CorSTAR
A TEKNEKRON INDUSTRIES AFFILIATE

WM DOCKET CENTER

'85 MAR 22 P3:26

March 21, 1985

NRC FIN B6985

WM-RES
WM Record File
B6985
Corstar

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

Distribution:
Brooks
Joan-ticket

(Return to WM, 623-SS)

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 February 1985

Dear Pauline:

This letter contains a management level summary of progress during the month of February. 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 - Benchmark Problem Report - Waste Package Codes

During February the draft Benchmark Problem Report for the Waste Package Codes was modified to incorporate preliminary comments received from the NRC and outside reviewers. Upon the formal receipt of all comments from the NRC, a final report will be prepared and submitted to the NRC for publication.

Tasks 4&5 - Siting Codes

There was no activity on this task during February.

Tasks 4&5 - Radiological Assessment Codes

During February, we attempted to rerun the ORIGEN problem runs and route all output to microfiche. As of the date of this progress report, we believe that we have determined the correct job control language to accomplish this.

Enclosed with the monthly letter progress report is a description of the method used to estimate the U-234 content of fresh uranium fuel. This methodology was used in order to allow a more accurate prediction of the U-234 content of spent fuel, the primary precursor to radium Ra-226, potentially significant radionuclide from a human health standpoint.

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

1942

Tasks 4&5 - Repository Design Codes

With the arrival of The ADINA and ADINAT codes from Adina Engineering, all applicable codes have been procured. No new codes were installed at Brookhaven this month. We are still awaiting installation of the ADINA and ADINAT codes on the Brookhaven system. This installation delay has caused us to fall behind schedule in meeting the proposed deadline date of March 15, 1985 for a draft report.

During the month, arrangements were made to run the code STEALTH at the INEL computer facility. The code HEATING6 will be run on the Oak Ridge National Laboratory computer. Both of these codes are available.

During the month, Problem 6.1-PSV was analyzed with SALT4. Selected temperature results from this run are summarized and included at the end of this report. A comparison of code predictions and field measured temperatures and displacements has not been made.

Problem 3.5 has been run with VISCOT. The preliminary results from this computer run indicate an error in the solution we presented in the Benchmark Problem Report. We are investigating this error and hope to have it resolved soon. Other problem and/or code difficulties that have been encountered are outlined in detail in the technical progress report. A brief summary of these difficulties are listed below:

- Problem 3.5 - Questions have arisen regarding the analytical solutions as given in the benchmark problems report (NUREG/CR-3636). We are currently investigating the source material for these solutions and will have this problem resolved soon.

- VISCOT Problem 5.2 (Salt) - The creep law and its parameters, which is stated for this problem in the benchmark problems report (NUREG/CR-3636), was derived from laboratory data and is not applicable for an extended length of time. Our use of this creep law for times up to 10,000 years, as called for in this problem, results in computer errors.

- VISCOT Problems 5.2 and 6.3 (BWIP) - Difficulties were encountered in setting up initial stress fields for these problems. The VISCOT code seems to contain a built-in lateral stress constraint which limits the horizontal stress to a fixed unspecified ratio of the vertical stress. This constraint results in unwanted stress redistributions which cause unlikely upward displacements on the model when there are no loads placed upon it.

- VISCOT Problem 6.1 (PSV) - The creep law given in the benchmark problems report (NUREG/CR-3636), which was developed specifically for use with this problem, is in a form that is not usable with VISCOT. We recommend trying the salt creep law used for VISCOT Problem 5.2 (Salt) which is of a usable form for VISCOT. It is not known at this time, however, if the same creep law difficulties will develop for this problem as they did for VISCOT Problem 5.2 (Salt) as stated above.

General

Our estimate of costs through the end of February (through March 2, 1985 for CorSTAR) is:

Actual costs this month:	35.5K
Actual costs this fiscal year:	229.3K
Actual costs to date:	3003.5K
Planned costs this month:	12K
Planned costs this fiscal year:	184K

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

TECHNICAL STATUS SUMMARY

Technical Status Summary -
Tasks 4&5 - Radiological Assessment Codes

ORIGEN results for benchmark problems 2.4 and 2.5 were in poor agreement with measured U-234 data. Since U-234 is a precursor of Ra-226, a potentially important radionuclide in estimating dose-to-man, better agreement was desired. In reviewing the benchmark problem inputs, the most likely source of error was the fuel initial U-234 content. To improve our estimate of U-234 content the following method was used.

Step 1: Estimate the number of enriching stages required to produce U-235 of the desired product enrichment. From Reference Benedict and Pigford (1957),

$$n_p = \frac{\mathrm{Ln}\left(\frac{x_p^{235}(1 - x_f^{235})}{(1-x_p^{235})\; x_f^{235}}\right)}{\mathrm{Ln}\;\beta^{235}} - 1$$

where:

n_p = number of stages in the enriching section of an ideal cascade

x_f^{235} = enrichment plant U-235 feed assay

x_p^{234} = enrichment plant U-235 product assay

$\beta^{235} = \sqrt{\alpha^{235}}$

α^{235} = separation factor for U-235

$= \sqrt{\frac{\text{mass of } U^{235}\ F6}{\text{mass of } U^{238}\ F6}}$

Knowing the number of product stages, the U-234 content can be estimated by:

$$x_p^{234} = \frac{1}{((1 + (\beta^{234})^{n_f}) - (1/(x_f^{234} - 1)}$$

where:

x_p^{234} = enrichment plant U-234 product

x_f^{234} = enrichment plant U-234 product assay

$\beta^{234} = \sqrt{\alpha^{234}}$

$\alpha^{234} = \sqrt{\frac{\text{mass of } U^{234} F6}{\text{mass of } U^{235} F6}}$

The U-234 product assay from a difusion enrichment plant for typical U-235 enrichments are given in the attached worksheet.

