



WM DOCKET CONTROL CENTER TEKNEKRON INDUSTRIES AFFILIATE

February 24, 1986

WM-RES
WM Record File
36985
CorStar

WM Project 10/11/16
Docket No. _____
PDR
LPDR B, M, S

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

Subject: Contract No. NRC-02-81-026
Benchmarking of Computer Codes and Licensing Assistance
Monthly Letter Progress Report for January 1986

Dear Pauline:

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

Task 3 - Benchmark Problem Report - Waste Package Codes

CorSTAR has recommended deleting the geochemistry problems in this report as they are not applicable to conditions near the waste package. By letter dated January 31, the NRC stated that they will be reassessing the geochemistry problems in this report to determine whether they are well-posed and applicable to appropriate repository conditions. The NRC stated that its review will be complete in one month.

Tasks 4 & 5 - Siting Codes

During the week of January 27, GeoTrans submitted a cost proposal for completion of this effort. During the week of February 3, we received notification from the NRC that a DCAA review of that proposal had been successfully conducted. A subcontract modification will be transmitted to GeoTrans during the week of February 10.

Tasks 4 & 5 - Radiological Assessment Codes

During January the draft report was typed and tables and figures were prepared.

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PDR WMRES EECCDRS
B-6985 PDR

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WASHINGTON, D.C.

INCLINE VILLAGE

2806

Tasks 4 & 5 - Repository Design Codes

On January 24, 1986, the last CDC 6600 mainframe computer, MFA, was taken out of service at Brookhaven National Laboratories. Prior to the removal of MFA, all files for the repository design codes were copied to the new CYBER 180/830 mainframe, MFC.

At the request of the NRC, Acres contacted Dr. Bathe of ADINA Engineering by telephone on February 3, 1986. A summary of the conversation with Dr. Bathe is included in the technical status summary report.

Acres has continued to encounter difficulties in obtaining a computer solution to problem 3.5. Considerable effort has been expended on this benchmark problem without obtaining a satisfactory computer solution. Acres believes that effort on this benchmark problem should be suspended and continued later if time and budget resources permit.

Thermal analyses of both the axisymmetric and planar models of problem 6.1 (project salt vault) have been successfully run using ADINAT. The results are discussed in the Technical Status Report.

Tasks 4 & 5 - Waste Package Codes

During January, we submitted a request to the NRC for Computer Resources at ORNL to run the HEATING code. We expect to get access to the ORNL computer by the end of February. During January, a magnetic tape containing code COVE was sent to a service bureau to be converted to an IBM-PC floppy disk. We believe that this format will give us more flexibility in running the benchmark problems.

We are discussing with the NRC which version of the WAPPA code should be benchmarked. The ADINA and ADINAT codes are now available at BNL.

Task 6 - Technology Transfer

During the reporting period, work continued on the QA plan and procedures. By the end of the month, a working draft report was available. During January we stated a review of reports describing other organizations' experiences with software errors, software quality assurance, and benchmarking.

General

On January 9, 1986, Dr. David Large of CorSTAR visited Acres offices in Buffalo to perform a Quality Assurance Audit. The results of that audit are summarized in the enclosed letter from Dr. Large to Mr. Lamb of Acres.

During the period January 27-29, Doug Vogt attended an NRC Division of Research Model Validation Workshop in Bethesda. A brief report summarizing that meeting was forwarded to the NRC by letter dated February 24, 1986.

On January 30, Pauline Brooks and Doug Vogt met with Marie Page of NRC Division of Contracts to discuss our letter proposal for completion of work on the repository design codes. At that time we were told that no problem existed that would prevent timely authorization to proceed with the work outlined in that proposal. Timely authorization to proceed with this work is required to avoid adverse cost and schedule impacts.

