CorSTAR
A TEKNEKRON INDUSTRIES AFFILIATE

NRC BIN B6985

October 10, 1985

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 September 1985

Dear Pauline:

This letter contains a management level summary of progress during the month of September. Also enclosed is a Technical Status Summary further describing work performed during this period.

Task 3 - Benchmark Problem Report - Waste Package Codes

There was no significant activity on this code area during the month. We are still waiting for formal receipt of the NRC comments on this report. The report has been revised using preliminary comments received from the NRC in the spring.

Tasks 4 & 5 - Siting Codes

On October 1, 1985 we met with GeoTrans in their offices in Reston, Virginia to further discuss the completion of this report.

Tasks 4 & 5 - Radiological Assessment Codes

There was no significant activity on this code area during the month.

Tasks 4 & 5 - Repository Design Codes

During the month the code ADINA was successfully compiled and run. Compilation difficulties previously encountered were corrected with the help of Mr. Lee Ho of ADINA Engineering. Because of the relatively small amount of small core memory at Brookhaven National Laboratory, difficulties may be encountered in setting up the large hypothetical and field validation problems for ADINA. Because of difficulties in obtaining the ADINA code and getting the code running on the Brookhaven computer, we are considerably behind schedule on this task.

The Brookhaven facility is phasing out both of its CDC 6600 machines. The removal of one machine has already resulted in some difficulty obtaining access to Brookhaven. When the final CDC 6600 machine is removed in December, it is

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possible that additional system congestion will result. Our best estimate at present is that we will not be able to complete our computer involvement at the Brookhaven computer prior to the removal of the second CDC 6600 machine. Additional schedule and cost impacts may result if significant effort is required to learn a new computer access system.

By letter dated September 27, 1985, CorSTAR made recommendations for benchmarking the computer code STEALTH. Significant modifications would be required to the version of the code STEALTH supplied by the NRC for benchmarking. Our proposed approach is to use modifications to the code developed by the San Leandro office of Science Applications, Inc. Our recommended approach for benchmarking the code was outlined in a letter to you dated September 27.

The results of benchmark problems run during the month are summarized in the Technical Status Summary.

Tasks 4 & 5 - Waste Package Codes

On September 17, 1985, CorSTAR executed a contract modification authorizing us to start work on Tasks 4 & 5 of the Waste Package Code.

Task 6 - Technology Transfer

On September 17, 1985, CorSTAR executed a contract modification authorizing us to proceed with Task 6 - Technology Transfer. By letter dated September 27, 1985, CorSTAR recommended a trial code and the order of remaining codes to be transferred to the NRC during the technology transfer task. On October 3, 1985, CorSTAR met with the NRC staff to review its recommendations. During this meeting it was agreed that the code ORIGEN would be the trial code. A preliminary order for the remaining code transfer was also established during the meeting.

General

Our estimate of costs through the end of September (through September 14, 1985 for CorSTAR) is:

Actual costs this month:	19.0K
Actual costs this fiscal year:	450.3K
Actual costs to date:	3195.0K
Planned costs this month:	0K
Planned costs this fiscal year:	240.0K

These 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
Project Manager

DKV/ks

TECHNICAL STATUS SUMMARY

TECHNICAL STATUS REPORT ATTACHMENT
TO PROGRESS REPORT FOR SEPTEMBER 1985

Repository Design Codes

Task 4 - Code Procurement

All applicable codes have been procured.

Code Installation

The ADINAT code has been successfully compiled and used to run sample problems supplied by ADINA Engineering and some of our analytical problems. In addition, the ADINA-PLOT code has also been compiled successfully. This code, however, has not yet been tested. Compilation of the ADINA-IN code was attempted. However, due to FORTRAN errors, which seem to be the result of the type of computer systems used at Brookhaven and not necessarily due to computer code errors, further debugging is required. Finally this month, the ADINA code was successfully compiled and run. The compilation difficulties previously encountered were corrected with the help of Mr. Lee Ho of ADINA Engineering. The correction entailed decreasing the amount of memory storage space called out internally within the ADINA code. The memory storage variable, MTOT, was reduced from 25000 to 20000. This solution, however, may result in possible storage problems in the running of the large hypothetical and field validation problems.

The lengthy installation delay of these codes has caused us to fall considerably behind schedule in meeting the proposed deadline date of March 15, 1985.

General Information

In a letter dated August 8, 1985, received from CorSTAR and initiated by the NRC, we were informed that Brookhaven is phasing out both of its CDC 6600 machines in addition to its CDC 7600 machine. The CDC 7600 machine is scheduled to be removed by the end of next year. This decision should have no effect on our work at this time. However, one CDC 6600 machine has already been removed from service while the other is to be removed possibly by December of this year. We currently use the CDC 6600 machines as our only method of communication with the Brookhaven system. The current reduction to one CDC 6600 machine should have a minimal immediate impact on our work. However, some accessing difficulties, due to system congestion, have already been felt. If these accessing difficulties continue to worsen, schedule delays and increased communication costs may result. The increased communication costs would be due to the fact that with a large number of users, we must "wait in line" to gain access to the computer. Not only is this "waiting" time unproductive, but it must be accomplished by remaining on the line where long distance phone charges are accumulating. In addition, excessive "waiting" time would lead to further schedule delays.

It is recommended that we attempt to finish our current computer involvement with Brookhaven prior to the removal of the last CDC 6600 machine. However, if the removal date of December of this year is accuate, our involvement will not be completed. In that event, schedule and cost changes may occur due to the learning of and data transfer to a different computer system.

Run Benchmark Problems

During the month, Problem 2.8 was run with ADINAT. The comparison of ADINAT results with the analytical and COYOTE solutions is included later in the report. As shown, the ADINAT surface temperature results compare very well with the analytical solution for the times shown. Additionally, Problem 2.10 has been set-up for use with ADINAT. This problem, however, has not yet been run successfully.

Both Problems 3.2b and 3.3c have been set-up and run with ADINA. The comparison of radial, circumferential, and longitudinal stresses between the ADINA results and analytical solution for both problems, are included later in the report. For Problem 3.2b, the ADINA results exhibit similar trends and are generally within 1% of the analytical solution. The only exception to this is in the case of the longitudinal stresses where the ADINA results in the plastic range do not match those of the analytical solution. It is felt that the ADINA code may not be able to properly deal with the discontinuous spike shown in this region. As a result, the code tries to solve for a continuous solution. Additionally, as shown in the circumferential stress solution ADINA calculates that the elastic-plastic transition point occurs closer toward the center of the circular tunnel than it does in the analytical solution. This error then affects those stresses calculated in the plastic region. For Problem 3.3c, the ADINA solution again shows good agreement with the analytical results and are within 5% of them.