Reference

Benedict, M. and T.H. Pigford, Nuclear Chemical Engineering, McGraw Hill, New York, 1957, p. 388.

WORKSHEET FOR U-234 IN ENRICHED URANIUM

U-235 ENRICHMENT	NUMBER OF ENRICHING STAGES	U-234 ENRICHMENT
1.0	161	0.008670
1.1	206	0.009860
1.2	247	0.011089
1.3	285	0.012357
1.4	320	0.013660
1.5	353	0.014998
1.6	383	0.016370
1.7	412	0.017774
1.8	439	0.019210
1.9	465	0.020676
2.0	489	0.022171
2.1	513	0.023695
2.2	535	0.025248
2.3	556	0.026828
2.4	577	0.028435
2.5	596	0.030069
2.6	615	0.031728
2.7	633	0.033414
2.8	651	0.035124
2.9	667	0.036859
3.0	684	0.038618
3.1	700	0.040401
3.2	715	0.042208
3.3	730	0.044038
3.4	744	0.045892
3.5	758	0.047768
3.6	772	0.049667
3.7	785	0.051588
3.8	798	0.053531
3.9	811	0.055496
4.0	823	0.057483
4.1	835	0.059491
4.2	847	0.061521
4.3	858	0.063572
4.4	869	0.065644
4.5	880	0.067737
4.6	891	0.069850
4.7	902	0.071984
4.8	912	0.074139
4.9	922	0.076314
5.0	932	0.078509

ALPHA-235	1.0042887974
ALPHA-234	1.0057307059
XF-235	0.00711
XF-234	0.00005477

TECHNICAL STATUS REPORT ATTACHMENT
TO PROGRESS REPORT FOR FEBRUARY 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. We are awaiting notice of 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 behind schedule in meeting the proposed deadline date of March 15, 1985.

Run Benchmark Problems

Problem 6.1-PSV was run this month using SALT 4. Temperature results from this run are summarized and included later in this report. One graph shows the temperature history for Room 1 for points at various offsets from the center of the array heaters and located 9 ft below the repository floor. The other graph shows the temperature history for Room 4 for points at various depths below the repository floor and located at an 8 ft offset from the center of the array heaters. A comparison against field measured temperatures has not been finalized as yet. Also, reduction of field and SALT 4 displacement results has not been completed.

Problem 3.5 has been run with VISCOT. The preliminary results from this run indicate a solution error which is causing extraordinarily large displacements to be calculated. We are looking into this error and hope to have a solution soon.

In addition to the difficulty stated previously with VISCOT Problem 3.5, other problem and/or code difficulties have been encountered. These difficulties are explained in detail below:

(1) Problem 3.5 - Questions have arisen regarding the analytical solutions as given in the benchmark problems Report (pp.81-83, NUREG/CR-3636). We are currently investigating the source references for these solutions and will have this problem resolved soon.

(2) VISCOT Problem 5.2 (Salt) - A problem with the creep law was initially discussed in a letter, dated November 16, 1984, from Acres to CorSTAR. The creep strains predicted by the VISCOT model are very large due to the long time frame and the modeled geometry involved. The exponential-time creep law and its parameters, which is given in the benchmark problems Report (pg. 114, NUREG/CR-3636), was developed from laboratory data and is not applicable for an extended length of time. This is also stated in ONWI-295, Review of Constitutive Laws Used to Describe the Creep of Salt, pp. 34-35, June 1983:

"However, the long times of interest for a repository have not been studied in the laboratory. Almost no data are available for times greater than about one hundred days......Therefore, prediction of long-time deformation requires the creep law to be extrapolated well beyond the data base.....If the character of the deformation changes at long times, then creep laws based on only short-time data will not be able to predict long-time deformations."

The use of a 10,000 year time frame for our problem is not reasonable if the creep law parameters were developed from data for only 100 days. As a result, since the creep law parameters cannot be changed to effectively model creep, Problem 5.2S (long-term creep deformation) is not solvable without further long-term studies.

(3) VISCOT Problems 5.2 and 6.3 (BWIP) - The execution of these problems with VISCOT requires the use of two separate runs, a geostatic run and a thermal load run. The geostatic run is needed to set up initial stresses in the model prior to thermal loading. The initial stresses are developed by using the gravity loading option as recommended in the VISCOT user manual (ONWI-437). When doing this for these problems, however, two unfavorable developments result. First, the VISCOT code seems to have a built in constraint which limits the initial horizontal stress to a fixed ratio of the initial vertical stress. This ratio, Kx, is based on the material's poisson ratio, ν, and is defined as:

$$Kx = \frac{\nu}{1-\nu}$$

where

- Kx is the coefficient of lateral pressure
- ν is the poisson ratio of the material

This limitation allows for no variation of the lateral pressure coefficient which is a severe constraint. The second unfavorable development is that the lateral coefficient constraint results in stress redistributions that cause unlikely upward displacements within the model when there is no loading placed upon it. The presence of the unlikely upward displacements cause us to question the applicability of the VISCOT code without further code explanation for these problems.