Our estimate of costs through the end of January (February 1, 1986 for Corstar) is:

Actual costs this month:	49K
Actual costs this fiscal year:	159K
Actual costs to date:	3,354K
Planned costs this fiscal year:	160K
Planned costs this month:	50K

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
Project Manager

DKV:kg

Enclosures



A TEKNEKRON INDUSTRIES AFFILIATE

January 17, 1986

Mr. D. W. Lamb
Acres International Corporation
424 Main Street, Suite 1000
Buffalo, New York 14202-3592

Re: Nuclear Regulatory Commission Contract 02-81-026
Subcontract with CorSTAR, Inc.
Quality Assurance Audit of 9 January 1986

Dear Bill:

You will recall my visit to your office on the above referenced date to perform a Quality Assurance Audit of your files relating to the above referenced contract. As we discussed, I found that the files were basically in order and that your indexing system conforms with the QA Procedure's guidelines. Furthermore, with the one exception described below, a random check of the file contents against your Control File Index failed to uncover any unaccounted for documents. There were, however, some problems with the backup files that we discussed, and which you agreed to rectify. For the record, these are as follows:

1. The QA plan requires that "back-up copies of the project tapes to which additions have been made shall be regenerated (updated) quarterly and stored on different premises from the primary tapes." My understanding is that the primary tapes for the COYOTE, DOT, MATLOC, VISCOT, SALT4, ADINA and ADINAT programs which you are benchmarking are stored at Brookhaven National Laboratory. Please see that copies of those tapes containing the latest versions of all of these programs excepting the last two (ADINA and ADINAT) are made and stored on your premises. CorSTAR will assume possession of them once your work under this subcontract is completed. (The responsibility of maintaining back-up copies of the proprietary codes ADINA and ADINAT lies with the Repository Projects Branch of the NRC.)
2. Paper copies of the original source codes and documentation of changes made thereto for all nonproprietary programs (i.e., all except for ADINA and ADINAT) are also to be kept in the QA file. The file P6678.573-COYOTE- "Code Listings & Updates" was empty during my visit. Please see that this absence is remedied.

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BERKELEY

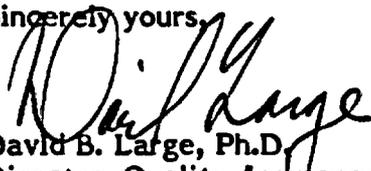
WASHINGTON, D.C.

INCLINE VILLAGE

Maintenance of a clear record of all changes you have made to the original source codes is of course a very critical aspect of your benchmarking effort. Most of the records in the QA file that I reviewed in this context showed no entries for a year or so. This may be appropriate, in that your work for some time has focused primarily on the proprietary codes ADINA and ADINAT. Also, I realize that the set of files kept by Mr. Swanson also document code changes. I would ask that you review your system for documenting code changes with Mr. Swanson to verify that records of changes have in fact been kept up to date. Should you find that any remedial actions are needed, I trust you will make them and report any changes to me.

Overall, we believe Acres has done an excellent job in the repository design area of this project, and your files support that view. I enjoyed meeting with you and look forward to another trip to your office sometime in the future.

Sincerely yours,



David B. Large, Ph.D.
Director, Quality Assurance
NRC Benchmarking Project

DBL:kg



February 5, 1986
P6678.00

Mr. Douglas K. Vogt
Vice President
CorSTAR Research, Inc.
2121 Allston Way
Berkeley, CA 94704

Dear Doug:

Contract No. NRC-02-28-026
Benchmarking of Computer Codes
Progress Report for January 1986

During the month of January, work continued on Task 4. A detailed Technical Status Report is attached. The following is a brief summary.

CODE PROCUREMENT

All applicable codes have been procured.

CODE INSTALLATION

All applicable codes have been compiled and used to run problems. Problems encountered while compiling the ADINA code led to a solution which may result in difficulties in setting up the large hypothetical and field validation problems.

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

GENERAL INFORMATON

The CDC 6600 (MFA) mainframe computer at Brookhaven National Laboratories (BNL) was permanently taken out of service on January 24, 1986. Prior to the removal of MFA, all of the project files were successfully copied to the MFC mainframe.

