 6.1 is a two-dimensional analysis of two adjacent rooms each with separate heater experiments. The heater experiment in Room 3 consists of a row of heaters parallel to the axis of the room. Room 4 contains a circular array of heaters. Due to the differing geometric layouts of heaters, the problem was divided into two separate problems. Problem 6.1P is a two-dimensional planar analysis of Room 3 and Problem 6.1A is a two-dimensional axisymmetric analysis of Room 4. The boundary between the two problems was defined to be in the pillar between Rooms 3 and 4, one meter from the edge of Room 3.

With this division of the problem into two meshes, the effect of the heaters in the adjacent room are not modeled. However, by locating the common outer boundary at a point where the temperatures are at a minimum (determined from field results), this inaccuracy is minimized. This is because with heat sources of the same order of magnitude, the reflected heat at the outer adiabatic boundary is approximately the same as the heat flux across the boundary in the actual validation test.

The finite element meshes for each problem are shown in Figures 6.5-1 and 6.5-2. Other input data is as follows:

Material Properties

1. Density 2160 kg/m^3
2. Conductivity and Specific Heat Table

Temperature (°C)	Conductivity (W/m°K)			Specific Heat (J/kg°K)
T	k_x	k_y	k_{xy}	C
0	6.109	6.109	0	930.97
25	5.524	5.524	0	930.97
50	5.020	5.020	0	930.97
75	4.590	4.590	0	930.97
100	2.226	2.226	0	930.97
150	3.666	3.666	0	930.97
200	3.277	3.277	0	930.97
250	2.997	2.997	0	930.97
300	2.763	2.763	0	930.97
500	1.051	1.051	0	930.97
*1000	1.000	1.000	0	930.97

*(Values for 1000°C are arbitrary to prevent temperatures from going out of range.)

Time Step Data

		Planar Analysis	Axisymmetric Analysis
1.	Number of Time Steps	16	40
2.	Print Interval	2	2
3.	Time Step Increment	1.297×10^6 sec	1.297×10^6 sec
4.	Time Step Increment	15 days	15 days
5.	Time of Start (806 Standard Days = 0)	3.1104×10^7 sec	0 sec
6.	Time at Start	360 days	0 days

Initial Conditions/Boundary Conditions

1.	Initial Temperature	23°C
2.	Environmental Temperature in Rooms	23°C
3.	Convection Coefficient	5.886 W/m°C
4.	Externally Supplied Heat Flux Functions	

Planar Analysis		Axisymmetric Analysis	
Time	Function Value	Time	Function Value
0.0 sec	0.0 W/m	0.0	243.5 W/rad/heater
3.144×10^7	0.0	3.749×10^7	243.5
3.145×10^7	1000.0	3.750×10^7	340.6
6.070×10^7	1000.0	4.976×10^7	340.6
6.071×10^7	0.0	4.977×10^7	0.0
1.0×10^8	0.0		0.0

5. The function value of the externally supplied heat flux is multiplied by the following factors to give nodal heat flux:

Planar Problem		Axisymmetric Problem		
Node	Factor	Node	Factor	
254	0.0833	183	0.0833	center heater
273	0.3333	200	0.3333	
289	0.16667	209	0.1667	
308	0.3333	226	0.3333	
324	0.0833	235	0.0833	
		187	0.50	6 - Peripheral Heaters
		202	2.00	
		213	1.00	
		228	2.00	
		239	0.50	

For both problems, the finite element mesh was extended vertically to a point where they could be considered adiabatic. The left boundary of the planar problem represents a symmetry line since Room 2 had the same heater arrangement and power levels. The outer boundary was assumed adiabatic for reasons described above.

Time step data and initial times were set up for both problems such that starting the array heaters in Room 4 was considered time zero (standard day 806 in the problem definition). Since the heaters in Room 3 were not turned on for almost 1 year, the 6.1P had a start time of 3.1104×10^7 sec (360 days).

Run Problem

Problem 6.1A was the first and only axisymmetric problem with nodal heat sources to be run with DOT. The manual was not clear with respect to the units for input of thermal flux at a node. From examination of the code, it was determined that computation is on a per radian basis and thus the nodal thermal fluxes were input on the same basis.

Results

The temperature histories are shown in Figures 6.5-3 and 6.5-4 for the planar problem and the axisymmetric problem, respectively.

The maximum temperature occurs at day 570 for the axisymmetric problem (Room 4) and at the end of the analysis (600 days) for the planar problem (Room 3). Temperature distributions have been plotted for both rooms at 570 days. Figures 6.5-5 and 6.5-6 show horizontal temperature distributions at mid-heater level on day 570 for Room 3 (planar) and Room 4 (axisymmetric), respectively. The temperature contours for both problems are plotted in Figure 6.5-7, together with measured temperature contours for Room 3.

6.6 - Problem 6.3 - In Situ Heater Test - Basalt Waste Isolation Project (BWIP)

Input Data

Problem 6.3 was modeled using two-dimensional, 8-noded axisymmetric solid elements. The heater itself was modeled as a heat generating "solid" material with specific heat, density, and conductivity values for air. The geometry and the finite elemet mesh utilized is shown in Figure 6.6-1. The axisymmetric model is not truly valid above the floor level; but in the region where the temperature distribution is to be calculated, the model is representative of actual conditions. The inclusion of the room and rock above the floor elevation provide a better representation of the boundary conditions than if they had not been included. Boundaries are set at a distance at which adiabatic boundary conditions can be assumed.

Input Data for Problem 6.3 was as follows:

Material Properties

1. Density of Basalt 2850 kg/m^3
2. Conductivity and Specific Heat Table for Basalt

Temperature (°C)	Conductivity (W/m°K)			Specific Heat (J/kg°K)
T	k_x	k_y	k_{xy}	C
0	1.53	1.53	0.0	1250
100	1.63	1.63	0.0	1240
200	1.73	1.73	0.0	1229
500	2.03	2.03	0.0	1196
1000	2.53	2.53	0.0	1142

3. Density of air 0.950 kg/m^3
4. Conductivity and Specific Heat Table for Air

Temperature (°C)	Conductivity (W/m°K)			Specific Heat (J/kg°K)
T	k_x	k_y	k_{xy}	C
0	0.0244	0.0244	0.0	1004
100	0.0320	0.0320	0.0	1010
200	0.0390	0.0390	0.0	1025
350	0.0490	0.0490	0.0	1054
1000	0.0820	0.0820	0.0	1159

Time Step Data

1. Number of Time Steps 24
2. Print Interval 2
3. Time Step Increment 1.296×10^6 sec
4. Time Step Increment 15 days

Initial Conditions/Boundary Conditions

1. Initial Temperature 15.5°C
2. Environmental Temperature in Room 25°C
3. Convection Coefficient 1.0 W/m^2 °C)
4. Internal Heat Generation Function

Time	Function Value (Total Heat Input)
0 sec	1000 W
7.776×10^6	1000
7.777×10^6	3000
1.9526×10^7	3000
1.9527×10^7	5000
4.5533×10^7	5000

5. Internal Heat Generation Multiplier (1/heat source volume) = $3.1831/m^3$

The material properties input for the air within the heater cavity do not truly represent the actual air properties. This is because there is no provision for temperature dependent density. Nevertheless, numerically the heat generation rate is correct as modeled. The only significance in the results of this inconsistency is an unrealistic air temperature. Although the air temperature will not be computed correctly, this is not a required output of the problem.

Run Problems

A constant time step was utilized and, therefore, restarts were not necessary. No significant code-related problems were encountered in running this problem.

Results

The temperature history for a point at mid-heater level and offset 0.4 m from the centerline of the heater is shown in Figure 6.6.2. Horizontal and vertical temperature distributions are shown for day 259 in Figures 6.6-3 and 6.6-4, respectively. The horizontal temperature distribution at day 350 (temperatures interpolated between time steps) is shown in Figure 6.6-5. For each of these figures, the computed temperatures are shown to agree very well with field measurements.

It should be noted that extensive modeling of the BWIP heater experiment has been carried out at the BWIP site. As a result, reported values of thermal conductivity and specific heat have likely been confirmed and very likely adjusted through the course of these experiments.

Although this may appear to be "fudging" the results, in fact it is the proper way in which any model should be used. The properties of an intact large scale rock mass are very much different from the properties obtained from a small laboratory sample. A proper modelling program would involve adjusting the model throughout the initial experiments, such as the BWIP heater test, on through construction, and even through initial operation of the repository. At each step, the accuracy of the model is both verified and improved as minor adjustments are made to overall rock properties.

DOT REFERENCES

1. Polivka, R.M. and E.L. Wilson, 1976. "Finite Element Analysis of Nonlinear Heat Transfer Problems," UC SESM 76-2, Department of Civil Engineering, University of California, Berkeley, California.

2. INTERA Environmental Consultants, Inc. "DOT: A Nonlinear Heat-Transfer Code for Analysis of Two-Dimensional Planar and Axi-symmetric Representations of Structures," ONWI-420 Prepared for Battelle Memorial Institute, Office of Nuclear Waste Isolation, April 1983.

3. Gartling, D.K. "COYOTE A Finite Element Computer Program for Nonlinear Heat Conduction Problems," Sandia National Laboratories, SAND 77-1332, October 1982.

4. Bradshaw, R.L. and W.C. McClain, "Project Salt Vault: A Demonstration of the Disposal of High-Activity Solidified Wastes in Underground Salt Mines," Prepared for U.S. Atomic Energy Commission by Oak Ridge National Laboratory, Report ORNL-4555, April 1971.

5. Wart, R.J., E.J. Shiba, and R.H. Curtis, "Benchmark Problems Appearing in Repository Design Models," prepared by Acres American Incorporated for the U.S. Nuclear Regulatory Commission, Report NUREG/CR-3097, 1984.