(4) VISCOT Problem 6.1 (PSV) - The creep law given in the benchmark problems Report (pg. 147, NUREG/CR-3636), which was developed specifically for use with this problem, is in a format that is not usable with VISCOT. In order to continue to model creep behavior, however, we recommend trying the salt exponential-time creep law used for VISCOT Problem 5.2 (Salt) which is of a usable form for VISCOT. It is not known at this time, however, whether the same long-term creep law difficulties will develop for this problem as they did for VISCOT Problem 5.2 (Salt) as stated in (2). Results from this change will be discussed when this revised computer run is made.

Finally, some of the finite element meshes that had been missing from previous Progress Reports have been completed and are included later in this report.

JAB
3/6/85
P6678.250

PROJECT STATUS

TABLE 3

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

Legend:

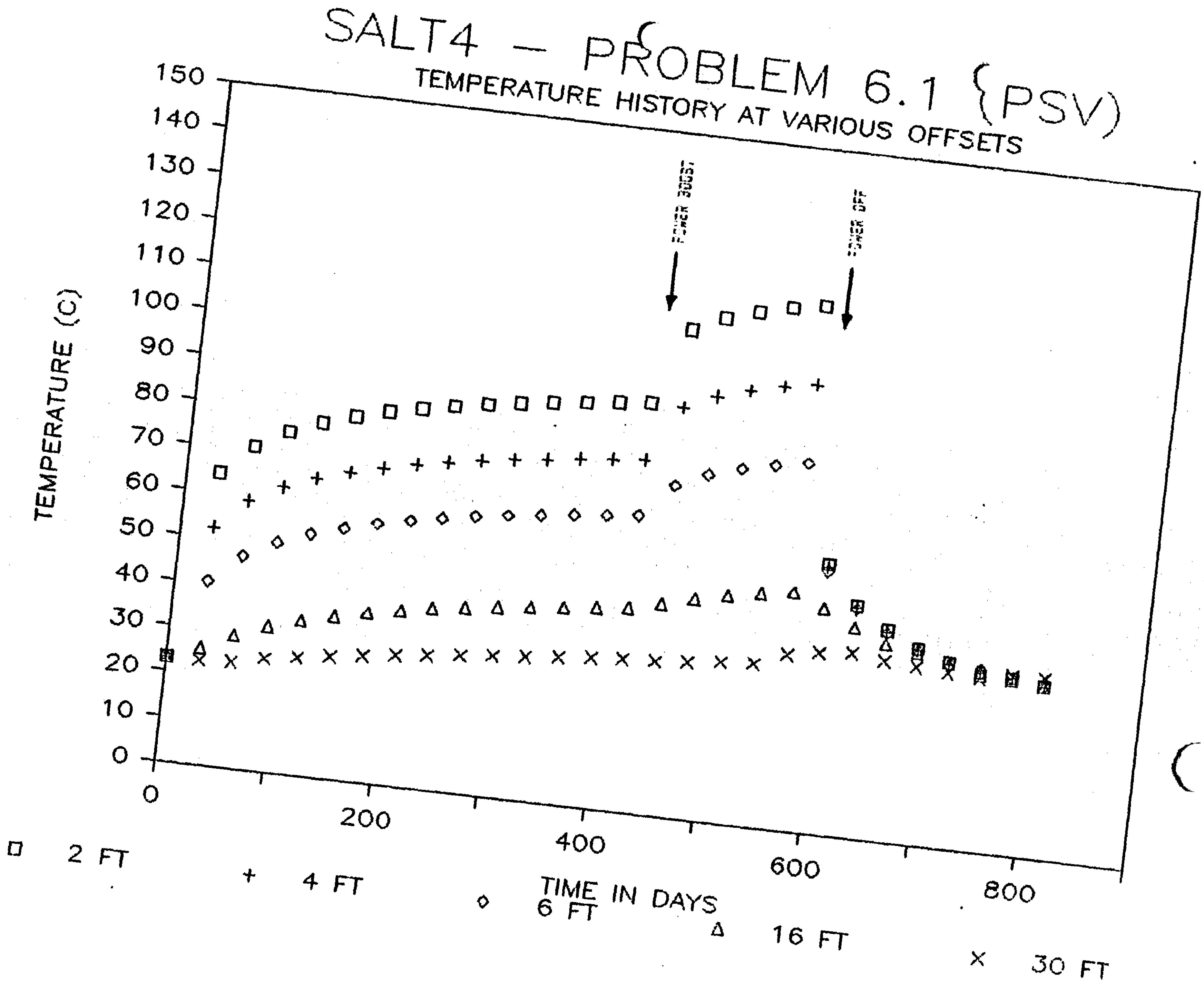
x Benchmark Problems by Acres.
0 Benchmark Problems by Teknekron.
(1) Requires 2 runs, one for MATLOC and one for VISCOT.
(2) Two-Dimensional Analysis.
(3) Requires 3 runs, one for MATLOC and two for VISCOT.
(4) Requires 2 runs, one for Salt and one for Basalt.
S - Problems run for Salt.
B - Problems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