Half of Problem 6.1 (PSV) has been run this month with VISCOT. In order to simplify the analysis, this problem was divided into axisymmetric and planar models. The axisymmetric model has been run successfully. For this problem, the creep law calculated for use was of a form that cannot be used with VISCOT. As a result, a compatible creep law for VISCOT, which is given for Problem 5.2, was substituted. The straight time-dependency of this new law results in larger creep strains and deformations that should be exhibited in the problem solution. Field measured and VISCOT floor uplift solution results are summarized for Room 4 at various times and are included later in the report. Both results compare favorably with each other for the first measuring interval. However, as expected, the VISCOT results start diverging from the field measured results as time progresses due to the effect of the new creep law. Vertical convergence results for VISCOT and field measured locations in room 4 are summarized and included at the end of the report. The field measured gage locations have to be determined before a comparison can be made. The planar model for Problem 6.1 has not yet been run successfully with VISCOT. The heater location, model configuration, and creep law used all seem to contribute to the difficulties encountered. A final solution for the planar model may not be attained.

Finally this month, VISCOT has been used to run Problem 5.2 (Basalt). The results of this analysis have not been summarized. In addition, Problem 5.2 (Salt) has not run successfully despite numerous attempts to correct it. The difficulties seem to arise from the straight time-dependent creep law used for this problem. This law was probably derived from laboratory data obtained for a few hundred days. Our use of this law to estimate the creep effects on an analysis of up to 10,000 years causes the creep strains and displacements to go out of range. In addition, the computer analysis does not seem to recognize when an opening has closed but instead continues to change the mesh shape until elements actually pass through each other. A solution for this problem may not be achieved.

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.

	AUINA - 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)	x	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					x		0
2.10 Steady Radiation Analysis of a Infinite Rectangular Opening (Rohsenow and Hartnett, 1973, pp. 15-32)				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	S,B	0	B			S,B	S	S	
5.2 Hypothetical Near Field Problem			(3)		x			(4)	x		0
5.3 Hypothetical Far Field Problem	(2)	(2)									0
6.0 FIELD VALIDATION PROBLEMS											
6.1 Project Salt Vault-Thermomechanical Response Simulation Problem	(2)	(2)	x								0
6.3 In Situ Heater Test-Basalt Waste Isolation Project	(2)	(2)	(1)		x			x	x		0

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

Problems completed

Problems attempted, results not analyzed

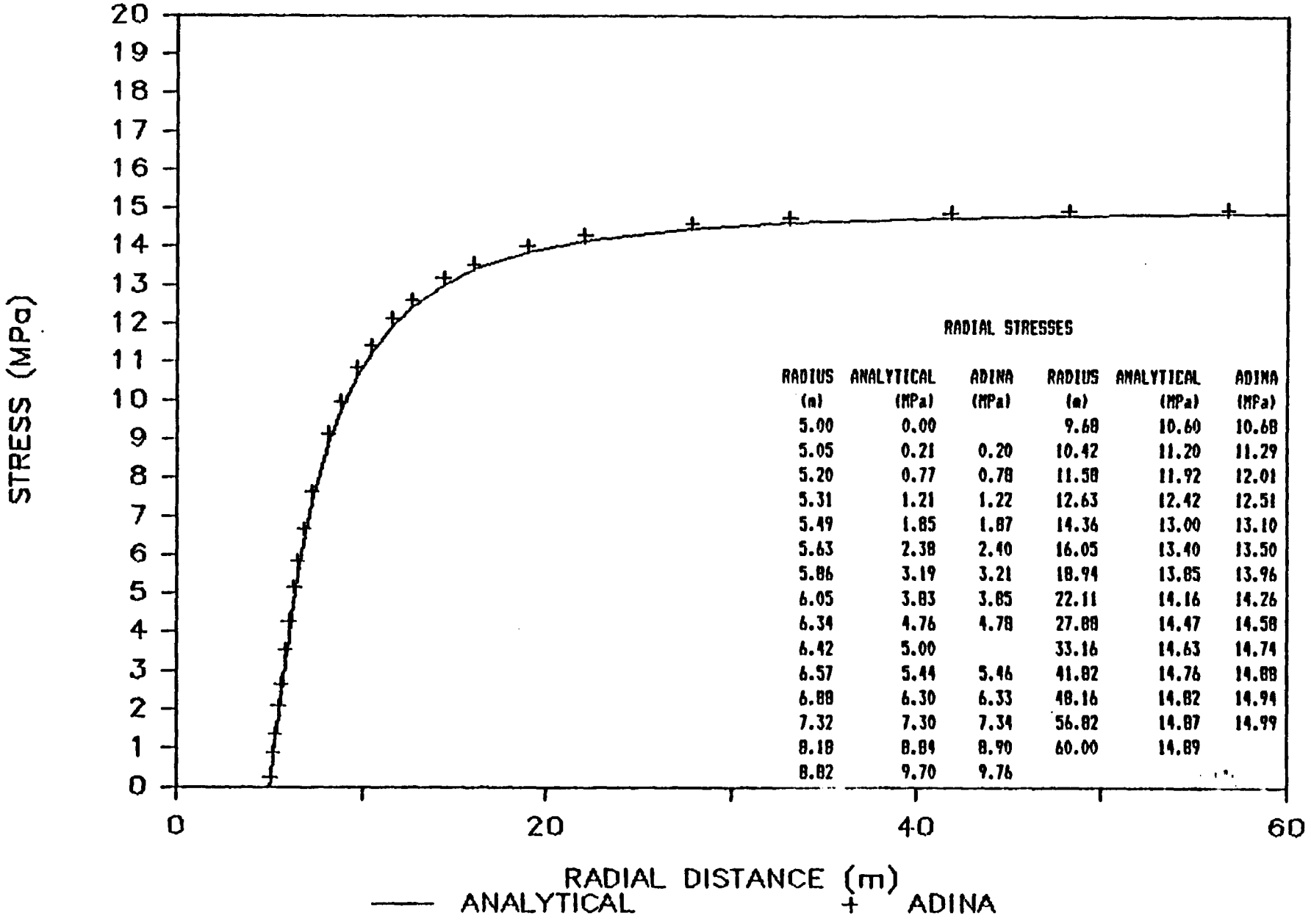
Problems attempted, difficulties encountered

Problem 2.8

Temperature Results Comparison

TIME (hr)	Surface Temperature (°C)		
	Analytical	COYOTE	ADINAT
0.0	260	260.0	260.0
2.3	174	166.5	174.1
4.6	154	149.4	155.2
7.0	141	137.6	142.3