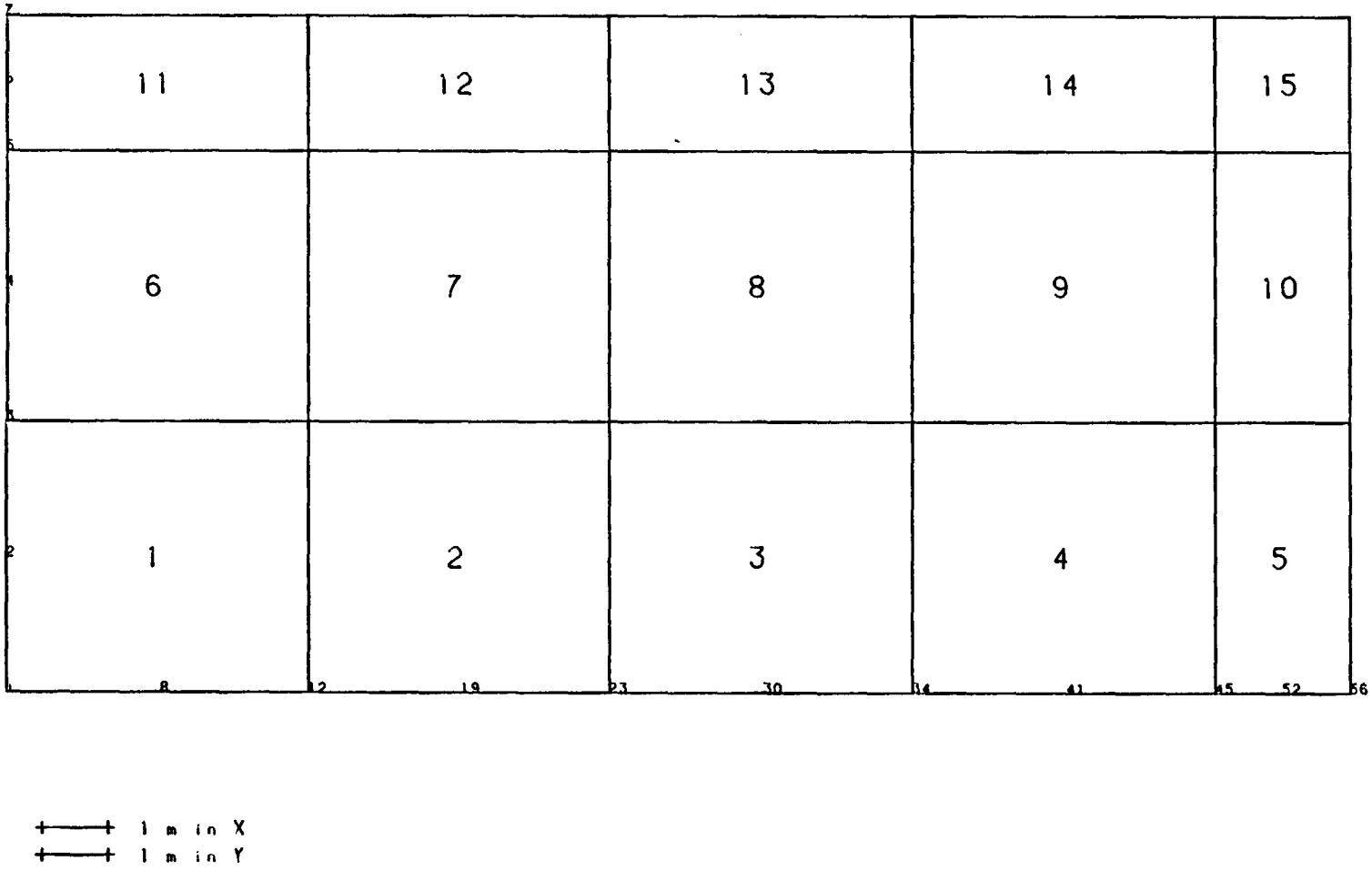
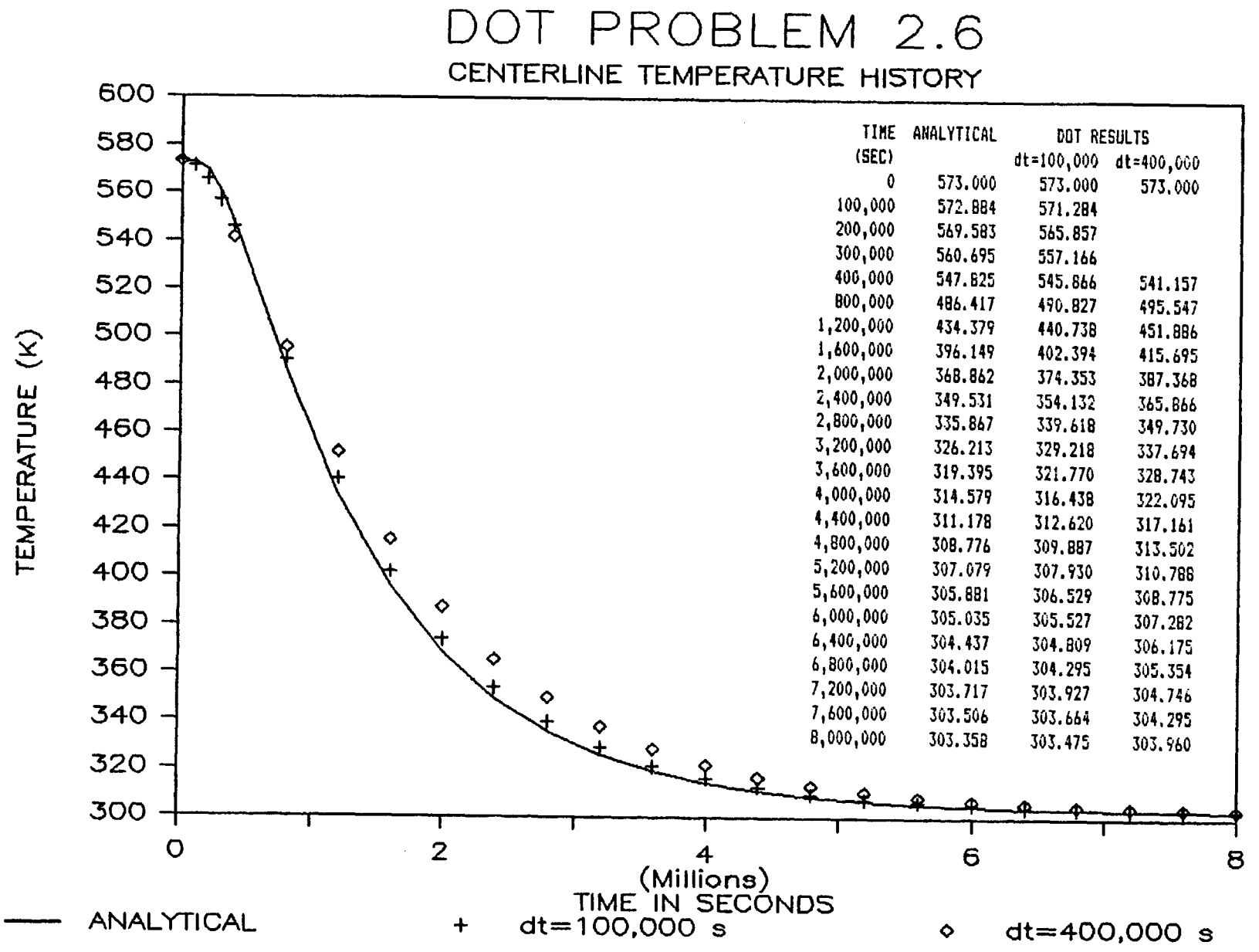
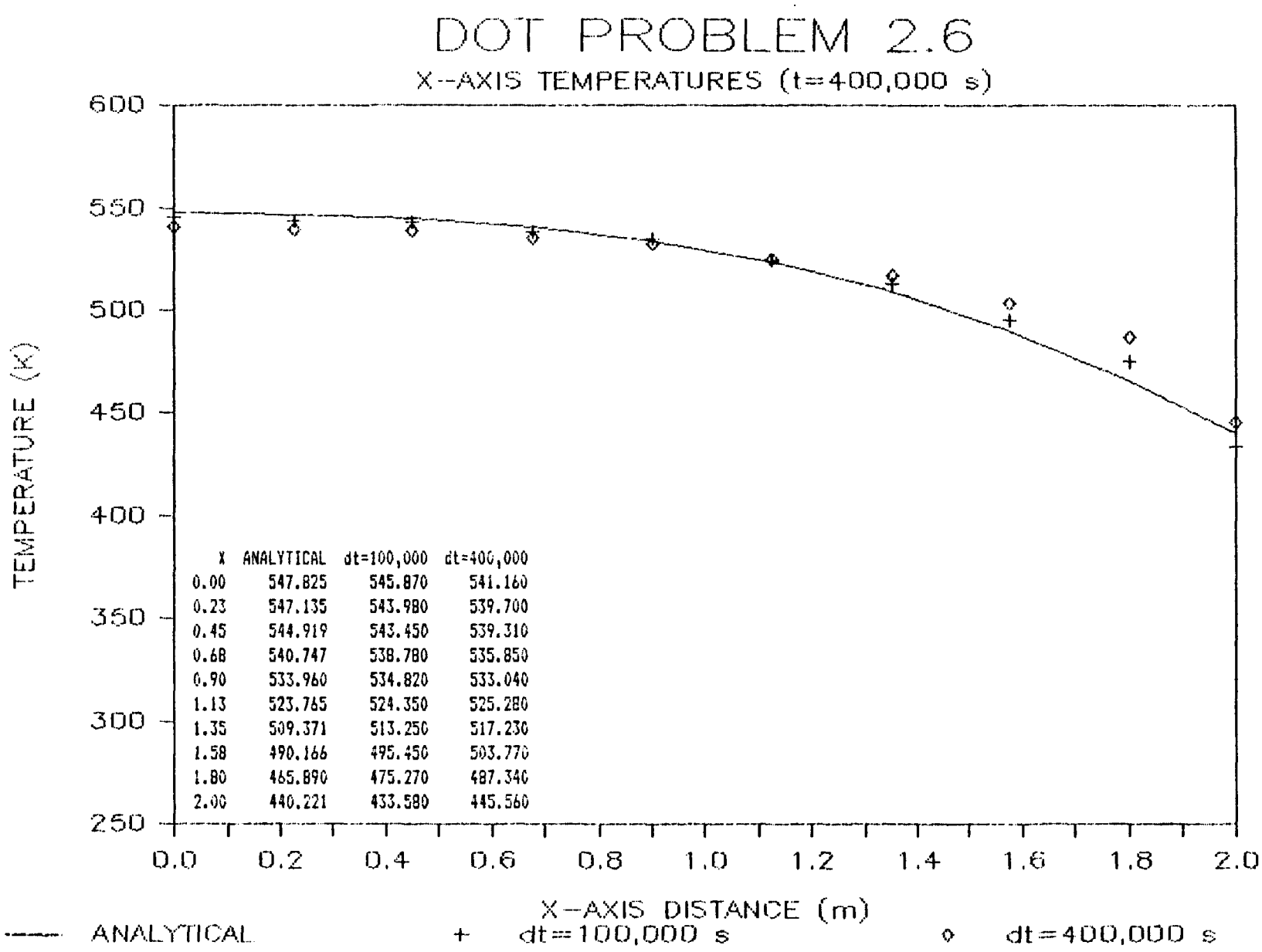


Figure 6.2-1 DOT Problem 2.6
Finite Element Mesh



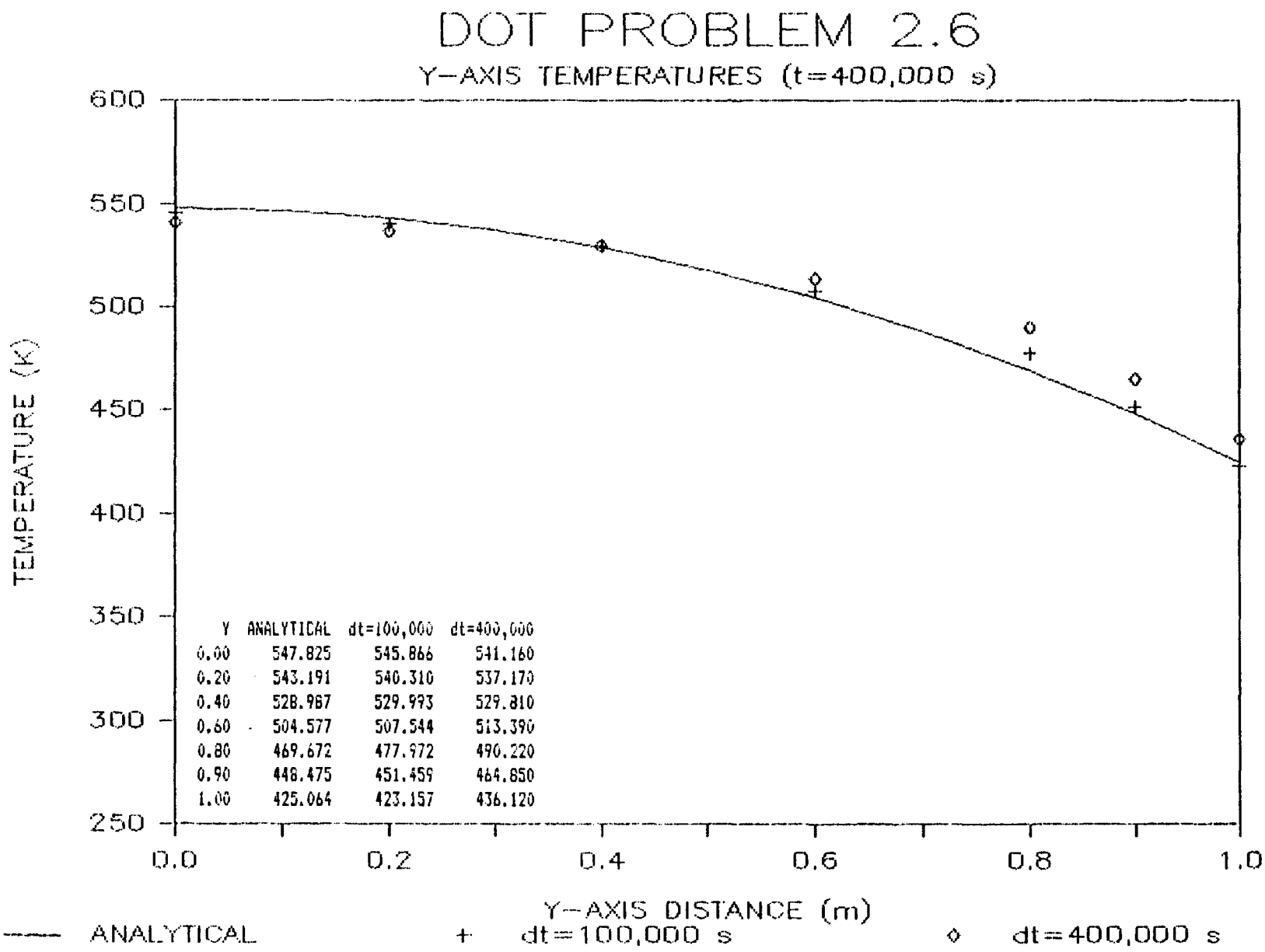
TIME (SEC)	ANALYTICAL	DOT RESULTS dt=100,000	dt=400,000
0	573.000	573.000	573.000
100,000	572.884	571.284	
200,000	569.583	565.857	
300,000	560.695	557.166	
400,000	547.825	545.866	541.157
800,000	486.417	490.827	495.547
1,200,000	434.379	440.738	451.886
1,600,000	396.149	402.394	415.695
2,000,000	368.862	374.353	387.368
2,400,000	349.531	354.132	365.866
2,800,000	335.867	339.618	349.730
3,200,000	326.213	329.218	337.694
3,600,000	319.395	321.770	328.743
4,000,000	314.579	316.438	322.095
4,400,000	311.178	312.620	317.161
4,800,000	308.776	309.887	313.502
5,200,000	307.079	307.930	310.788
5,600,000	305.881	306.529	308.775
6,000,000	305.035	305.527	307.282
6,400,000	304.437	304.809	306.175
6,800,000	304.015	304.295	305.354
7,200,000	303.717	303.927	304.746
7,600,000	303.506	303.664	304.295
8,000,000	303.358	303.475	303.960

Figure 6.2-2 DOT Problem 2.6
Centerline Temperature History



X	ANALYTICAL	dt=100,000	dt=400,000
0.00	547.825	545.870	541.160
0.23	547.135	543.980	539.700
0.45	544.919	543.450	539.310
0.68	540.747	538.780	535.850
0.90	533.960	534.820	533.040
1.13	523.765	524.350	525.280
1.35	509.371	513.250	517.230
1.58	490.166	495.450	503.770
1.80	465.890	475.270	487.340
2.00	440.221	433.580	445.560

Figure 6.2-3 DOT Problem 2.6
X-Axis Temperature Distribution
at Time = 400,000 sec.



Y	ANALYTICAL	dt=100,000	dt=400,000
0.00	547.825	545.866	541.160
0.20	543.191	540.310	537.170
0.40	528.987	529.993	529.810
0.60	504.577	507.544	513.390
0.80	469.672	477.972	490.220
0.90	448.475	451.459	464.850
1.00	425.064	423.157	436.120

Figure 6.2-4 DOT Problem 2.6
Y-Axis Temperature Distribution
at Time = 400,000 sec.