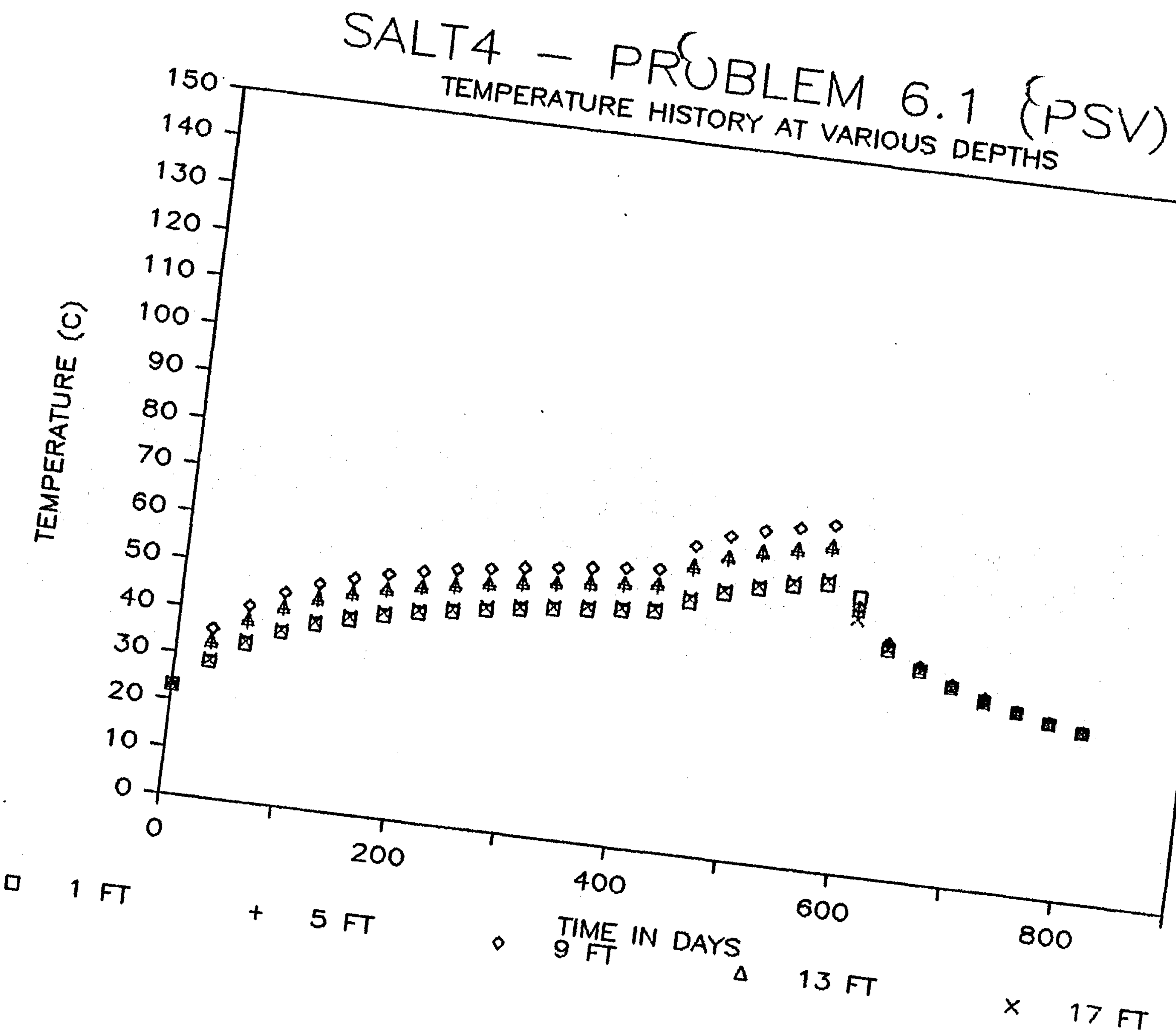
* From NUREG/CR-3636, Benchmark Problems for Repository Design Models, February 1984.

Problems Completed

Problems run, results not analyzed



SALT4 – PROBLEM 6.1 (PSV)
TEMPERATURE HISTORY AT VARIOUS OFFSETS
POWER BOOST
POWER OFF
TEMPERATURE (C)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
200
400
600
800
TIME IN DAYS
□ 2 FT
+ 4 FT
◇ 6 FT
Δ 16 FT
× 30 FT


SALT4 - PROBLEM 6.1 (PSV)
TEMPERATURE HISTORY AT VARIOUS DEPTHS
TEMPERATURE (C)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
0
200
400
600
800
TIME IN DAYS
□ 1 FT
+ 5 FT
◇ 9 FT
Δ 13 FT
× 17 FT