On January 9, 1986, Dr. David Large of CorSTAR visited Acres offices in Buffalo to perform a Quality Assurance Audit of the files related to this project. In his letter of January 17, 1986 to Acres, a copy of which is presented later in this report, Dr. Large reported that he found Acres files to be in order with two notable exceptions:

ACRES INTERNATIONAL CORPORATION

Engineers, Architects and Planners
Suite 1000, Liberty Building, 424 Main Street,
Buffalo, New York 14202-3592
Telephone 716-853-7525 Telex 91-6423

February 5, 1986

- (1) Backup copies of the project tapes to which additions or changes have been made were not stored on premises different from the primary tapes.
- (2) The file P6678.573-COYOTE-"Code Listings & Updates" which contains the original source code and documents changes to the program, was empty during Dr. Large's visit.

On February 3, 1986, Acres contacted Dr. Bathe of ADINA Engineering by telephone and discussed our experiences with the ADINA codes to date. A detailed summary of the conversation is included in the Technical Status Report.

Run Benchmark Problems

Problem 3.5 has required an unusually large amount of time to solve, and as a result, we have consumed all of the time allocated for this problem according to the revised schedule of December 9, 1985. We have, therefore, suspended work on Problem 3.5 and will continue later as time and budget constraints permit.

The thermal analysis of both the Axisymmetric and Planar models of Problem 6.1 (PSV) have been set-up and successfully run using the ADINAT code. The results are discussed in detail in the Technical Status Report.

WRITE-UP RESULTS

We have begun to write up the results for the ADINAT code. At this time, the write-up is not ready for your review.

PROJECT CONTROL

The lengthy delay caused by the unavailability of the ADINA and ADINAT codes have caused us to fall well behind the schedule in meeting the proposed Draft Task Summary Report deadline of March 15, 1985. Our revised schedule, as presented in last month's Report, more accurately reflects the outstanding work.

During the month of January, a total 220 man-hours were expended which, together with direct costs, represent a cost of approximately \$10,600.

Very truly yours,



D. W. Lamb
Manager
Project Operations

DWL:sd

TECHNICAL STATUS SUMMARY

TECHNICAL STATUS REPORT ATTACHMENT
TO PROGRESS REPORT FOR JANUARY 1986

Repository Design Codes

Task 4 - 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 all of our analytical problems. In addition, the ADINA-PLOT code had also been compiled successfully. This code, however, has not yet been tested. Compilation of the ADINA-IN code has not been completed due to FORTRAN errors which stem from the type of computer at the Brookhaven facility and not computer code errors. Further compilation of the ADINA-IN code will not be attempted. The ADINA code was successfully compiled with the assistance 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 its original value of 25000 to 20000. This solution, however, may result in storage problems when large hypothetical or field validation problems are run.

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

The CDC 6600 (MFA) mainframe computer at Brookhaven National Laboratories (BNL) was permanently taken out of service on January 24, 1986. Prior to the removal of MFA, all of the project files were successfully copied to the recently installed CYBER 180/830 (MFC) mainframe via the CDC 7600 (MFZ) mainframe. The method used to move the files from MFA to MFC was presented at a seminar given by the NRC on December 11, at their offices in Bethesda, MD.

On January 9, 1986, Dr. David Large of CorSTAR visited Acres' office in Buffalo to perform a Quality Assurance Audit of the files related to this project. In his letter of January 17, 1986 to Acres, a copy of which is presented later in this report, Dr. Large reported that he found Acres' files to be in order with two notable exceptions:

1. Backup copies of the project tapes to which additions or changes have been made were not stored on premises different from the primary tapes.

Acres has identified four (4) tapes previously sent to Brookhaven specifically for this purpose. A batch job has been submitted to store the source codes and the most recently used versions of the COYOTE, DOT, MATLOC, SALT4, and VISCOT codes on one of the tapes. Files pertaining to codes provided by ADINA-PLOT are also being stored on a separate tape. We will review our records to assure that microfiche and hard copies of the above-mentioned codes are also obtained. The tape, microfiche and hard copies of these codes will be stored at Acres office in Buffalo until the completion of this project.

2. The file P6678.573-COYOTE-"Code Listings & Updates" which contains the original source code and documents changes to the program, was empty during Dr. Large's visit.

We are reviewing our files to locate this information and correct the oversight.