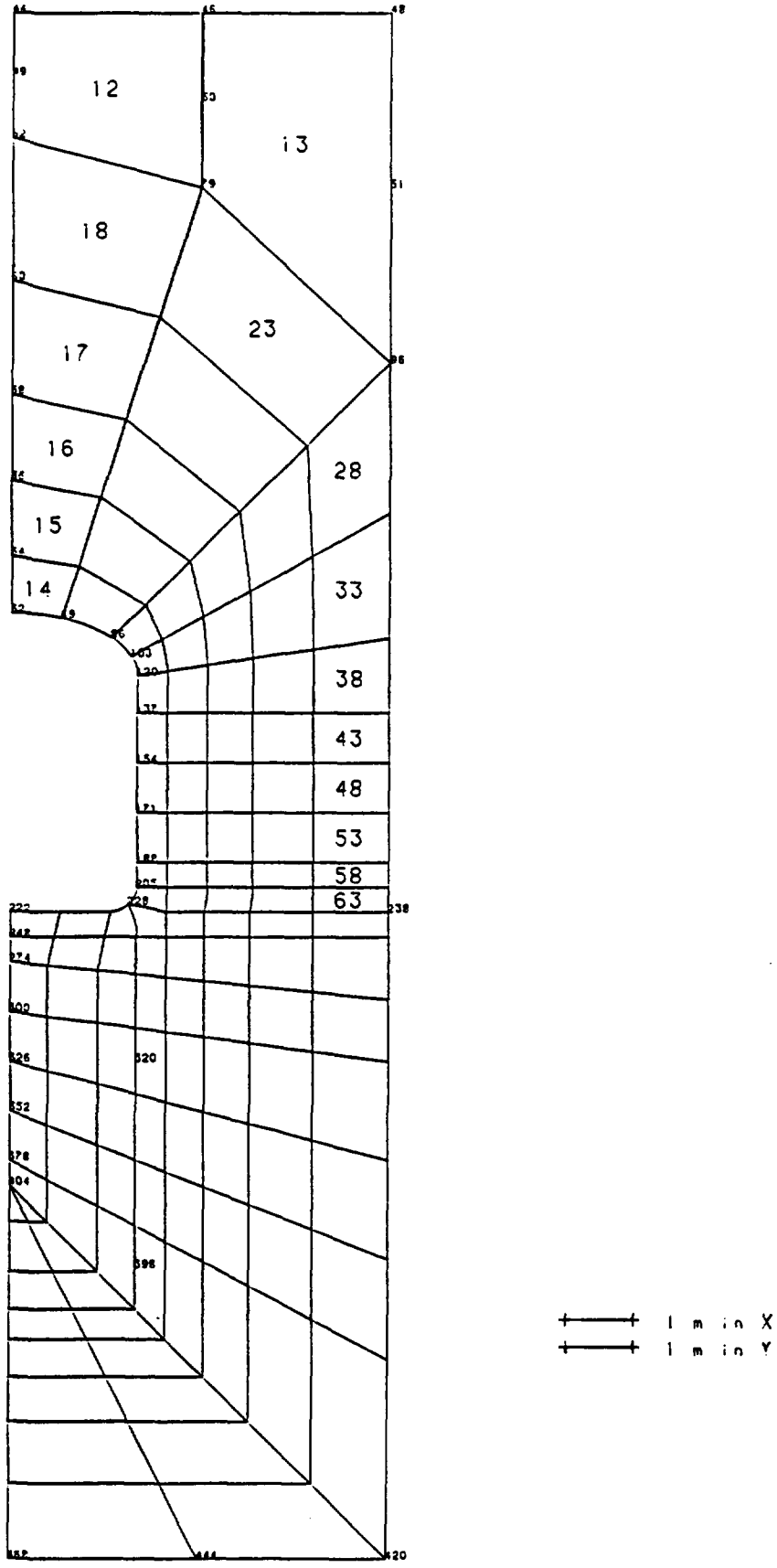
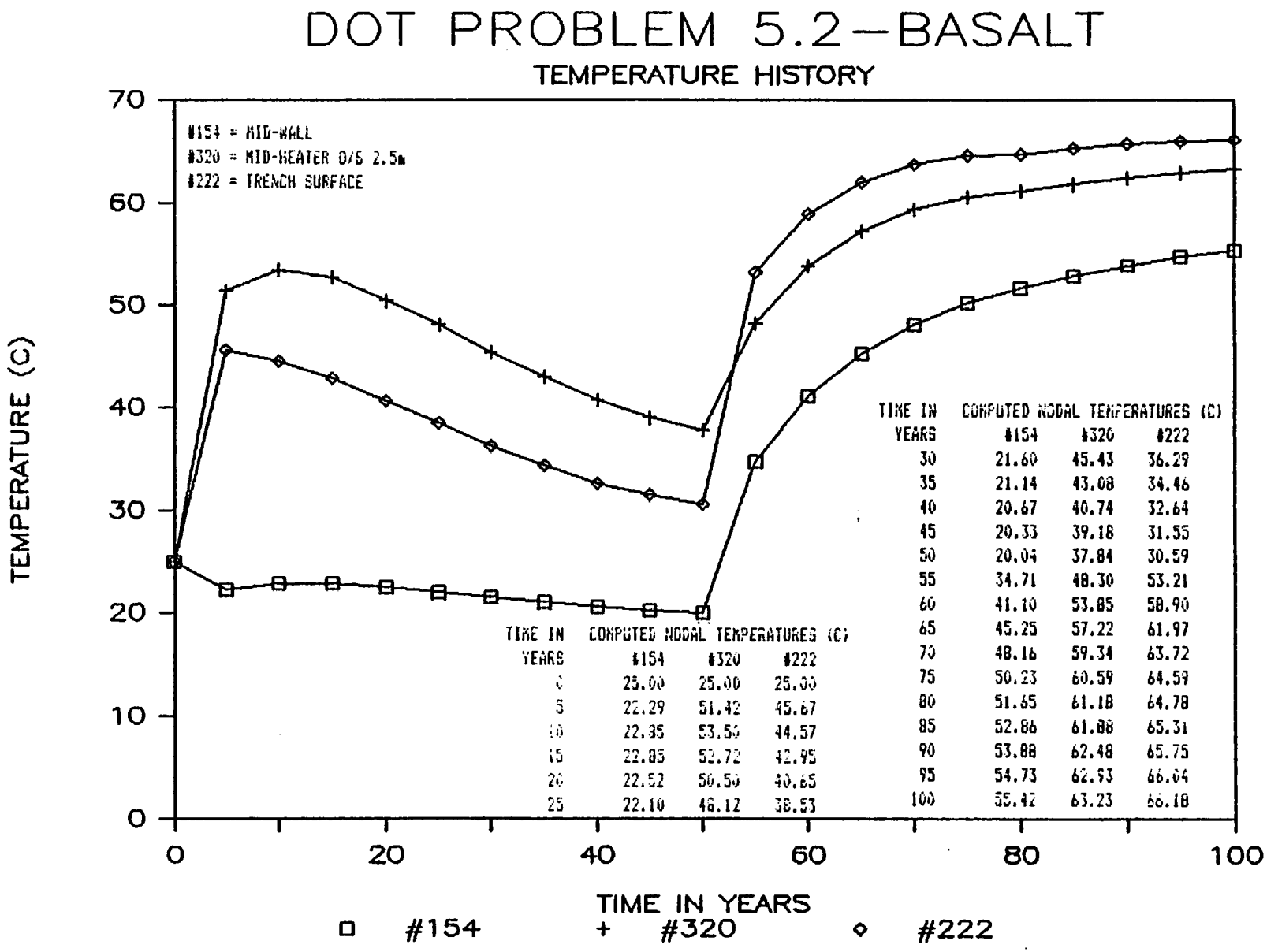


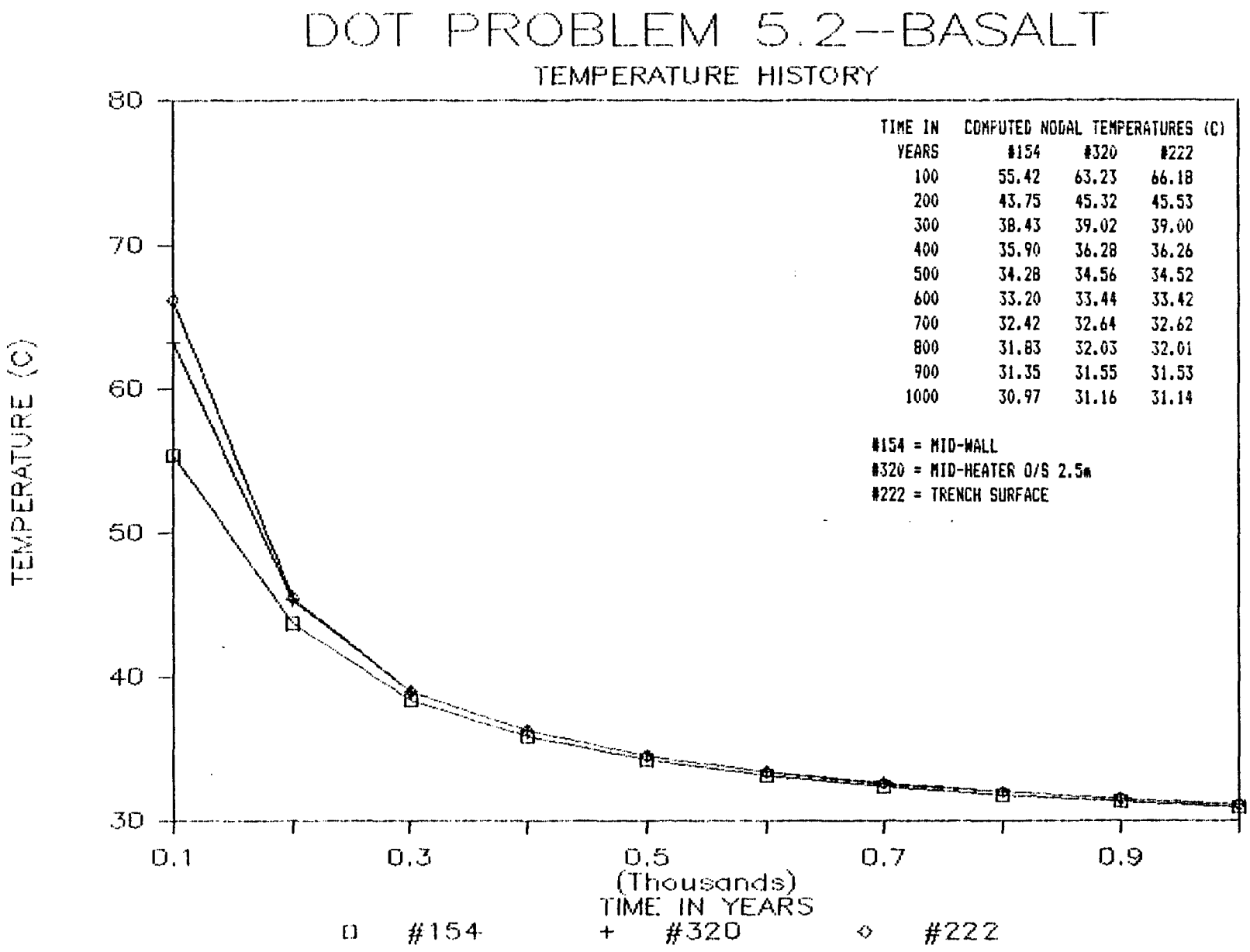
Figure 6.3-1 DOT Problem 5.2
Finite Element Mesh



TIME IN YEARS	COMPUTED NODAL TEMPERATURES (C) #154	#320	#222
0	25.00	25.00	25.00
5	22.29	51.42	45.67
10	22.35	53.59	44.57
15	22.05	52.72	42.95
20	22.52	50.50	40.65
25	22.10	46.12	38.53

TIME IN YEARS	COMPUTED NODAL TEMPERATURES (C) #154	#320	#222
30	21.60	45.43	36.29
35	21.14	43.08	34.46
40	20.67	40.74	32.64
45	20.33	39.18	31.55
50	20.04	37.84	30.59
55	34.71	48.30	53.21
60	41.10	53.85	58.90
65	45.25	57.22	61.97
70	48.16	59.34	63.72
75	50.23	60.59	64.59
80	51.65	61.18	64.78
85	52.86	61.88	65.31
90	53.88	62.48	65.75
95	54.73	62.93	66.04
100	55.42	63.23	66.18

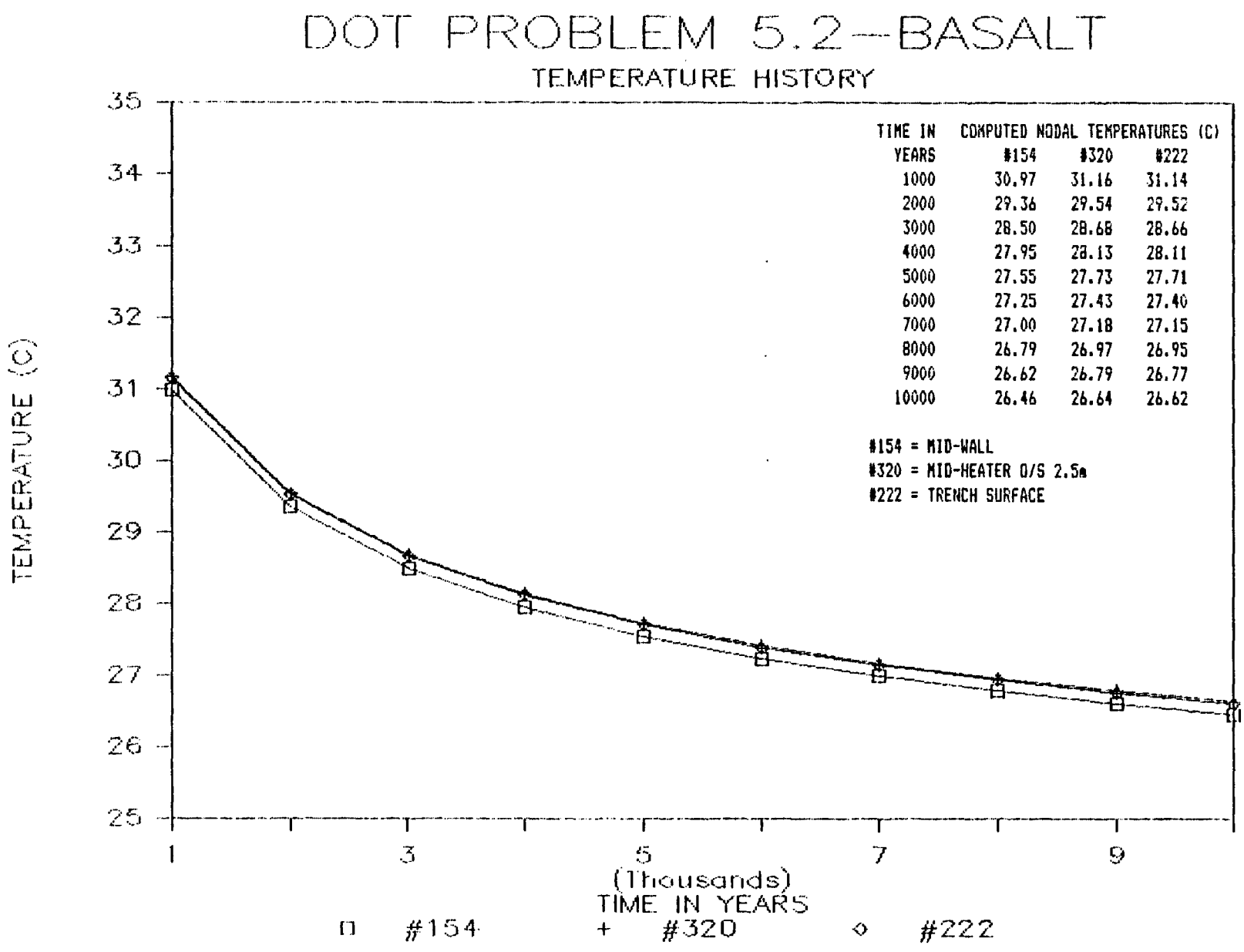
Figure 6.3-2 DOT Problem 5.2 - Basalt Temperature History 0-100 Years



TIME IN YEARS	COMPUTED NODAL TEMPERATURES (C) #154	#320	#222
100	55.42	63.23	66.18
200	43.75	45.32	45.53
300	38.43	39.02	39.00
400	35.90	36.28	36.26
500	34.28	34.56	34.52
600	33.20	33.44	33.42
700	32.42	32.64	32.62
800	31.83	32.03	32.01
900	31.35	31.55	31.53
1000	30.97	31.16	31.14