ADINA — PROBLEM 3.2b



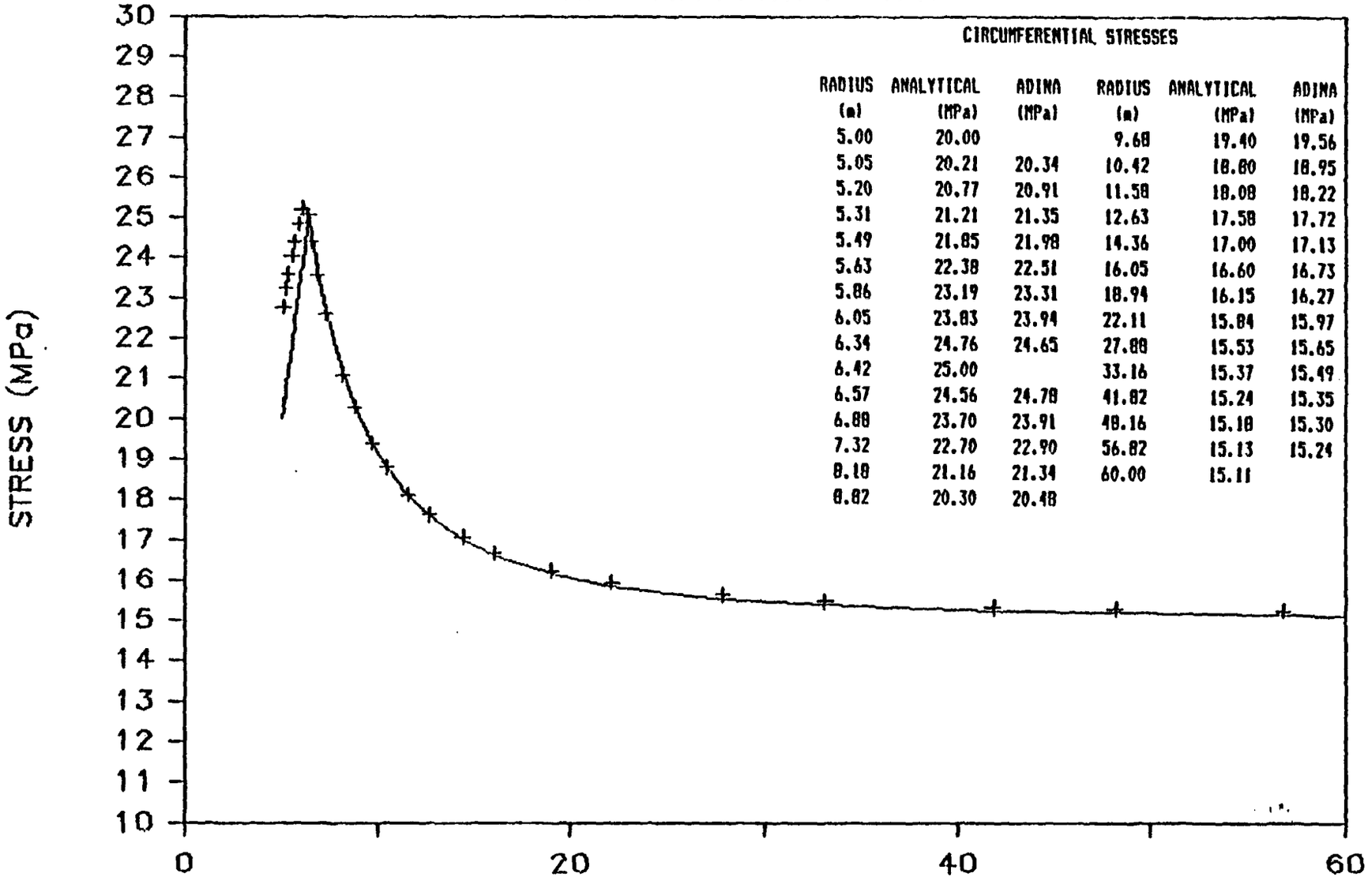
RADIAL STRESSES

RADIUS (m)	ANALYTICAL (MPa)	ADINA (MPa)	RADIUS (m)	ANALYTICAL (MPa)	ADINA (MPa)
5.00	0.00		9.68	10.60	10.68
5.05	0.21	0.20	10.42	11.20	11.29
5.20	0.77	0.78	11.58	11.92	12.01
5.31	1.21	1.22	12.63	12.42	12.51
5.49	1.85	1.87	14.36	13.00	13.10
5.63	2.38	2.40	16.05	13.40	13.50
5.86	3.19	3.21	18.94	13.85	13.96
6.05	3.83	3.85	22.11	14.16	14.26
6.34	4.76	4.78	27.88	14.47	14.58
6.42	5.00		33.16	14.63	14.74
6.57	5.44	5.46	41.82	14.76	14.88
6.88	6.30	6.33	48.16	14.82	14.94
7.32	7.30	7.34	56.82	14.87	14.99
8.18	8.84	8.90	60.00	14.89	
8.82	9.70	9.76			