On February 3, 1986, Acres contacted Dr. Bathe of ADINA Engineering by telephone and discussed our experience with the ADINA codes to date. Dr. Bathe was particularly interested in the problems that we have encountered with the ADINA codes. We reported to him that the ADINAT code has been used successfully for analytical and field validation problems without storage requirement restrictions. We discussed the problems related to the ADINA code in greater detail, specifically those caused by the limited storage space available at Brookhaven. Dr. Bathe confirmed that our mesh sizes must be relatively small due to the limitation of MTOT to 20000. We told him that one field validation problem, Problem 6.3 (BWIP), was run with ADINAT but was too large to be run with ADINA. He suggested that we try grouping the elements into several element groups before redefining the mesh. This would allow us to use the output from the ADINAT run. If this does not work, it will then be necessary to redefine the mesh, which would require another ADINAT run to obtain the temperatures at the proper nodal points.

We also discussed a problem encountered in Problem 3.2B with Dr. Bathe. In this problem, the code must compute the radius of the plastic/elastic interface for a cylindrical opening in an elastic/plastic medium exposed to a hydrostatic stress field. The Von Mises failure criterion was used with no strain hardening. The results indicate that the radius to the plastic/elastic interface does not agree with the analytical solution, and that a longitudinal stress discontinuity exists at this interface. Dr. Bathe suggested that we run the problem again using a strain hardening factor of 1% and send the results to him for his review.

Run Benchmark Problems

The analytical solutions for both parts of Problem 3.5, using the Von Mises and Drucker-Prager failure criteria, were reviewed. A LOTUS-123 Spreadsheet, which was received from CorSTAR in December, was used to calculate the analytical solutions. The problem has been set-up and run using ADINA, but the results have not been analyzed. This problem has required an unusually large amount of time to solve, and as a result, we have consumed all of the time allocated for this problem according to the revised schedule of December 9, 1985. We have therefore suspended work on Problem 3.5 and will continue later as time and budget constraints permit.

The thermal analysis of both the Axisymmetric and Planar models of Problem 6.1 (PSV) have been set-up and successfully run using the ADINAT code. The finite element meshes used for previous analyses with the DOT code were used. Temperature histories at mid-heater level at various offsets, and the horizontal temperature profile at various depths on Day 690 were prepared for Room 3 (Planar model). Since no field data were provided from Room 3, the results can only be compared to those obtained from the analysis done with the DOT code. For Room 4 (Axisymmetric model), field data were given in two graphs. The first shows temperature histories at various depths in a hole offset 2.4m from the center of the room. The second plot shows temperature histories at various offsets at a constant depth of 2.7m below the room floor. We have prepared plots of the field and ADINAT results for each of these data sets. These plots are presented later in this report.

TABLE 3
MATRIX OF CODE/PROBLEM COMBINATIONS*
(Revised 12/5/85)

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.