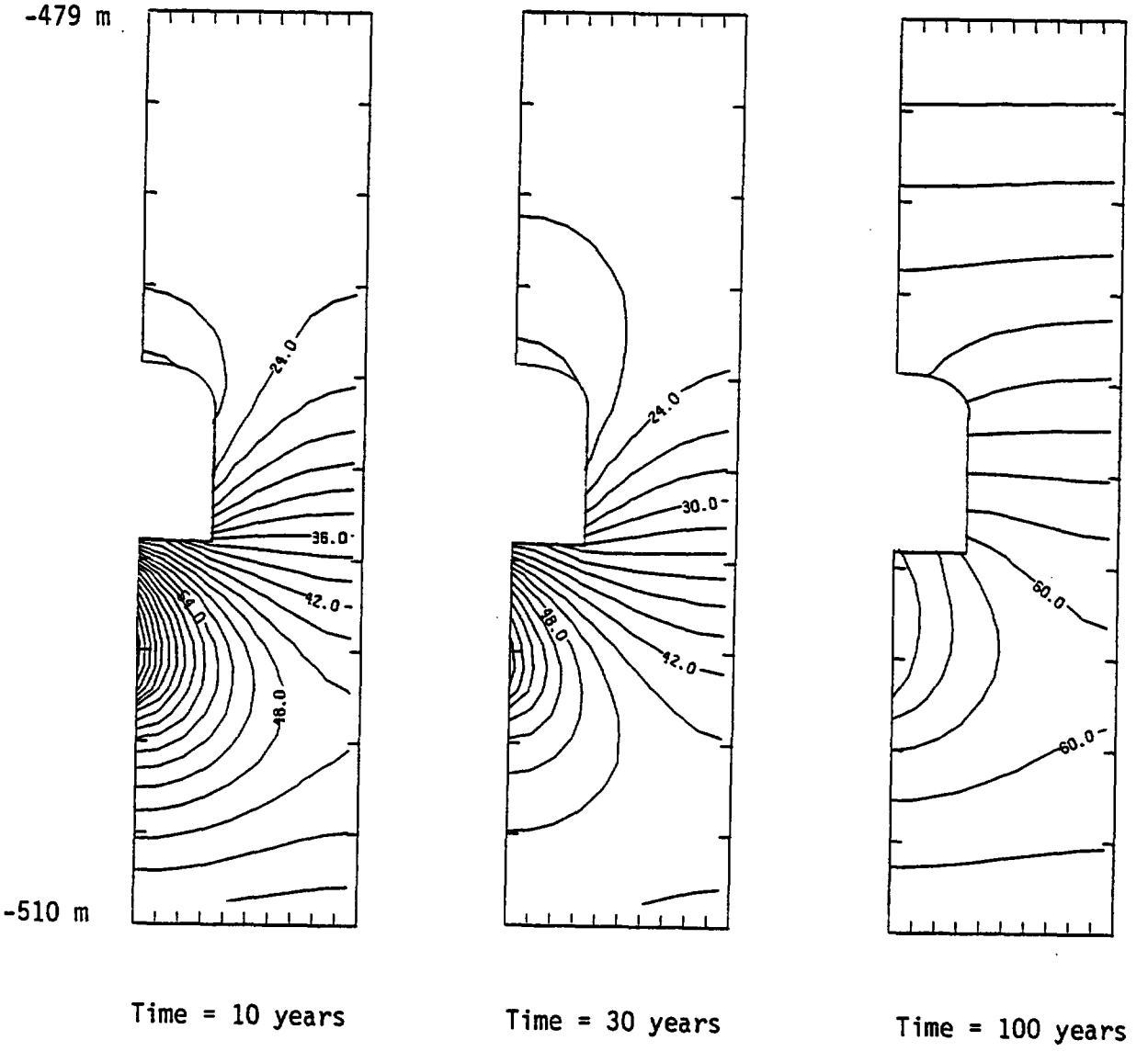
#154 = MID-WALL
#320 = MID-HEATER O/S 2.5m
#222 = TRENCH SURFACE

Figure 6.3-3 DOT Problem 5.2-Basalt
Temperature History 100-1,000 years



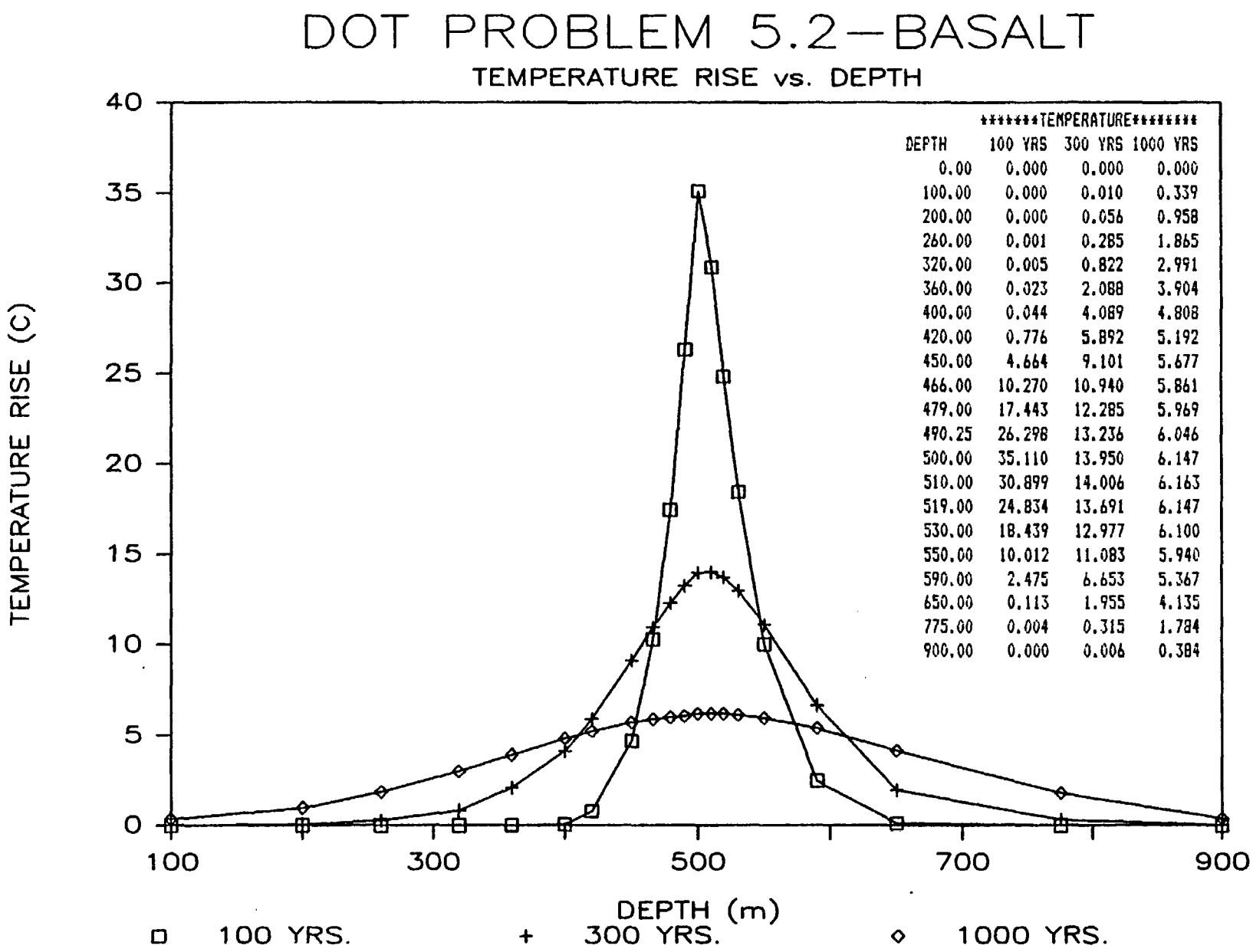
TIME IN YEARS	COMPUTED NODAL TEMPERATURES (C) #154	#320	#222
1000	30.97	31.16	31.14
2000	29.36	29.54	29.52
3000	28.50	28.68	28.66
4000	27.95	28.13	28.11
5000	27.55	27.73	27.71
6000	27.25	27.43	27.40
7000	27.00	27.18	27.15
8000	26.79	26.97	26.95
9000	26.62	26.79	26.77
10000	26.46	26.64	26.62

Figure 6.3-4 DOT Problem 5.2-Basalt
Temperature History 1,000-10,000 years



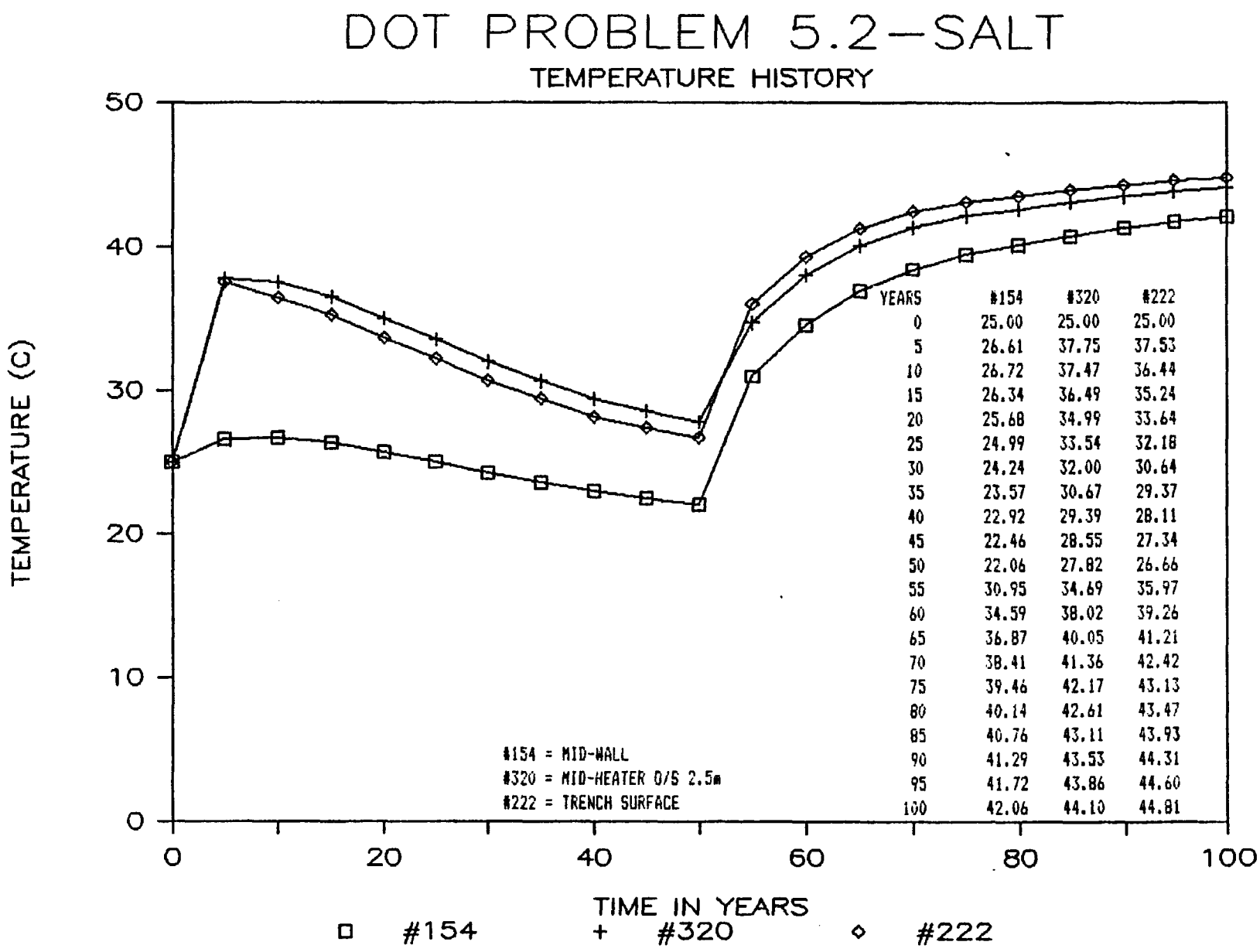
Temperature in °C
Contour Interval = 2°C
Initial Temperature = 25°C

Figure 6.3-5 DOT Problem 5.2-Basalt
Temperature Rises (0-100 years)



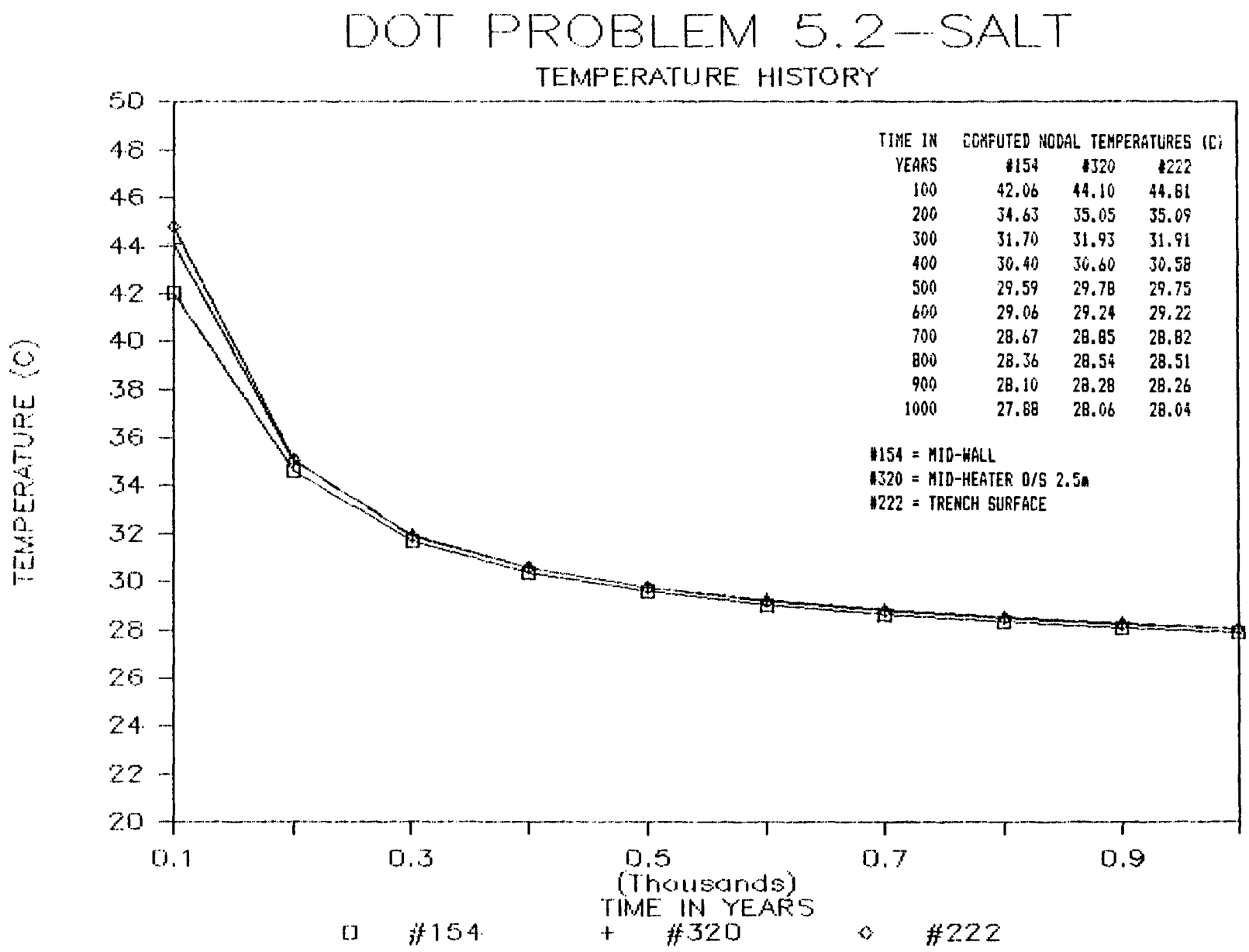
DEPTH	*******TEMPERATURE******** 100 YRS	300 YRS	1000 YRS
0.00	0.000	0.000	0.000
100.00	0.000	0.010	0.339
200.00	0.000	0.056	0.958
260.00	0.001	0.285	1.865
320.00	0.005	0.822	2.991
360.00	0.023	2.088	3.904
400.00	0.044	4.089	4.808
420.00	0.776	5.892	5.192
450.00	4.664	9.101	5.677
466.00	10.270	10.940	5.861
479.00	17.443	12.285	5.969
490.25	26.298	13.236	6.046
500.00	35.110	13.950	6.147
510.00	30.899	14.006	6.163
519.00	24.834	13.691	6.147
530.00	18.439	12.977	6.100
550.00	10.012	11.083	5.940
590.00	2.475	6.653	5.367
650.00	0.113	1.955	4.135
775.00	0.004	0.315	1.784
900.00	0.000	0.006	0.384

Figure 6.3-6 DOT Problem 5.2-Basalt
Temperature Rise (100-1,000 years)