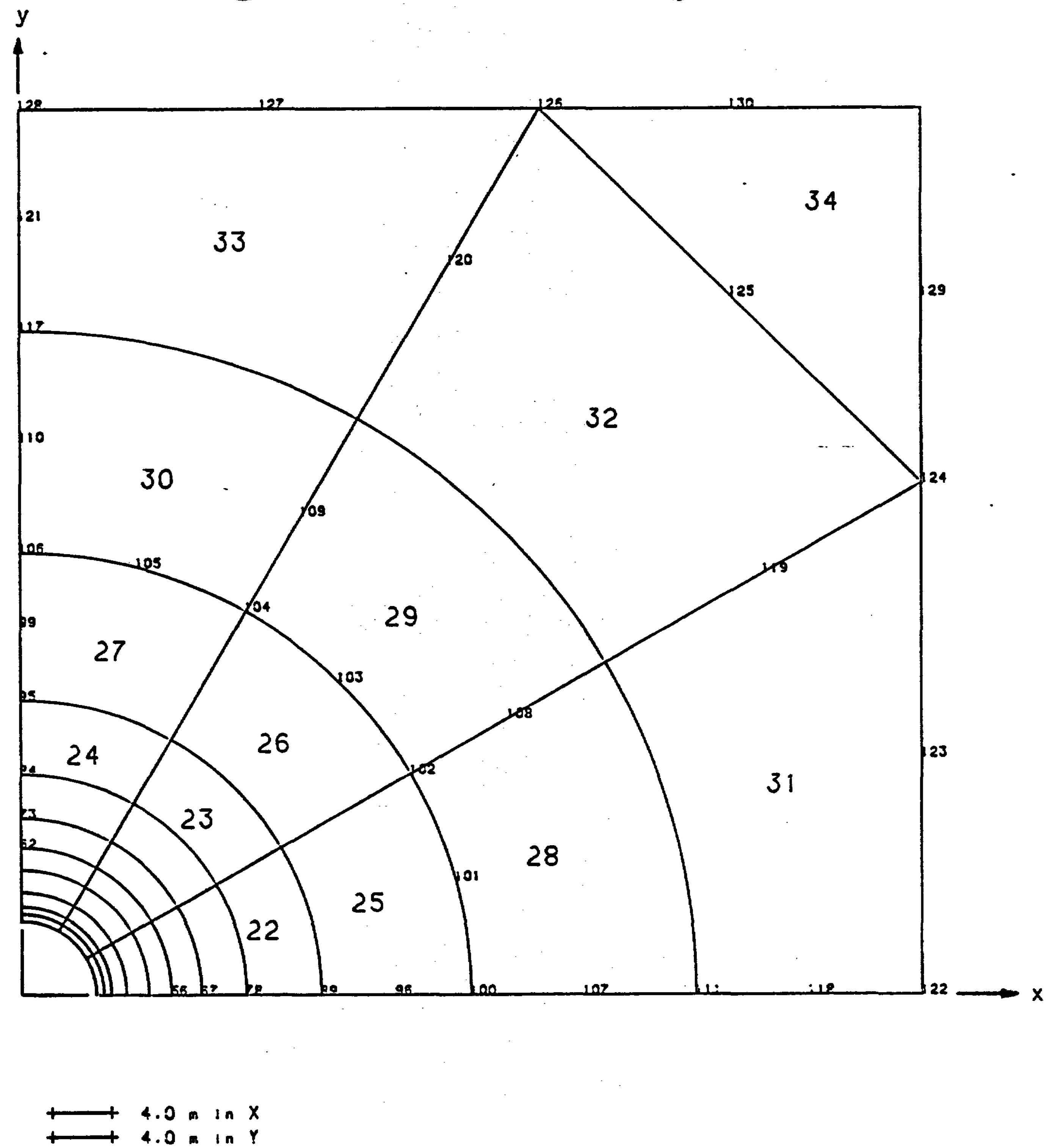


Figure 7.2-1 MATLOC Problem 3.2a
Finite Element Mesh

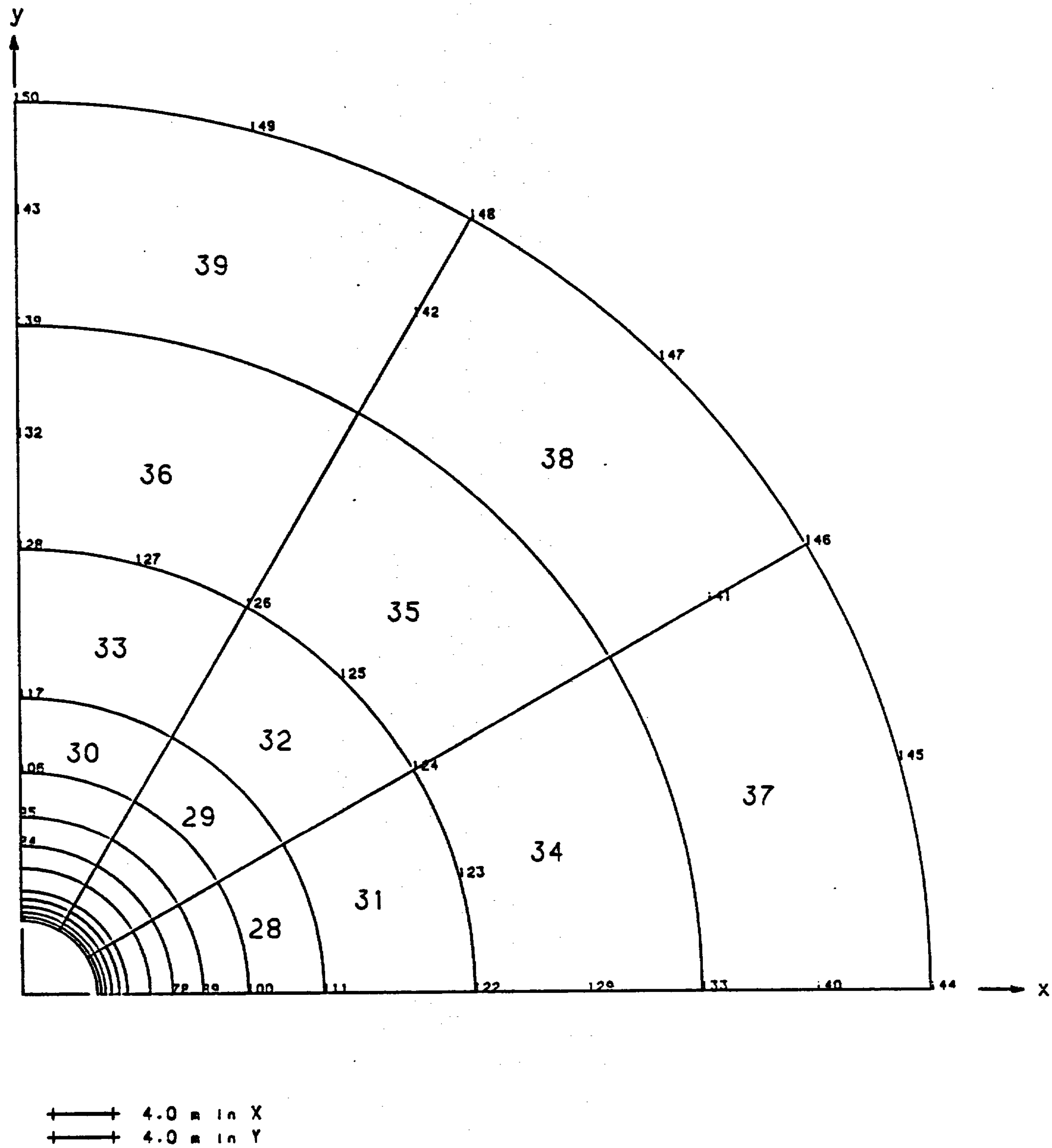