ADINA Problem 3.2b
RADIAL STRESS COMPARISON

ADINA — PROBLEM 3.2b

CIRCUMFERENTIAL STRESS

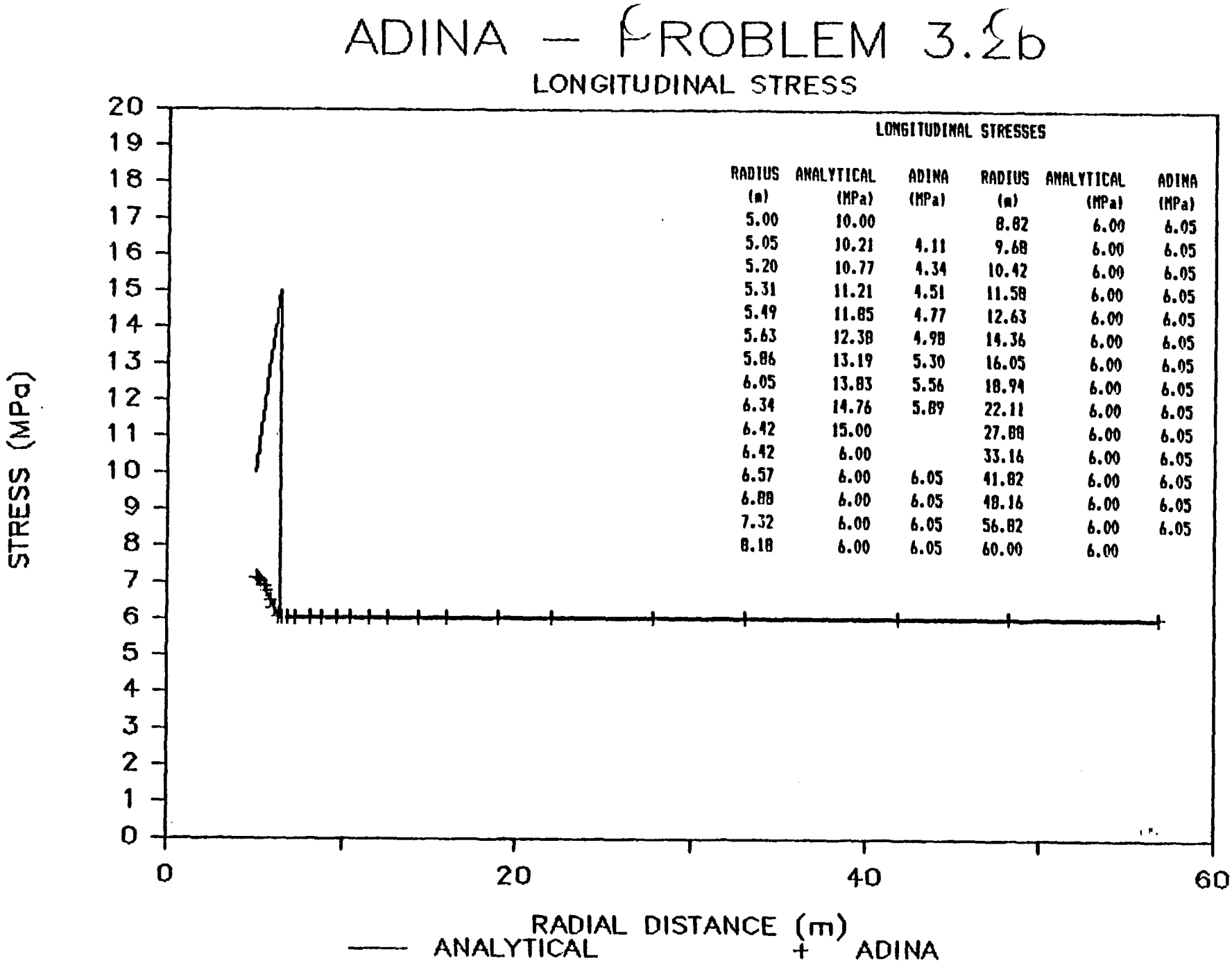


CIRCUMFERENTIAL STRESSES

RADIUS (m)	ANALYTICAL (MPa)	ADINA (MPa)	RADIUS (m)	ANALYTICAL (MPa)	ADINA (MPa)
5.00	20.00		9.68	19.40	19.56
5.05	20.21	20.34	10.42	18.80	18.95
5.20	20.77	20.91	11.58	18.08	18.22
5.31	21.21	21.35	12.63	17.58	17.72
5.49	21.85	21.98	14.36	17.00	17.13
5.63	22.38	22.51	16.05	16.60	16.73
5.86	23.19	23.31	18.94	16.15	16.27
6.05	23.83	23.94	22.11	15.84	15.97
6.34	24.76	24.65	27.88	15.53	15.65
6.42	25.00		33.16	15.37	15.49
6.57	24.56	24.78	41.82	15.24	15.35
6.88	23.70	23.91	48.16	15.18	15.30
7.32	22.70	22.90	56.82	15.13	15.24
8.18	21.16	21.34	60.00	15.11	
8.82	20.30	20.48			