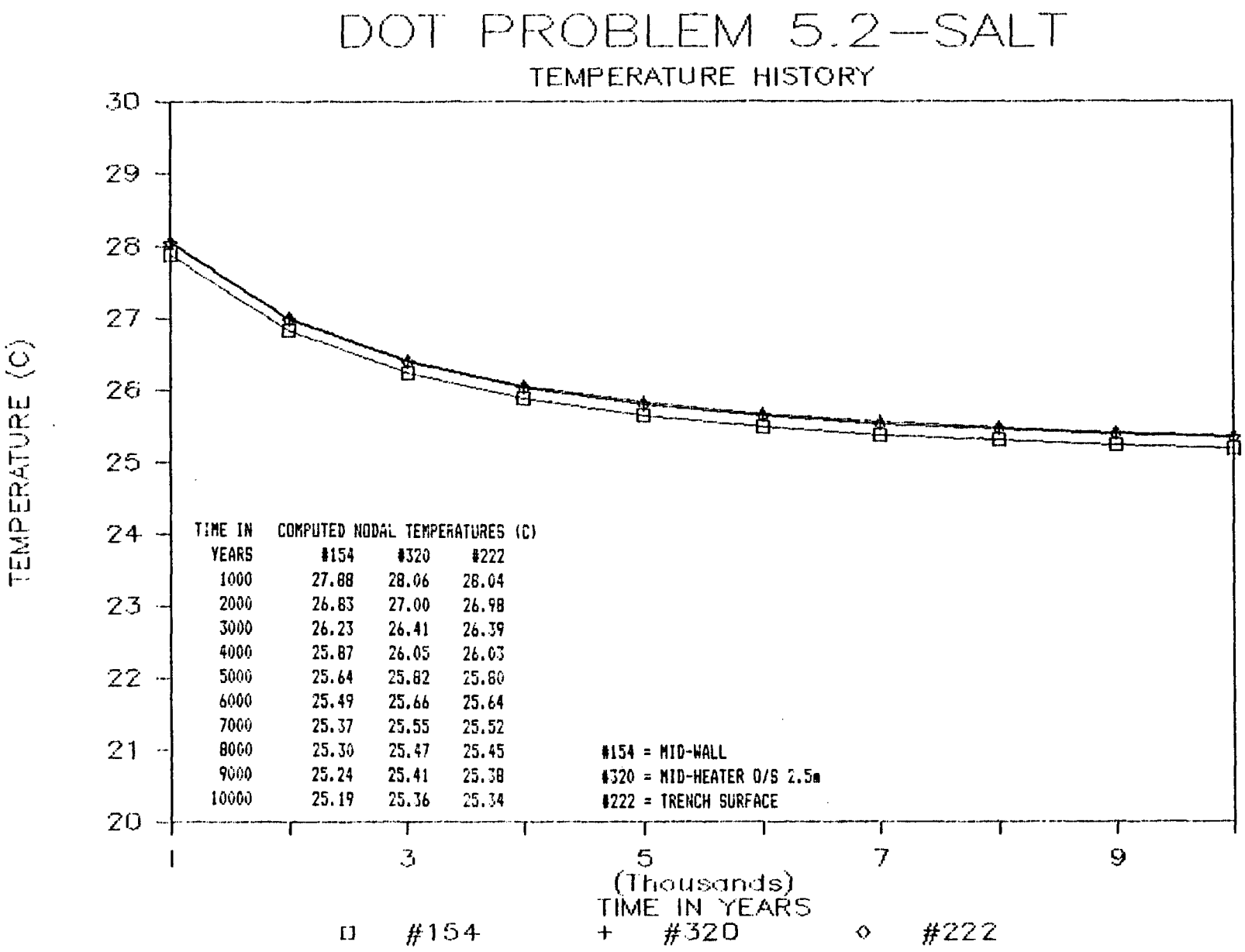
YEARS	#154	#320	#222
0	25.00	25.00	25.00
5	26.61	37.75	37.53
10	26.72	37.47	36.44
15	26.34	36.49	35.24
20	25.68	34.99	33.64
25	24.99	33.54	32.18
30	24.24	32.00	30.64
35	23.57	30.67	29.37
40	22.92	29.39	28.11
45	22.46	28.55	27.34
50	22.06	27.82	26.66
55	30.95	34.69	35.97
60	34.59	38.02	39.26
65	36.87	40.05	41.21
70	38.41	41.36	42.42
75	39.46	42.17	43.13
80	40.14	42.61	43.47
85	40.76	43.11	43.93
90	41.29	43.53	44.31
95	41.72	43.86	44.60
100	42.06	44.10	44.81

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



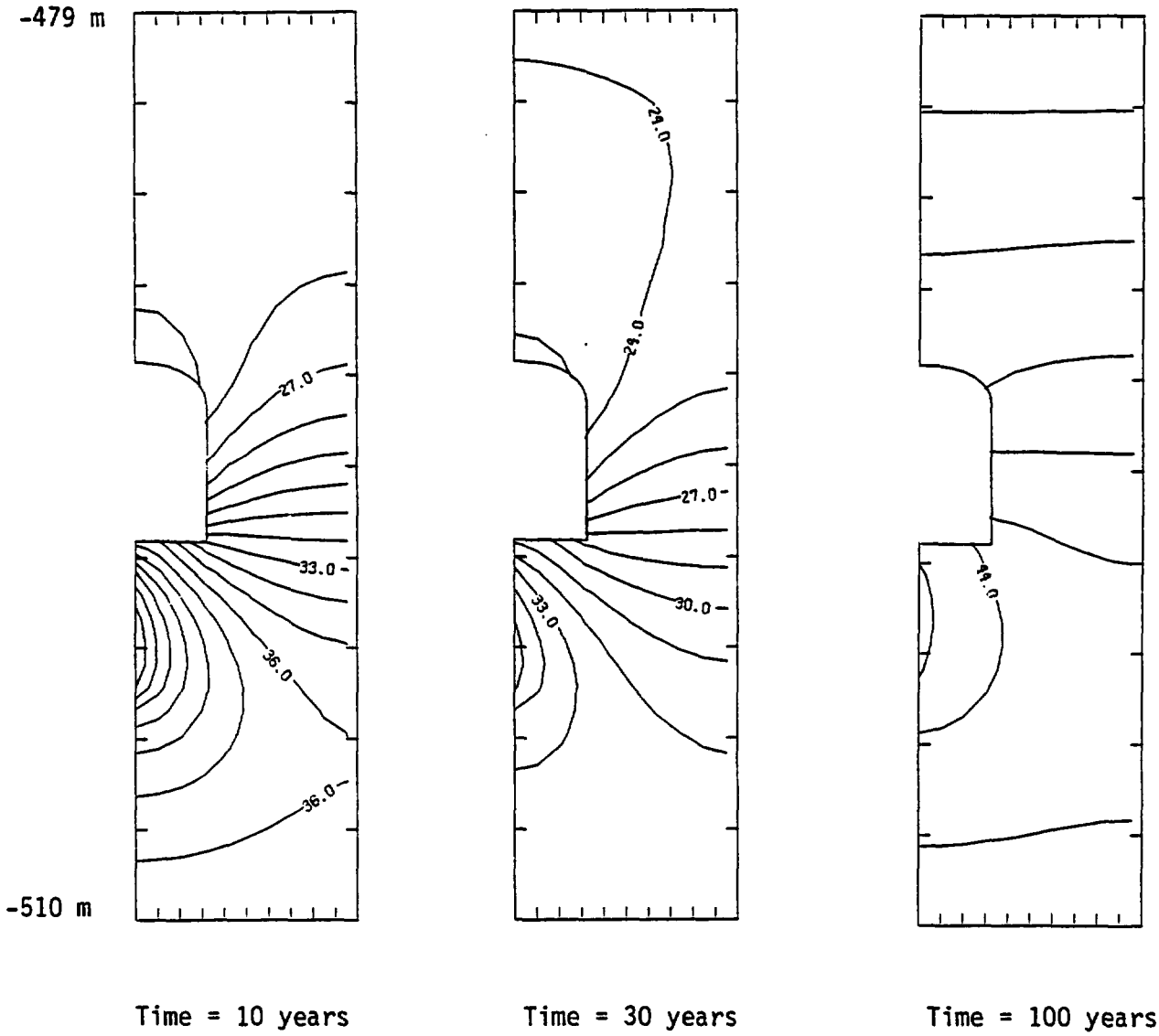
TIME IN YEARS	COMPUTED NODAL TEMPERATURES (C) #154	#320	#222
100	42.06	44.10	44.81
200	34.63	35.05	35.09
300	31.70	31.93	31.91
400	30.40	30.60	30.58
500	29.59	29.78	29.75
600	29.06	29.24	29.22
700	28.67	28.85	28.82
800	28.36	28.54	28.51
900	28.10	28.28	28.26
1000	27.88	28.06	28.04

Figure 6.4-2 DOT Problem 5.2-Salt
Temperature History 100-1,000 years



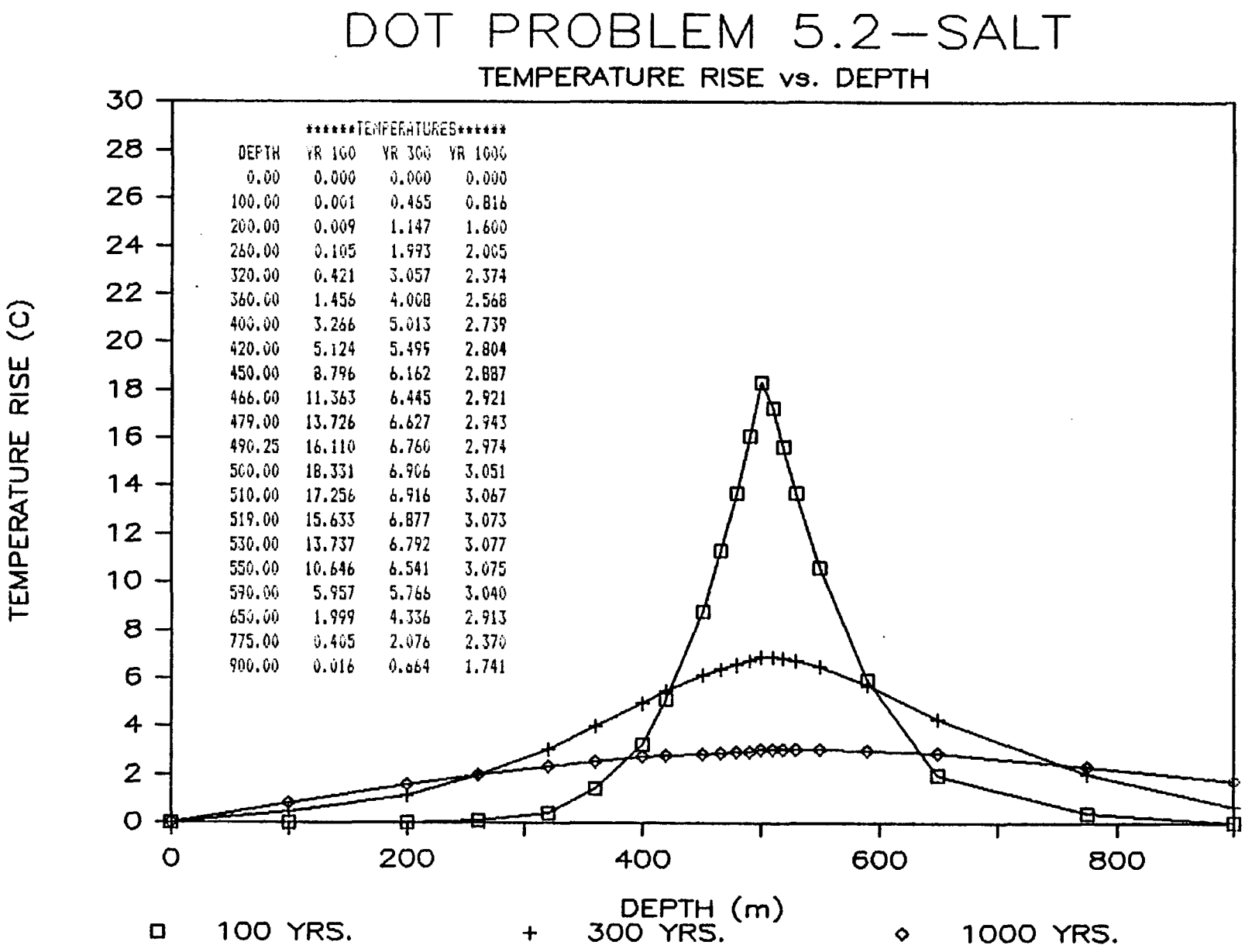
TIME IN YEARS	COMPUTED NODAL TEMPERATURES (C) #154	#320	#222
1000	27.88	28.06	28.04
2000	26.83	27.00	26.98
3000	26.23	26.41	26.39
4000	25.87	26.05	26.03
5000	25.64	25.82	25.80
6000	25.49	25.66	25.64
7000	25.37	25.55	25.52
8000	25.30	25.47	25.45
9000	25.24	25.41	25.38
10000	25.19	25.36	25.34

Figure 6.4-3 DOT Problem 5.2-Salt
Temperature History 1,000-10,000 years



Temperature in °C
Contour Interval = 1°C
Initial Temperature = 25°C

Figure 6.4-4 DOT Problem 5.2-Salt Temperature Contours



DEPTH	******TEMPERATURES****** YR 100	YR 300	YR 1000
0.00	0.000	0.000	0.000
100.00	0.001	0.465	0.816
200.00	0.009	1.147	1.600
260.00	0.105	1.993	2.005
320.00	0.421	3.057	2.374
360.00	1.456	4.008	2.568
400.00	3.266	5.013	2.739
420.00	5.124	5.499	2.804
450.00	8.796	6.162	2.887
466.00	11.363	6.445	2.921
479.00	13.726	6.627	2.943
490.25	16.110	6.760	2.974
500.00	18.331	6.906	3.051
510.00	17.256	6.916	3.067
519.00	15.633	6.877	3.073
530.00	13.737	6.792	3.077
550.00	10.646	6.541	3.075
590.00	5.957	5.766	3.040
650.00	1.999	4.336	2.913
775.00	0.405	2.076	2.370
900.00	0.016	0.664	1.741