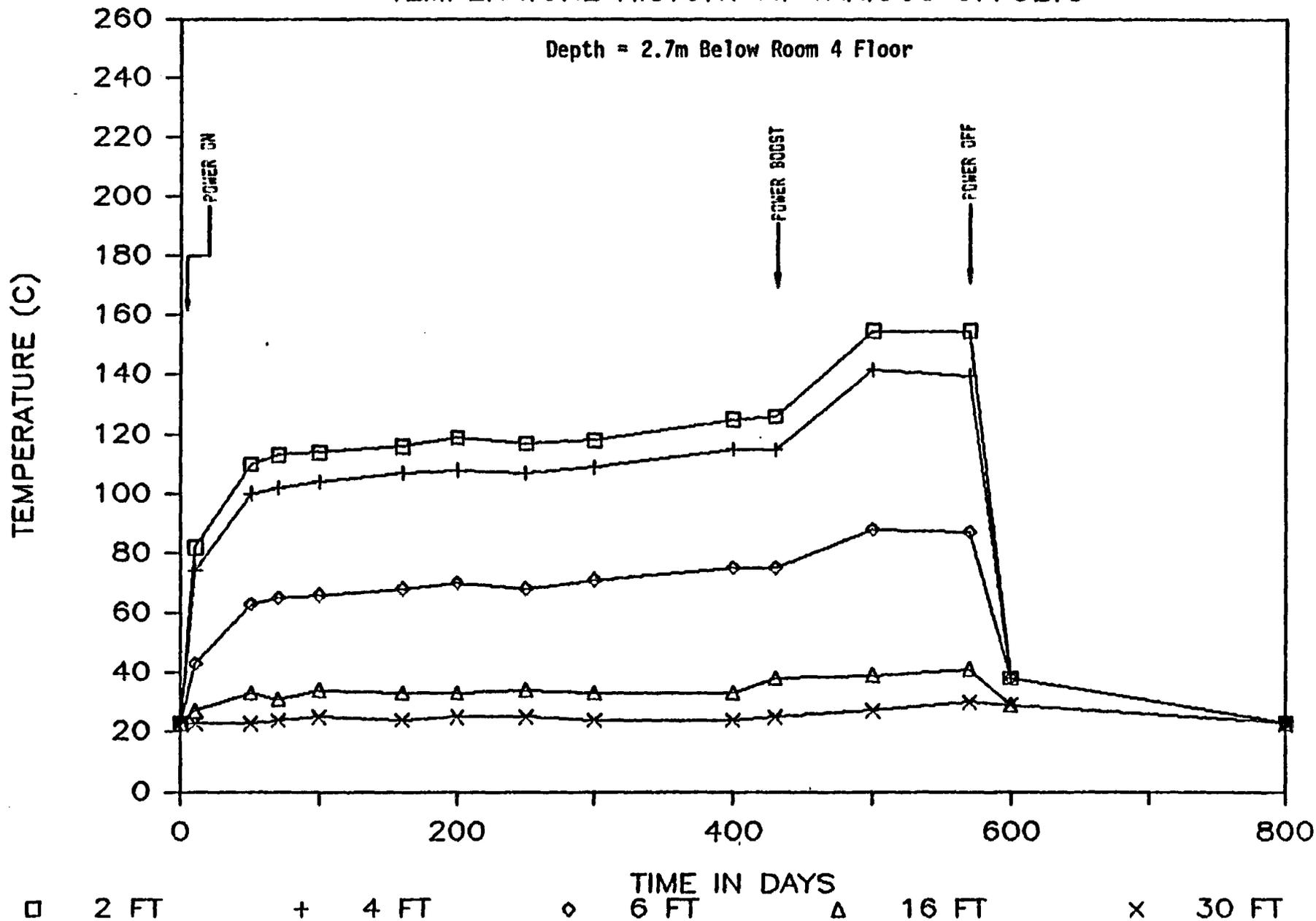
	ADINA - 3D	ADINAT - 3D	DOT	HEATING	MATLOC	SPECTROM 11	SPECTROM 41	VISCOT	COYOTE	SALT 4	STEALTH
2.0 THERMAL ANALYSIS CASE PROBLEMS											
2.6 Transient Temperature Analysis of an Infinite Rectangular Bar With Anisotropic Conductivity (Schneider, 1955, pp. 261)					0						0
2.8 Transient Temperature Response to the Quench of an Infinite Slab With a Temperature-Dependent Convection Coefficient (Kreith, 1958, pp. 161)					0						0
2.9 Transient Temperature Response of a Slab Exposed to a Uniform Radiative Environment (Rohsenow and Hartnett, 1973, pp. 3-49)					0						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											0
3.3 Thick-Walled Cylinder Subjected to Internal and/or External Pressure c) Plane strain - creep											0
3.5 Plane Strain Compression of an Elastic-Plastic Material von Mises; Drucker, Prager											0
5.0 HYPOTHETICAL REPOSITORY DESIGN PROBLEMS											
5.1 Hypothetical Very Near Field Problem					0						0
5.2 Hypothetical Near Field Problem											0
5.3 Hypothetical Far Field Problem										x	0
6.0 FIELD VALIDATION PROBLEMS											
6.1 Project Salt Vault-Thermomechanical Response Simulation Problem											0
6.3 In Situ Heater Test-Basalt Waste Isolation Project											0

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

- Problems completed
- Problems not yet attempted
- Problems attempted, difficulties encountered