ADINA Problem 3.2b
CIRCUMFERENTIAL STRESS COMPARISON

ADINA — PROBLEM 3.2b

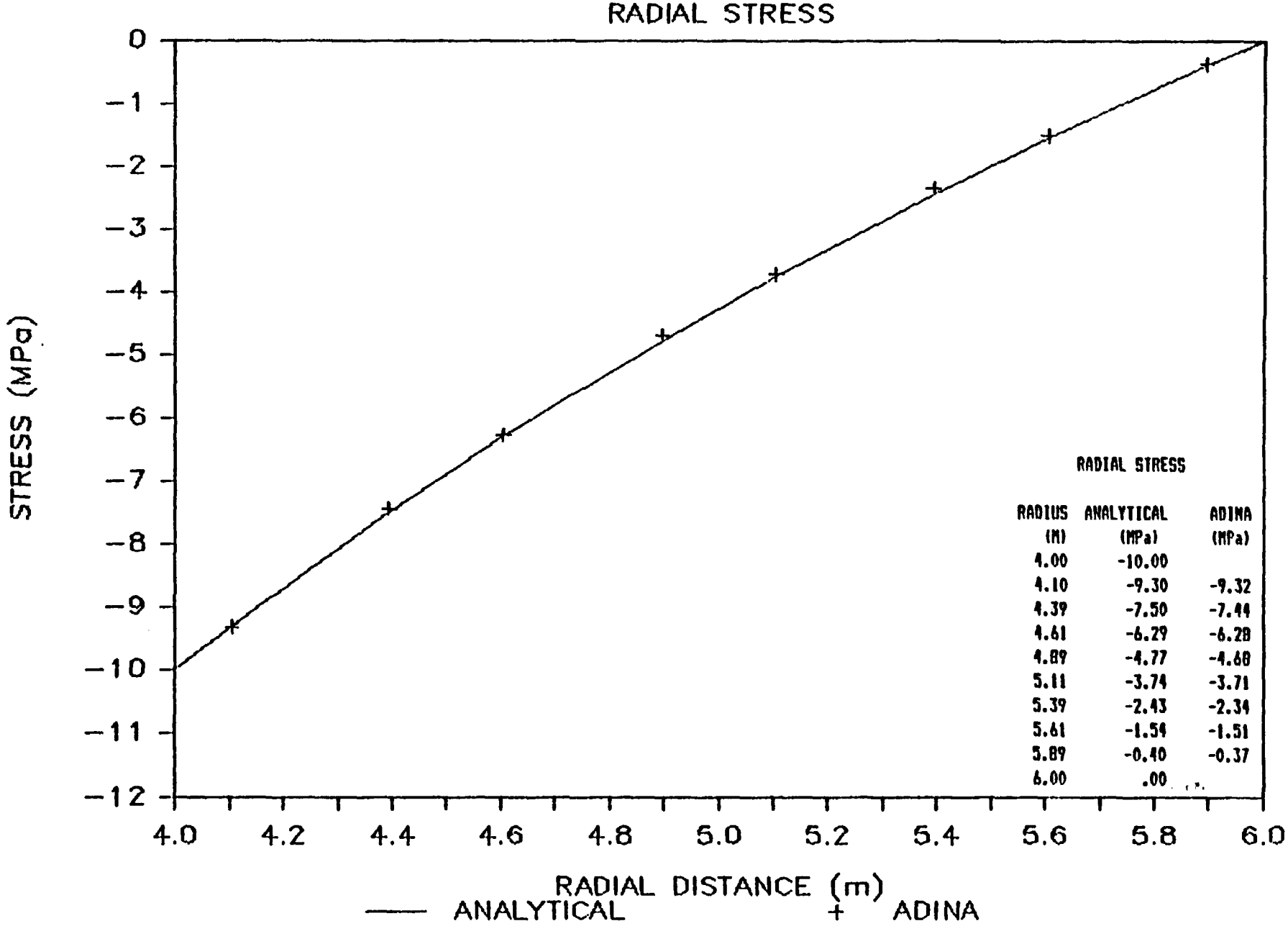


LONGITUDINAL STRESSES

RADIUS (m)	ANALYTICAL (MPa)	ADINA (MPa)	RADIUS (m)	ANALYTICAL (MPa)	ADINA (MPa)
5.00	10.00		8.82	6.00	6.05
5.05	10.21	4.11	9.68	6.00	6.05
5.20	10.77	4.34	10.42	6.00	6.05
5.31	11.21	4.51	11.58	6.00	6.05
5.49	11.85	4.77	12.63	6.00	6.05
5.63	12.38	4.98	14.36	6.00	6.05
5.86	13.19	5.30	16.05	6.00	6.05
6.05	13.83	5.56	18.94	6.00	6.05
6.34	14.76	5.89	22.11	6.00	6.05
6.42	15.00		27.88	6.00	6.05
6.42	6.00		33.16	6.00	6.05
6.57	6.00	6.05	41.82	6.00	6.05
6.88	6.00	6.05	48.16	6.00	6.05
7.32	6.00	6.05	56.82	6.00	6.05
8.18	6.00	6.05	60.00	6.00	

ADINA Problem 3.2b
LONGITUDINAL STRESS COMPARISON

ADINA — PROBLEM 3.3c

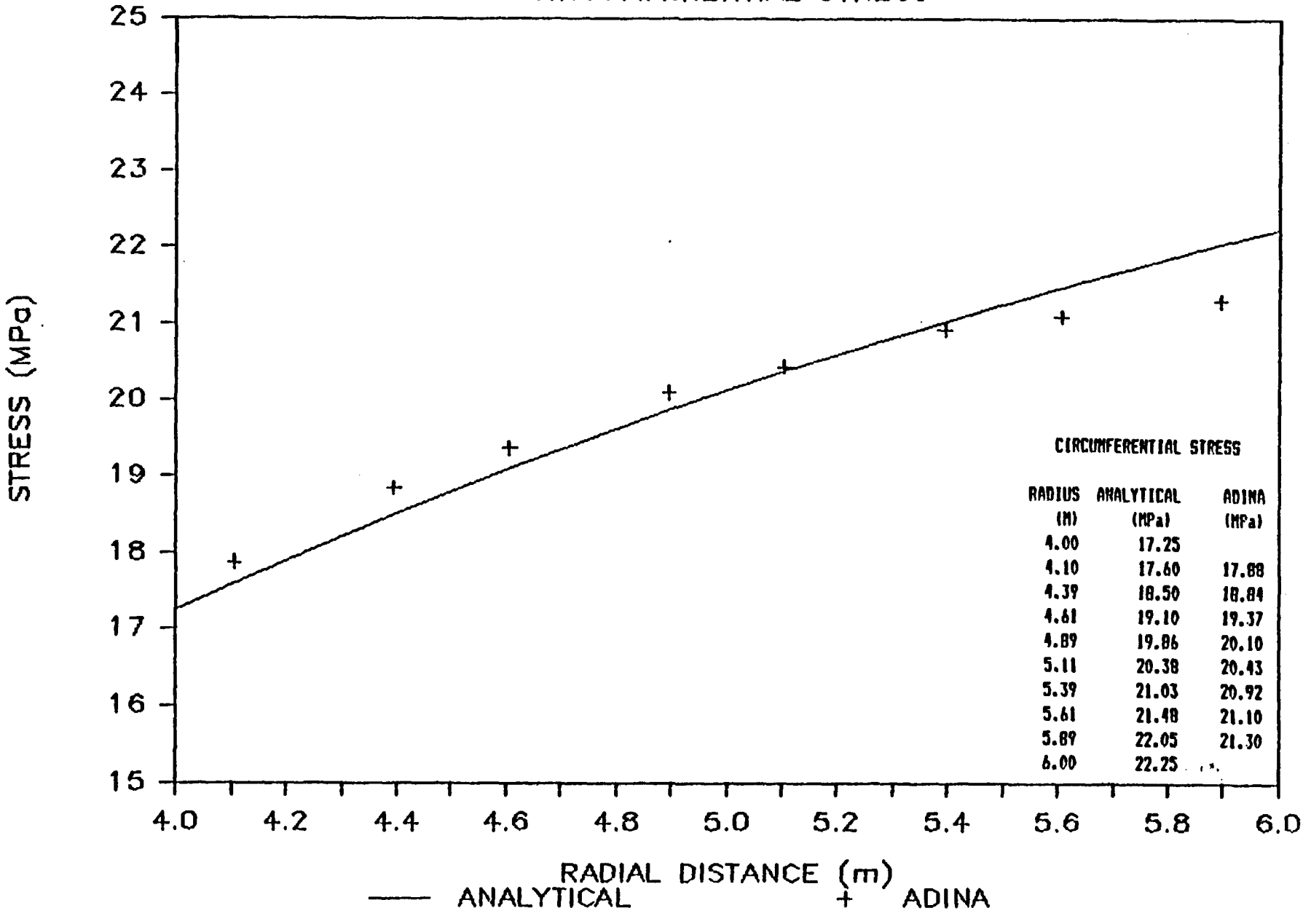


RADIAL STRESS

RADIUS (M)	ANALYTICAL (MPa)	ADINA (MPa)
4.00	-10.00	
4.10	-9.30	-9.32
4.39	-7.50	-7.44
4.61	-6.29	-6.28
4.89	-4.77	-4.68
5.11	-3.74	-3.71
5.39	-2.43	-2.34
5.61	-1.54	-1.51
5.89	-0.40	-0.37
6.00	.00	