Figure 6.4-5 DOT Problem 5.2 - SALT
Temperature Rise vs. Depth
100-1000 Years

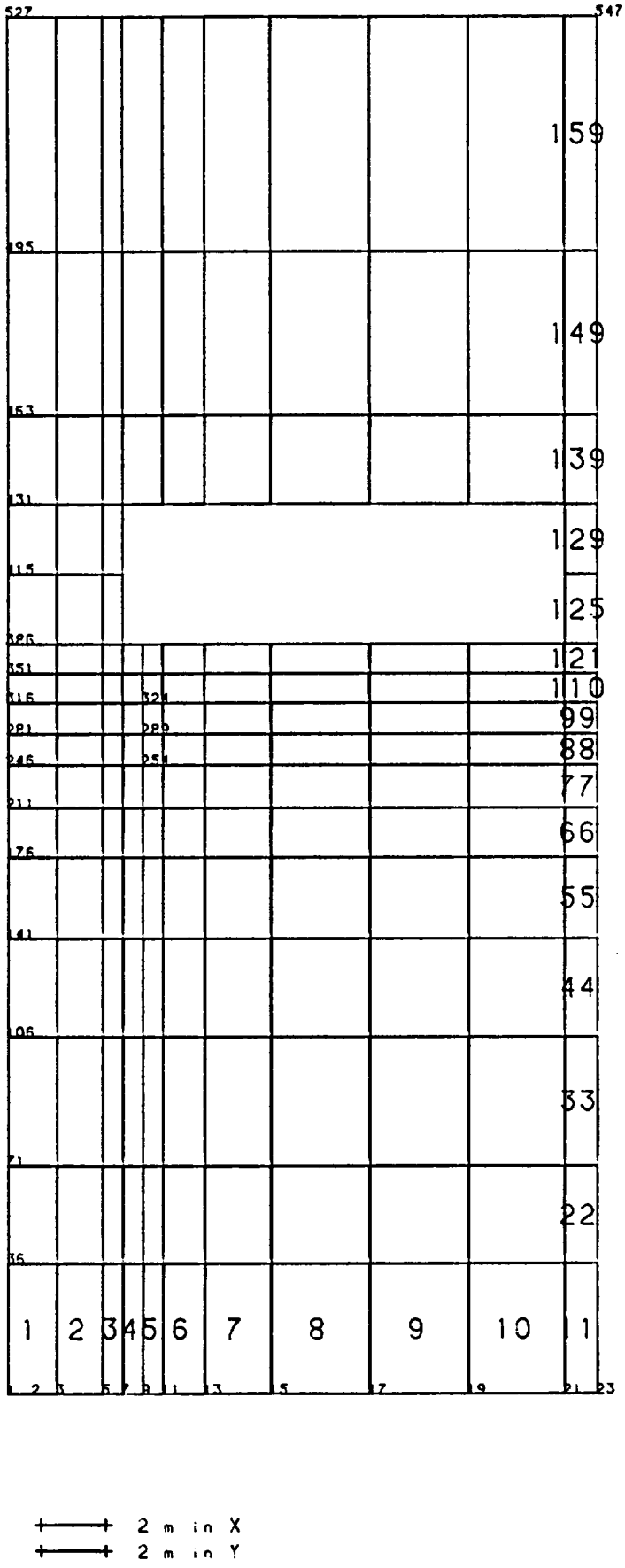


Figure 6.5-1 DOT Problem 6.1P - Room 3
Finite Element Mesh

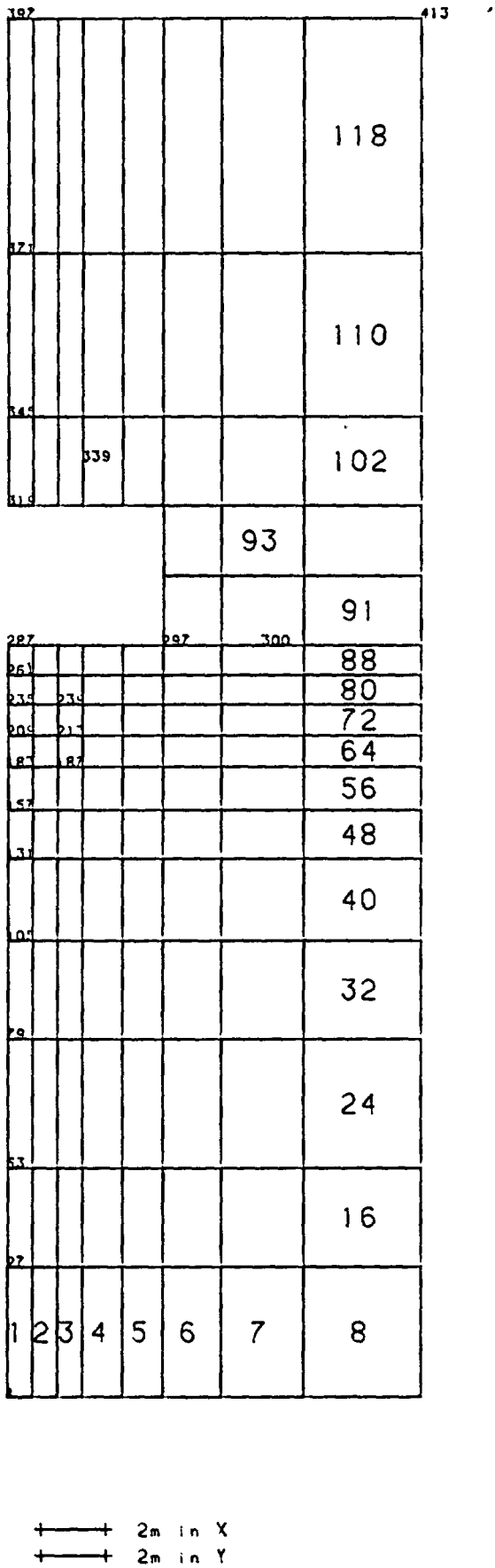


Figure 6.5-2 Problem 6.1A - Room 4
Finite Element Mesh

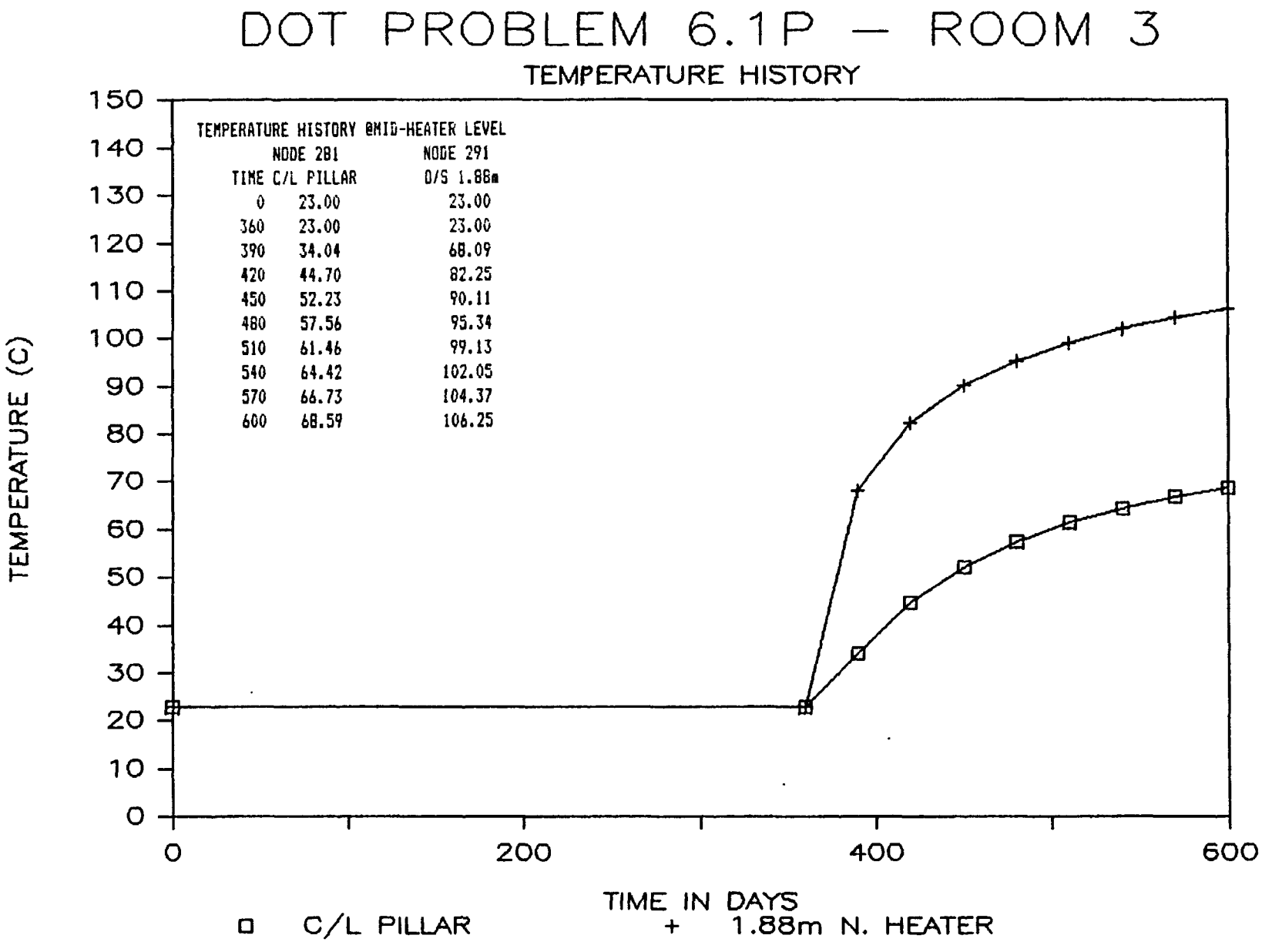


Figure 6.5-3 DOT Problem 6.1P - Room 3
Temperature History

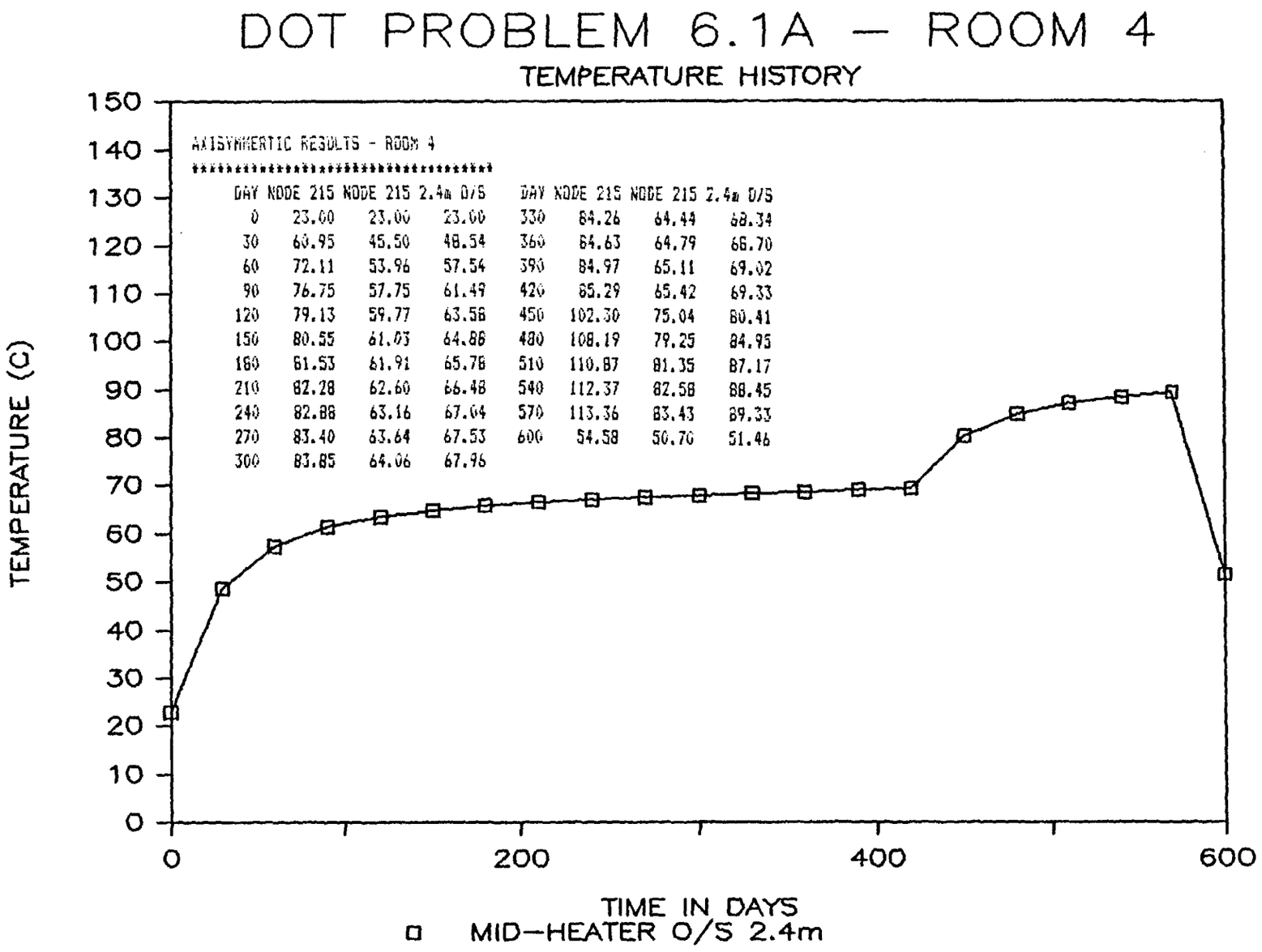