PROBLEM 6.1 (PSV) FIELD VALUES

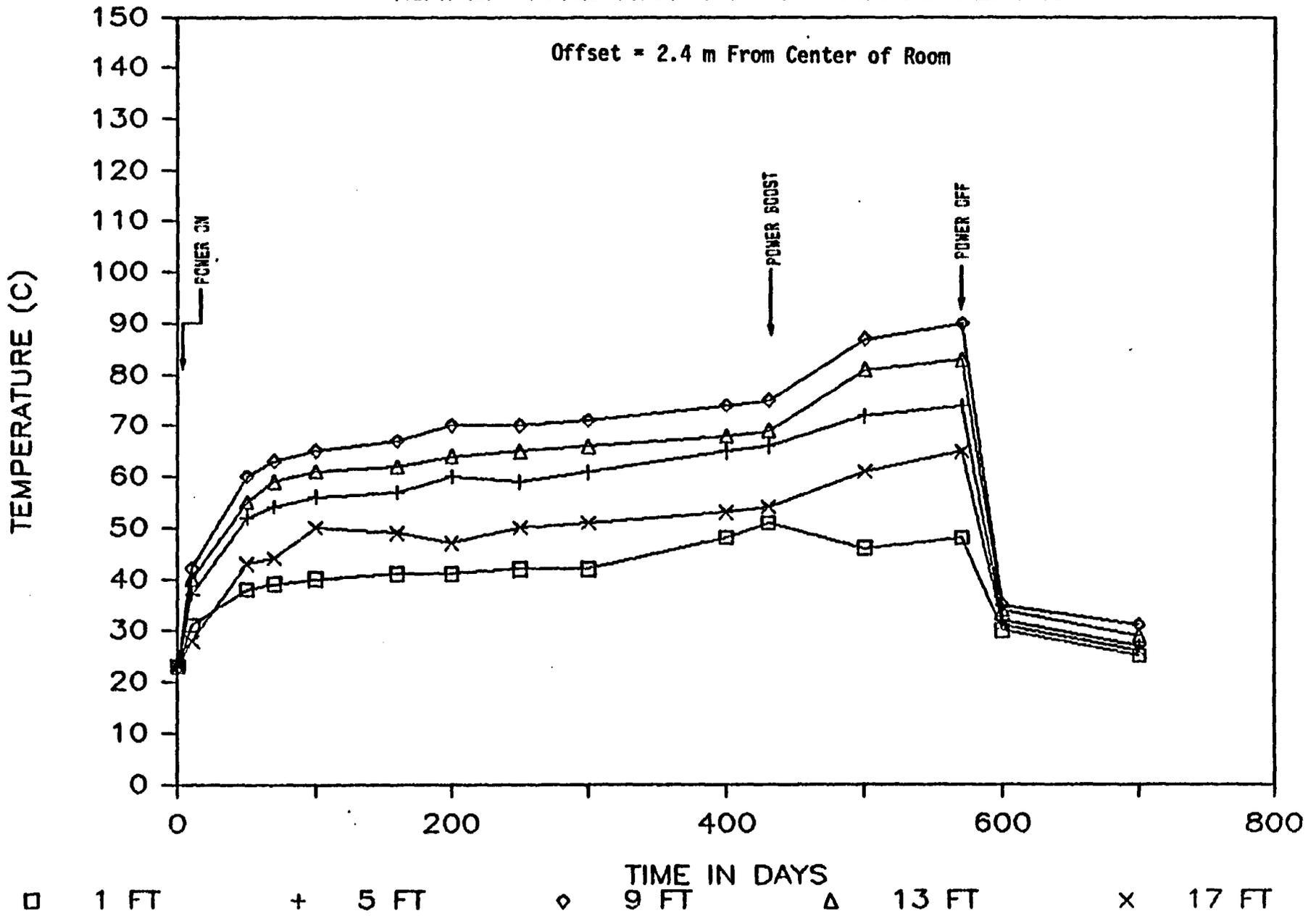
TEMPERATURE HISTORY AT VARIOUS OFFSETS



Problem 6.1A-Room 4
Temperature History at Various Offsets at Depth = 2.7m
Field Values