ADINA Problem 3.3c
RADIAL STRESS COMPARISON

ADINA — PROBLEM 3.3c

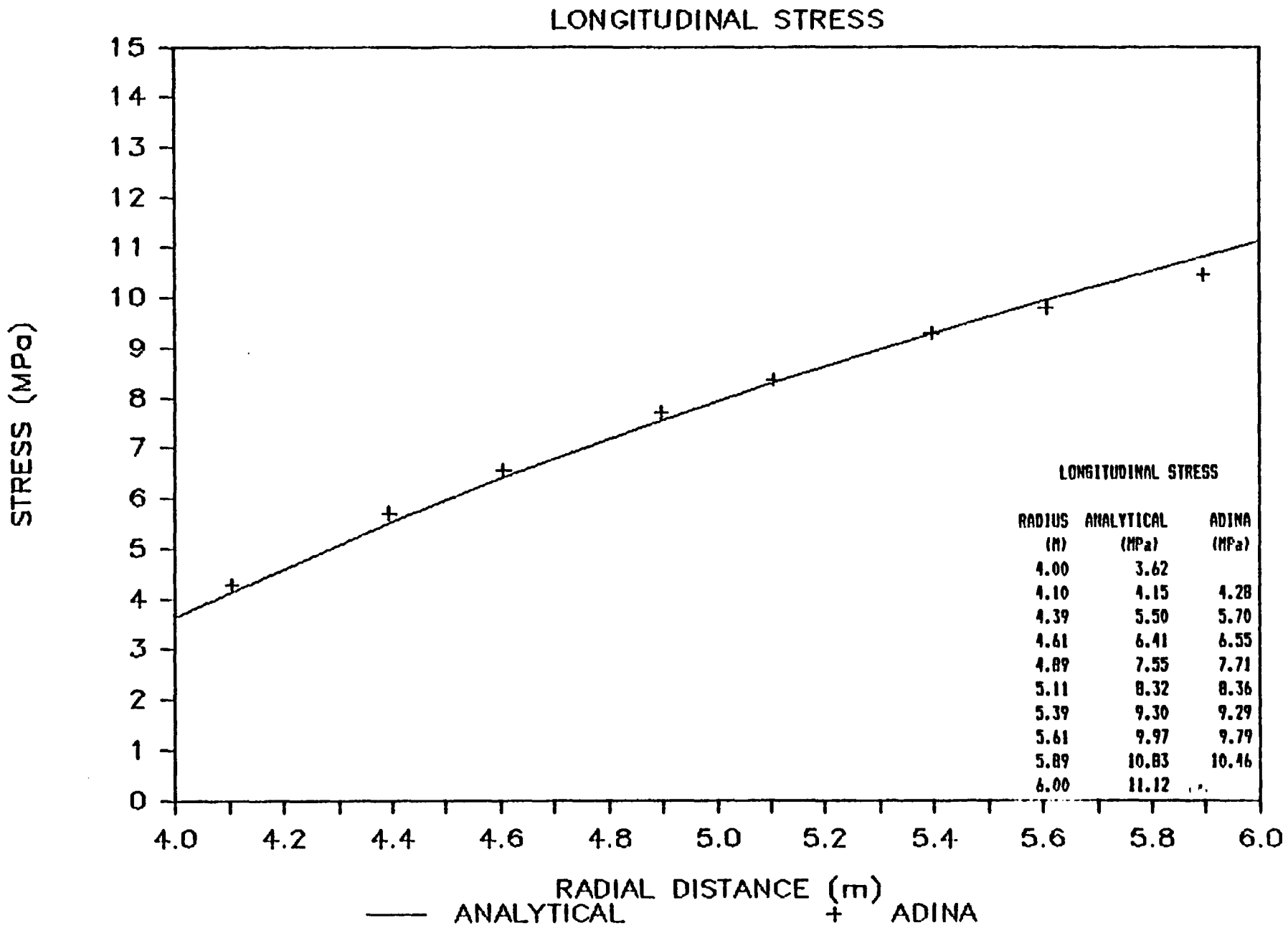


CIRCUMFERENTIAL STRESS

RADIUS (M)	ANALYTICAL (MPa)	ADINA (MPa)
4.00	17.25	
4.10	17.60	17.88
4.39	18.50	18.84
4.61	19.10	19.37
4.89	19.86	20.10
5.11	20.38	20.43
5.39	21.03	20.92
5.61	21.48	21.10
5.89	22.05	21.30
6.00	22.25	