Figure 8.2-1 VISCOT Problem 3.2b
Finite Element Mesh

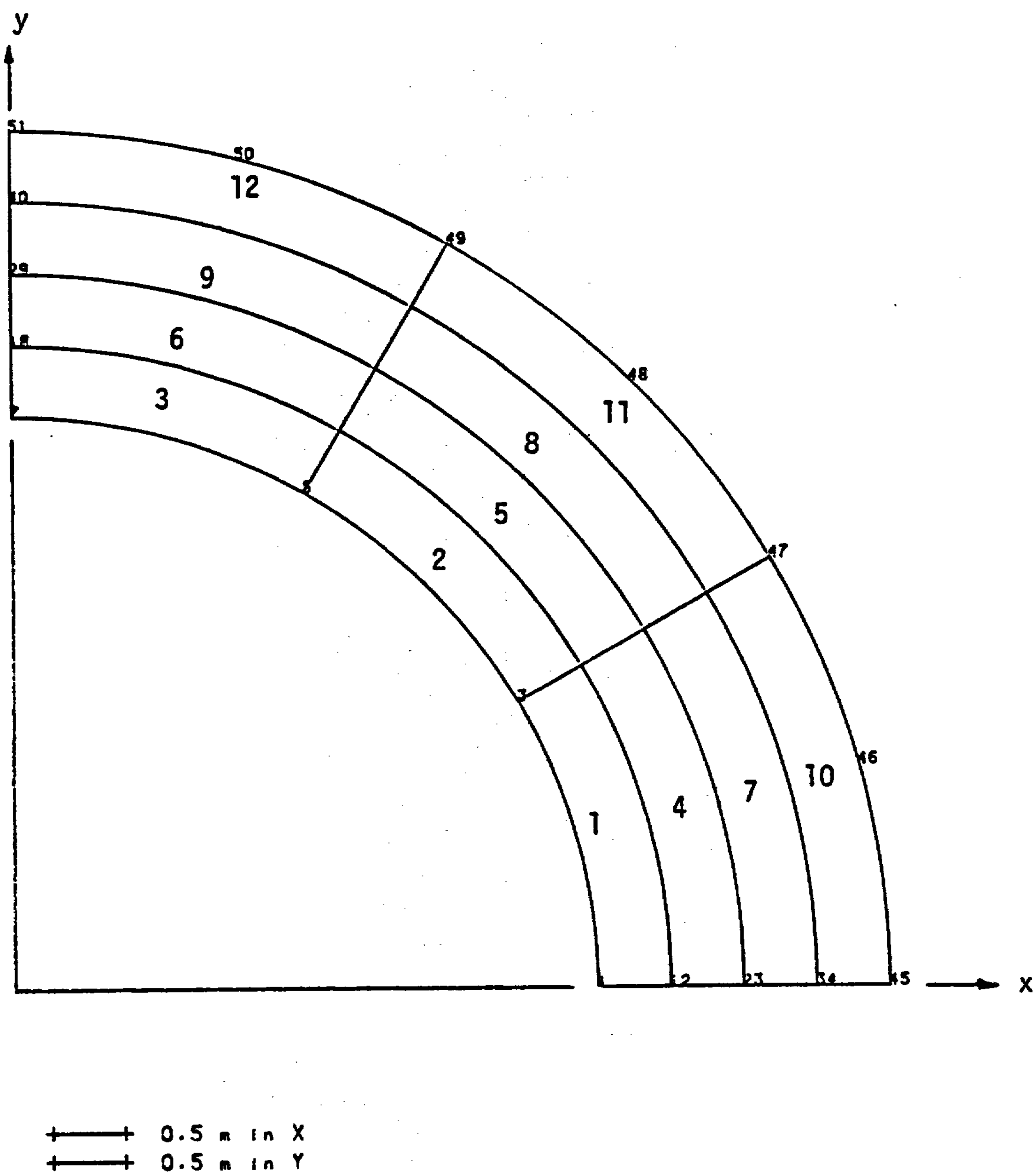


Figure 8.3-1 VISCOT Problem 3.3c
Finite Element Mesh