Figure 6.5-4 DOT Problem 6.1A - Room 4
Temperature History

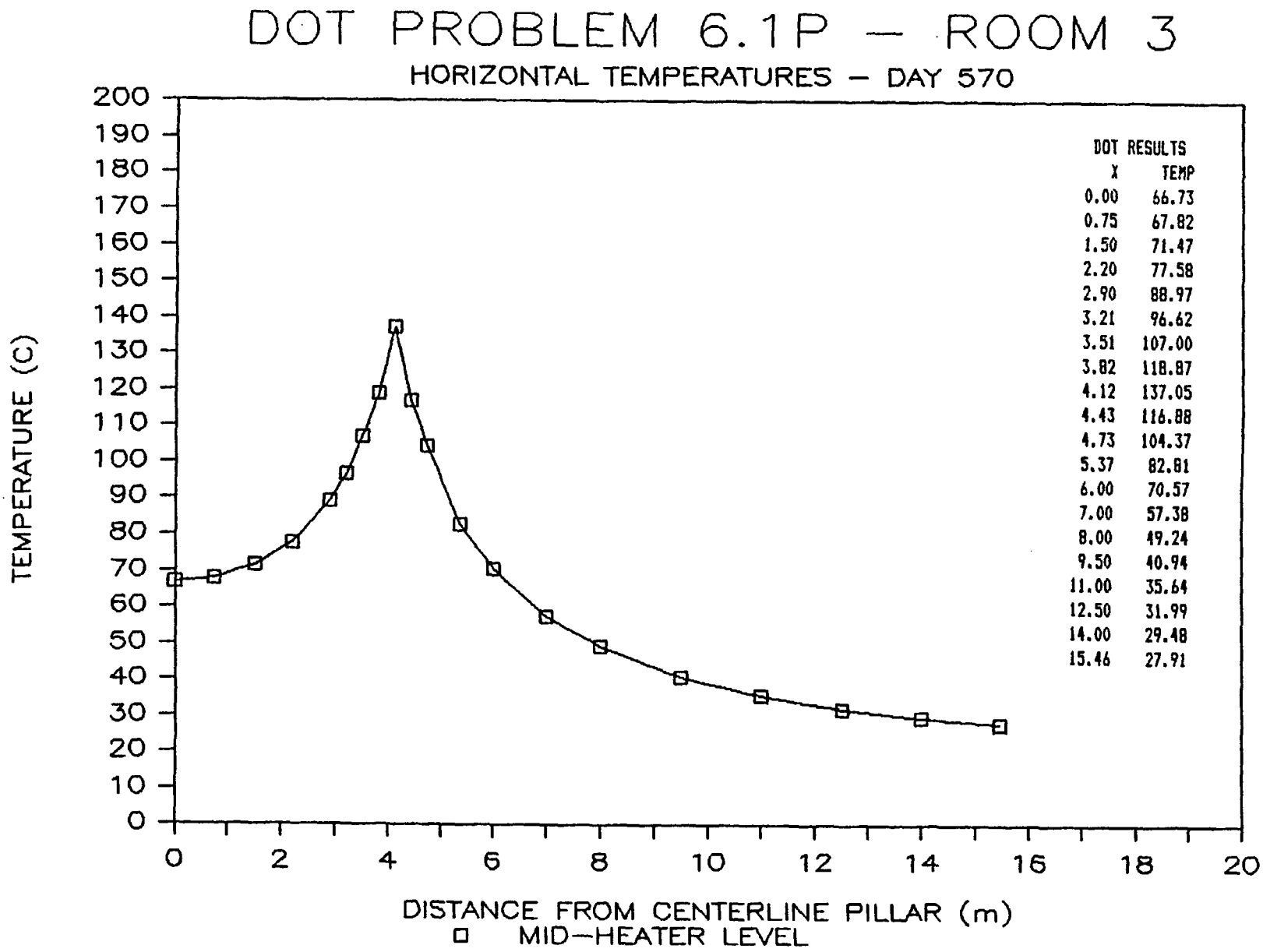


Figure 6.5-5 DOT Problem 6.1P
Horizontal Temperatures

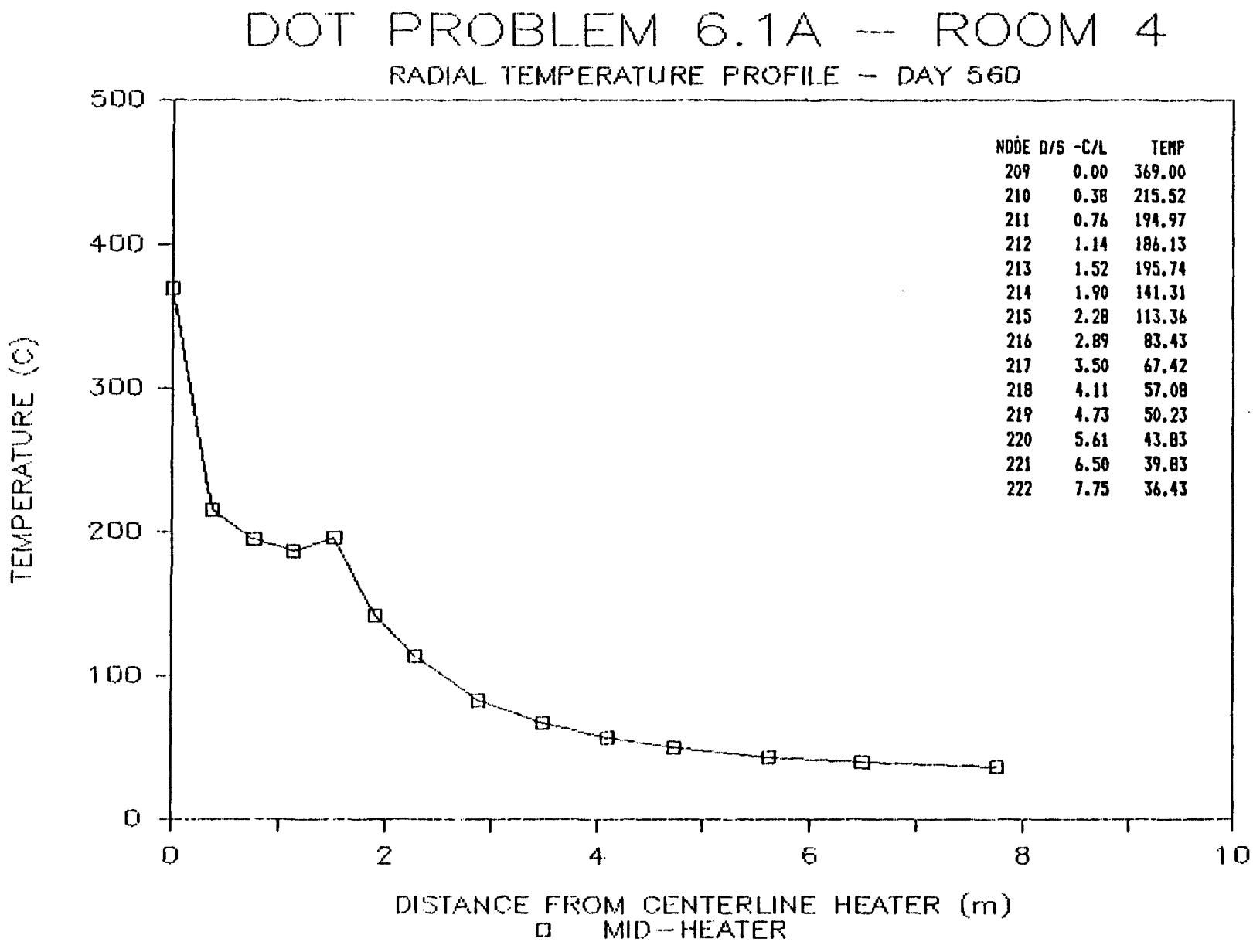
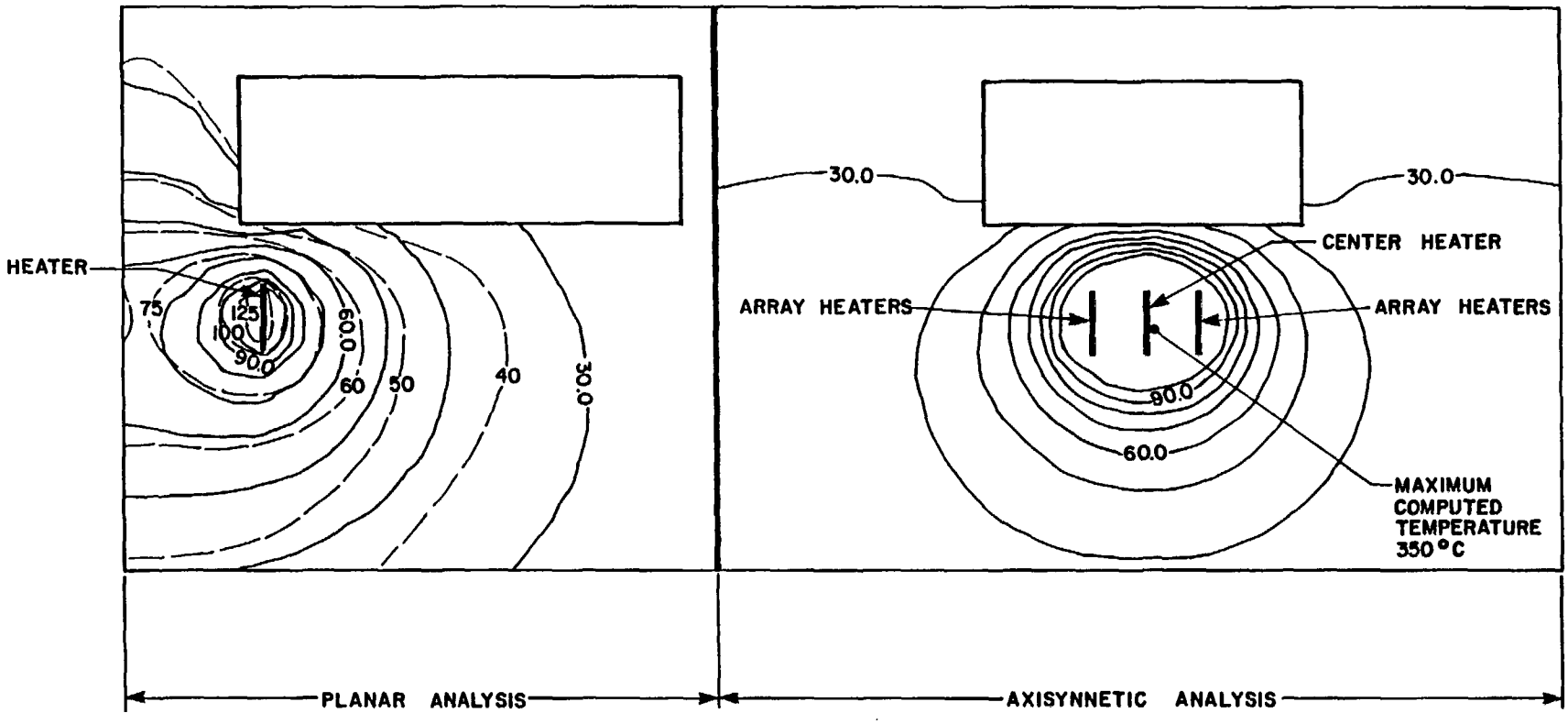


Figure 6.5-6 DOT Problem 6.1A Radial Temperature Profile



TEMPERATURE IN °C

——— DOT RESULTS CONTOUR INTERVAL = 10.0°

— — — MEASURED RESULTS (Bradshaw & Mc Clain, 1971)