ADINA Problem 3.3c
CIRCUMFERENTIAL STRESS COMPARISON

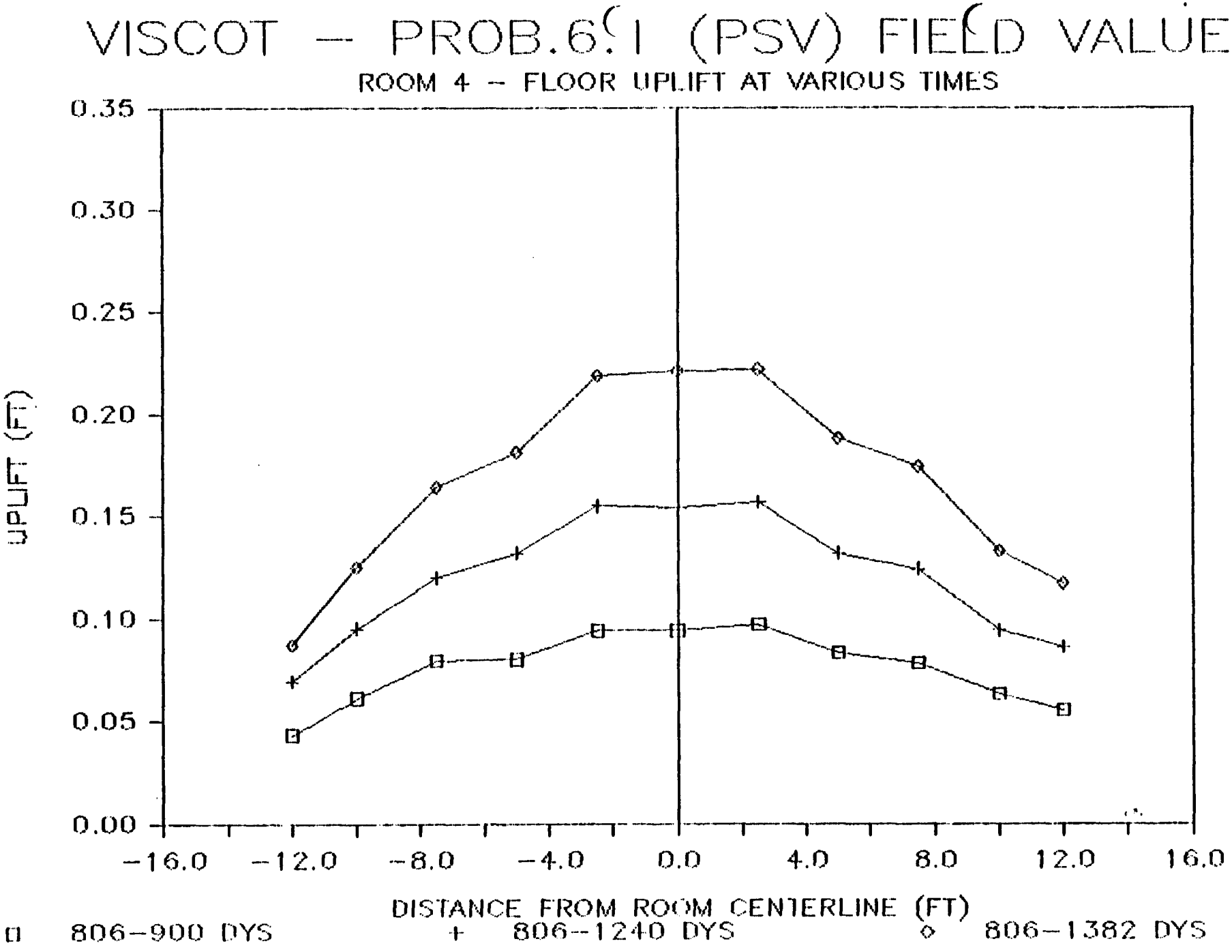
ADINA — PROBLEM 3.3c



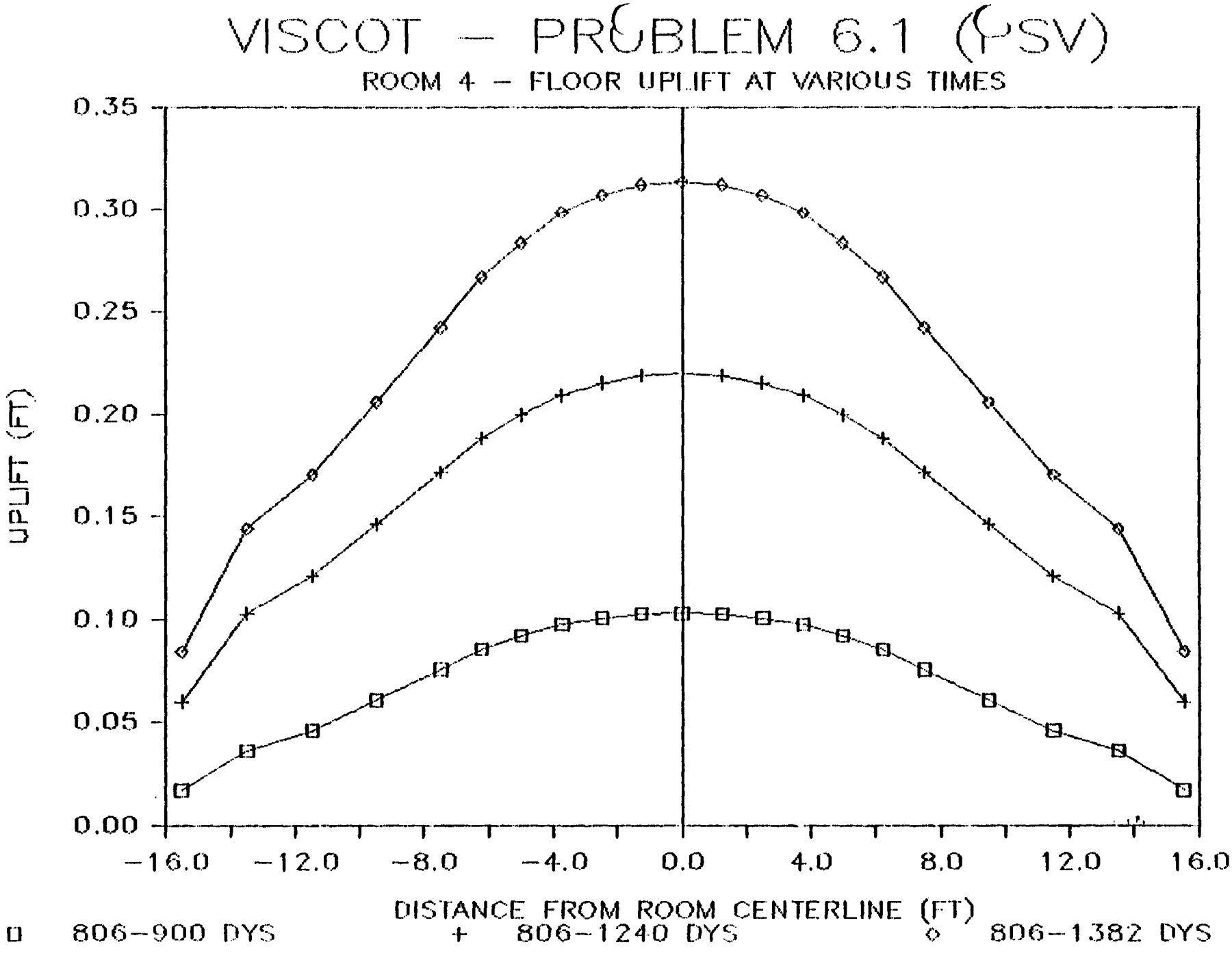
LONGITUDINAL STRESS

RADIUS (M)	ANALYTICAL (MPa)	ADINA (MPa)
4.00	3.62	
4.10	4.15	4.28
4.39	5.50	5.70
4.61	6.41	6.55
4.89	7.55	7.71
5.11	8.32	8.36
5.39	9.30	9.29
5.61	9.97	9.79
5.89	10.83	10.46
6.00	11.12	