PROBLEM 6.1 (PSV) FIELD VALUES

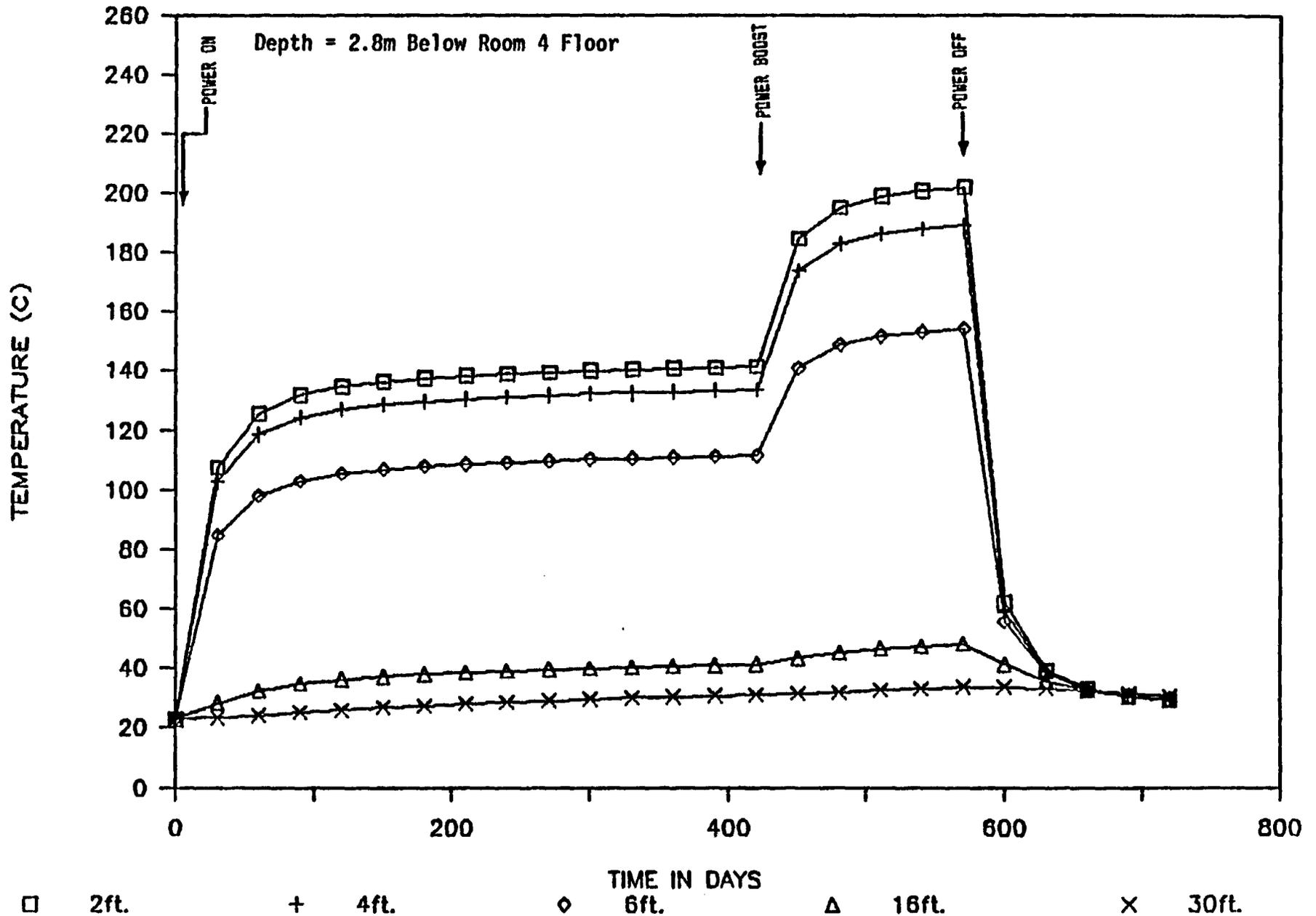
TEMPERATURE HISTORY AT VARIOUS DEPTHS



Problem 6.1A-Room 4
 Temperature History at Various Depths at Offset = 2.4m
 Field Values