Figure 6.5-7 DOT Problem 6.1
Temperature Contours at Day 570

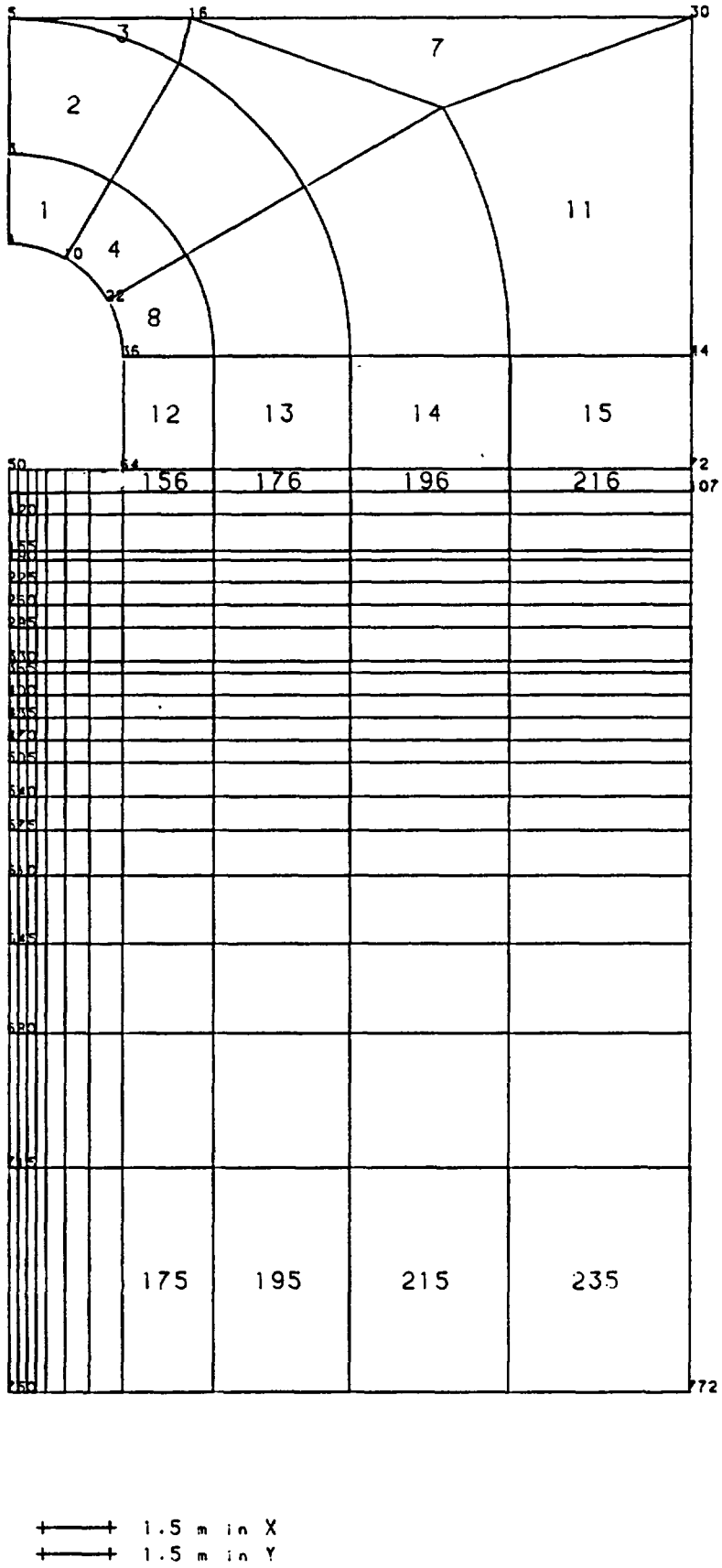


Figure 6.6-1 Problem 6.3
Finite Element Mesh

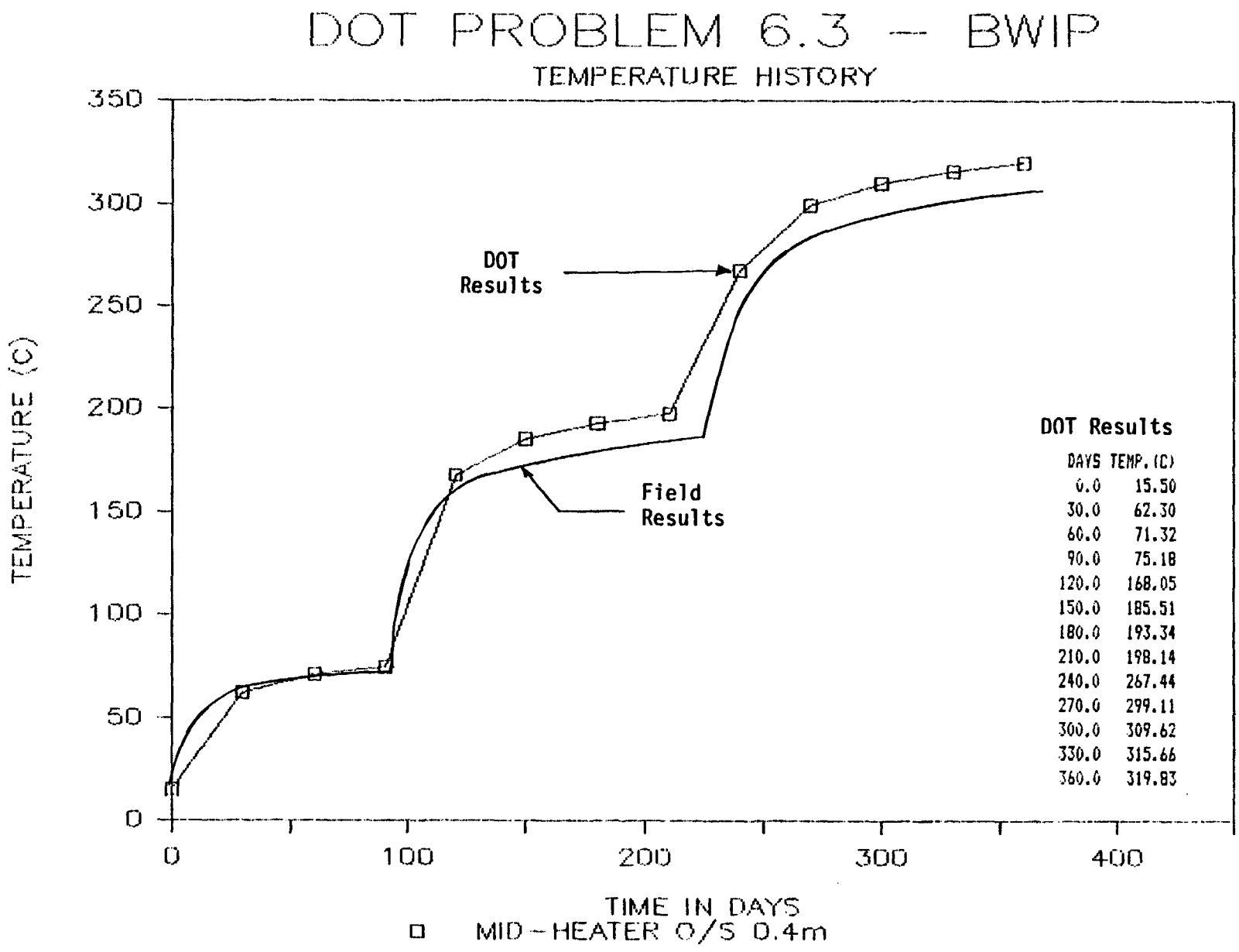
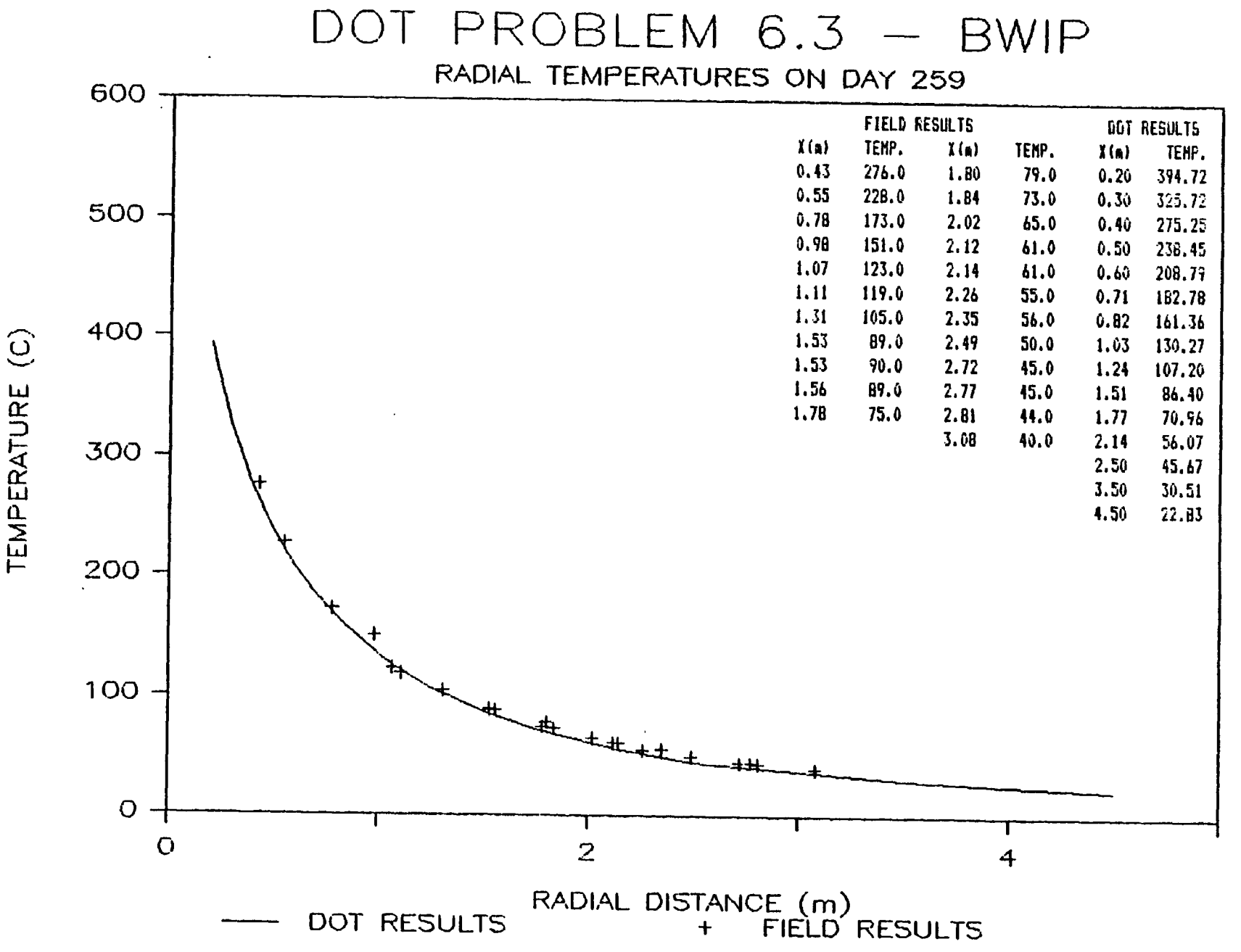
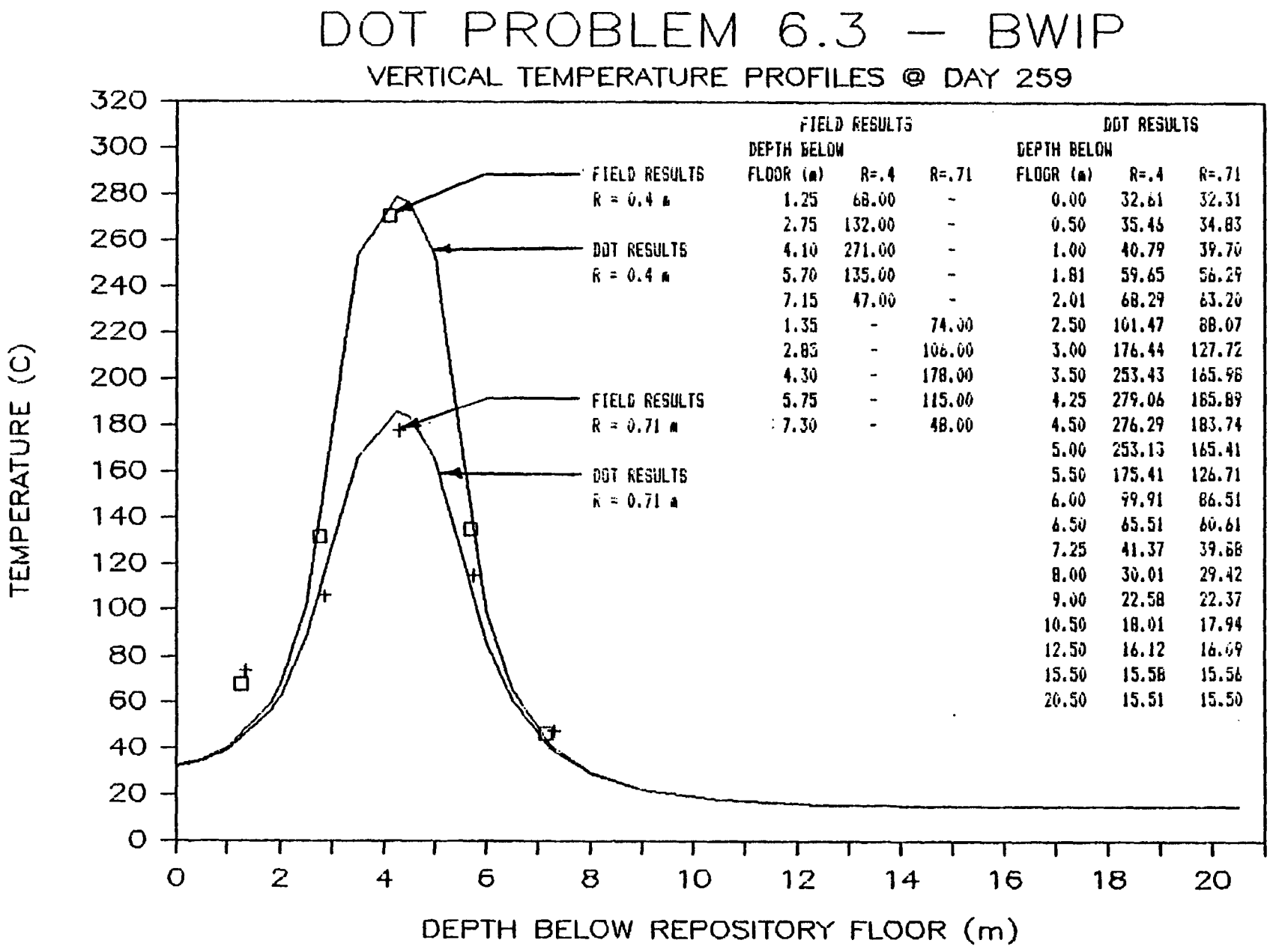


Figure 6.6-2 DOT Problem 6.3
Temperature History



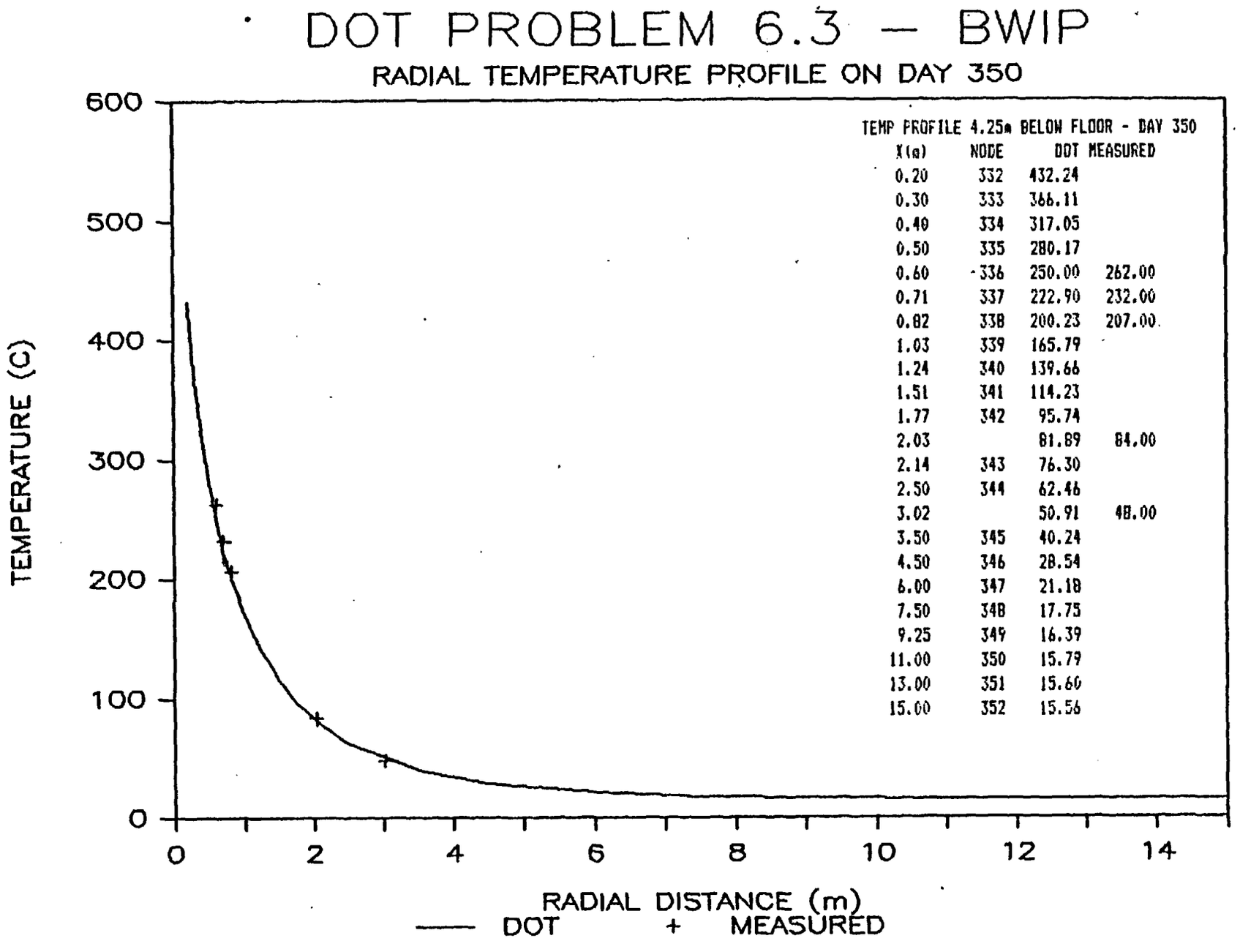
FIELD RESULTS				DOT RESULTS	
X(m)	TEMP.	X(m)	TEMP.	X(m)	TEMP.
0.43	276.0	1.80	79.0	0.20	394.72
0.55	228.0	1.84	73.0	0.30	325.72
0.78	173.0	2.02	65.0	0.40	275.25
0.98	151.0	2.12	61.0	0.50	238.45
1.07	123.0	2.14	61.0	0.60	208.79
1.11	119.0	2.26	55.0	0.71	182.78
1.31	105.0	2.35	56.0	0.82	161.36
1.53	89.0	2.49	50.0	1.03	130.27
1.53	90.0	2.72	45.0	1.24	107.20
1.56	89.0	2.77	45.0	1.51	86.40
1.78	75.0	2.81	44.0	1.77	70.96
		3.08	40.0	2.14	56.07
				2.50	45.67
				3.50	30.51
				4.50	22.83

Figure 6.6-3 DOT Problem 6.3
Radial Temperature Distribution
Day 259



FIELD RESULTS			DOT RESULTS		
DEPTH BELOW FLOOR (m)	R=.4	R=.71	DEPTH BELOW FLOOR (m)	R=.4	R=.71
1.25	68.00	-	0.00	32.61	32.31
2.75	132.00	-	0.50	35.46	34.83
4.10	271.00	-	1.00	40.79	39.70
5.70	135.00	-	1.81	59.65	56.29
7.15	47.00	-	2.01	68.29	63.20
1.35	-	74.00	2.50	101.47	88.07
2.83	-	106.00	3.00	176.44	127.72
4.30	-	178.00	3.50	253.43	165.96
5.75	-	115.00	4.25	279.06	165.89
7.30	-	48.00	4.50	276.29	183.74
			5.00	253.13	165.41
			5.50	175.41	126.71
			6.00	99.91	86.51
			6.50	65.51	60.61
			7.25	41.37	39.68
			8.00	30.01	29.42
			9.00	22.58	22.37
			10.50	18.01	17.94
			12.50	16.12	16.09
			15.50	15.58	15.56
			20.50	15.51	15.50

Figure 6.6-4 DOT Problem 6.3
Vertical Temperature Profiles
Day 259



TEMP PROFILE 4.25m BELOW FLOOR - DAY 350

X(m)	NODE	DOT	MEASURED
0.20	332	432.24	
0.30	333	366.11	
0.40	334	317.05	
0.50	335	280.17	
0.60	336	250.00	262.00
0.71	337	222.90	232.00
0.82	338	200.23	207.00
1.03	339	165.79	
1.24	340	139.66	
1.51	341	114.23	
1.77	342	95.74	
2.03		81.89	84.00
2.14	343	76.30	
2.50	344	62.46	
3.02		50.91	48.00
3.50	345	40.24	
4.50	346	28.54	
6.00	347	21.18	
7.50	348	17.75	
9.25	349	16.39	
11.00	350	15.79	
13.00	351	15.60	
15.00	352	15.56	

Figure 6.6-5 DOT Problem 6.3 Radial Temperature Distribution on Day 350