ADINA Problem 3.3c
LONGITUDINAL STRESS COMPARISON

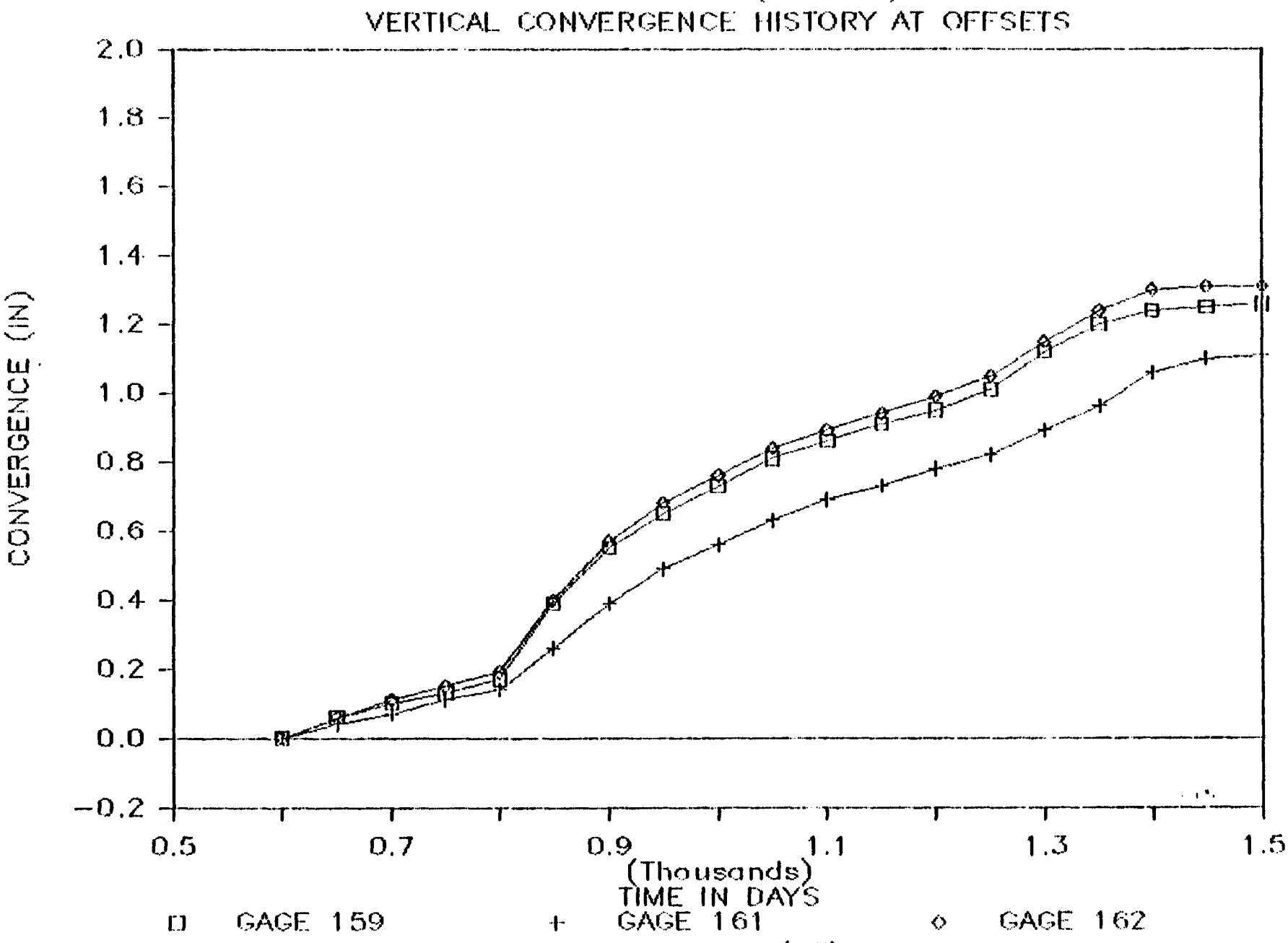


VISCOT Problem 6.1 (PSV)
FIELD MEASURED FLOOR UPLIFT
IN ROOM 4 AT VARIOUS TIMES

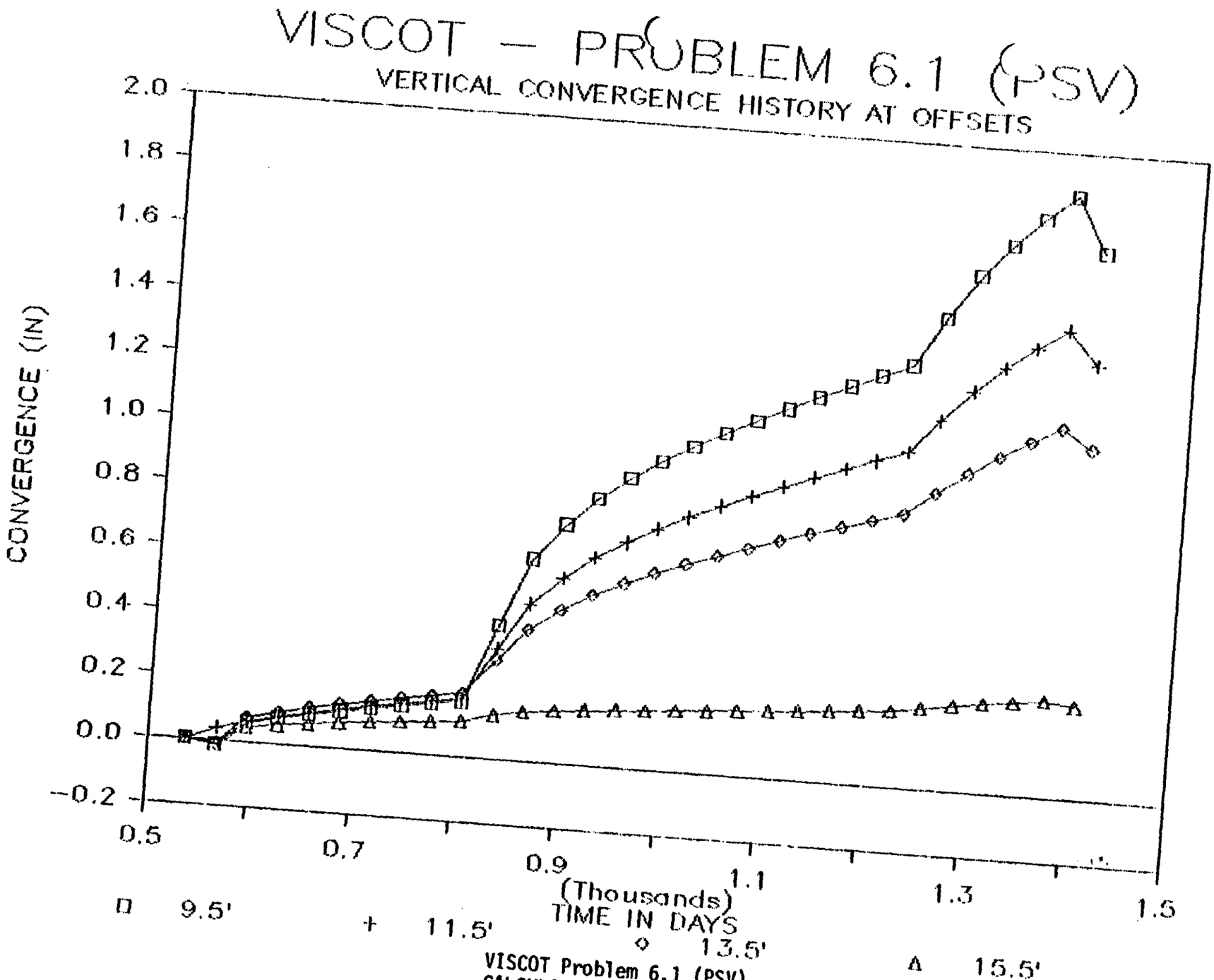


VISCOT Problem 6.1 (PSV)
CALCULATED FLOOR UPLIFT IN
ROOM 4 AT VARIOUS TIMES

VISCOT – PROB. 6.1 (PSV) FIELD VALUES



VISCOT Problem 6.1 (PSV)
FIELD MEASURED VERTICAL CONVERGENCE
IN ROOM 4 AT VARIOUS GAGES AND TIMES



VISCOT Problem 6.1 (PSV)
CALCULATED VERTICAL CONVERGENCE IN ROOM 4
AT VARIOUS TIMES AND OFFSETS FROM ARRAY HEATERS