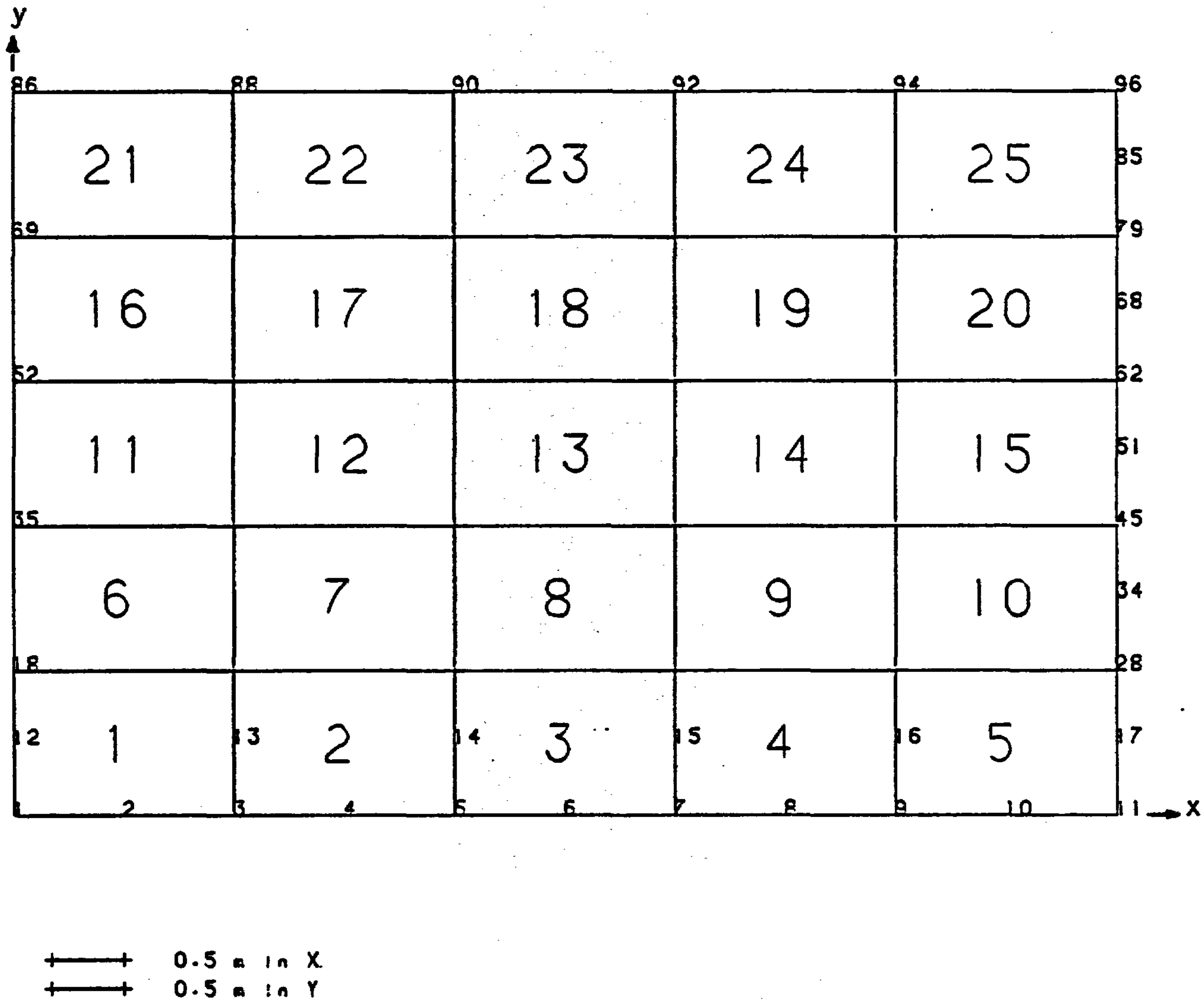


Figure 8.4-1 VISCOT Problem 3.5
Finite Element Mesh

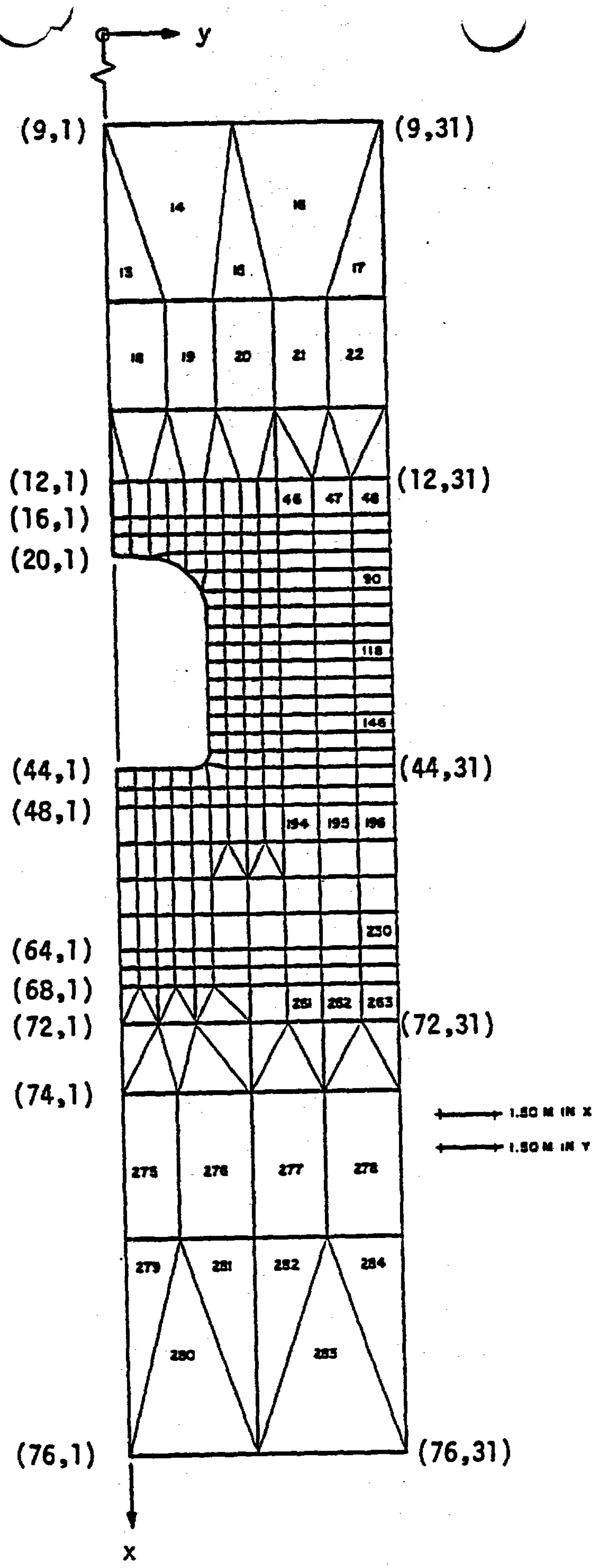


Figure 10.5-1 COYOTE Problem 5.2S
Finite Element Mesh

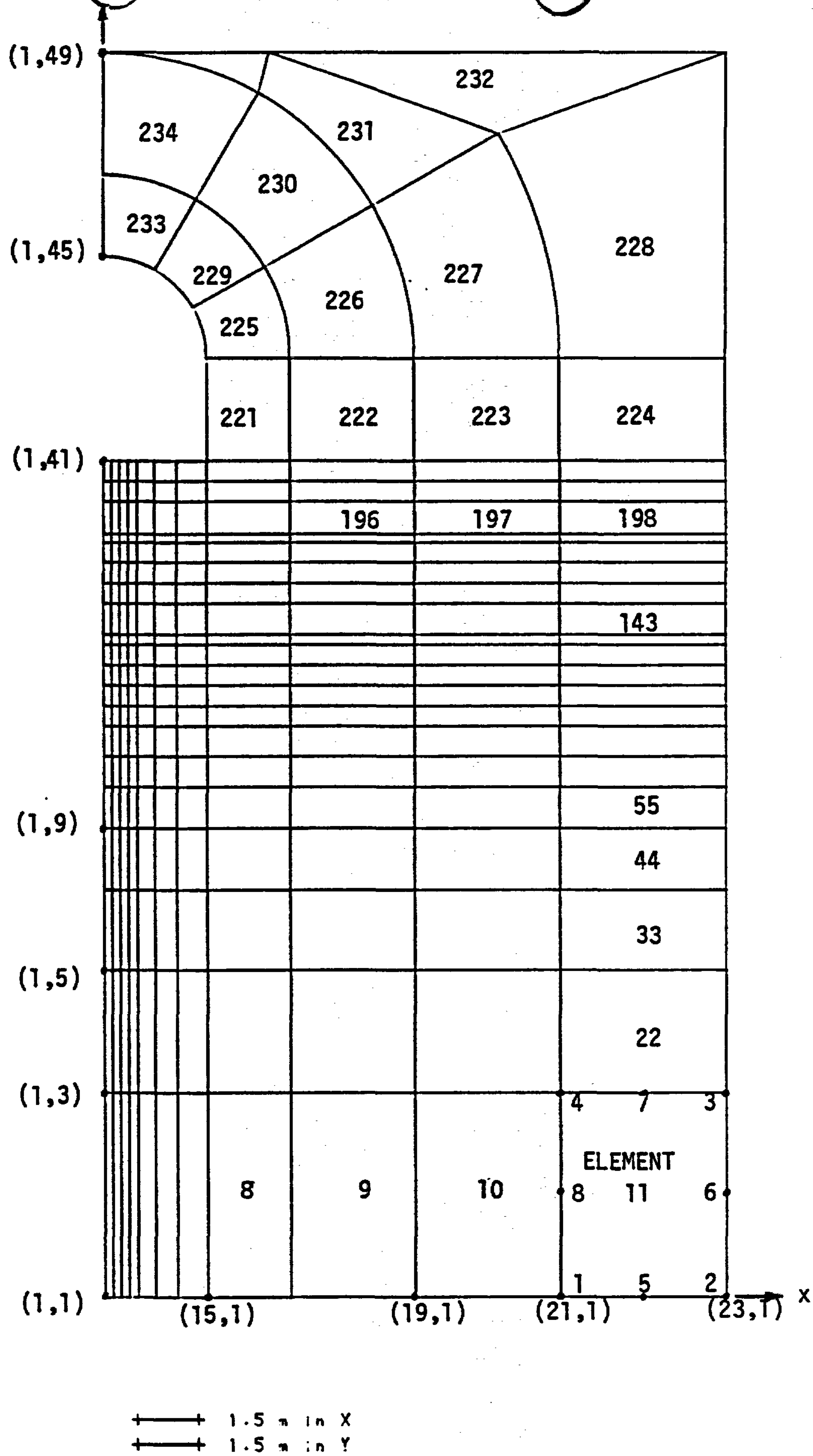


Figure 10.6-1 COYOTE Problem 6.3
Finite Element Mesh