ADINAT PROBLEM 6.1A - ROOM 4

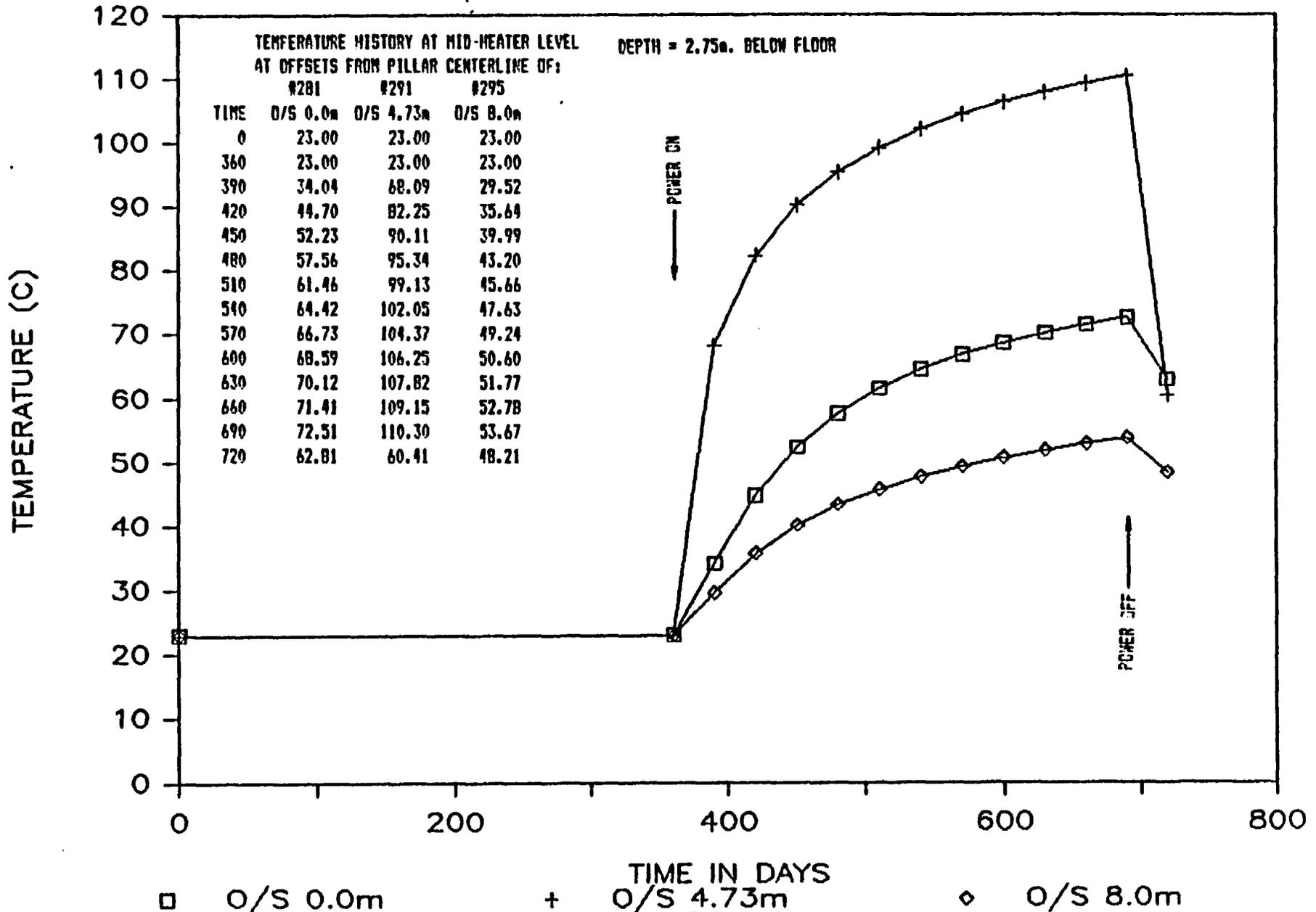
TEMPERATURE HISTORIES AT VARIOUS OFFSETS



Problem 6.1A-Room 4
Temperature History at Various Offsets at Depth = 2.8m
ADINAT Values

DOT PROBLEM 6.1P - ROOM 3

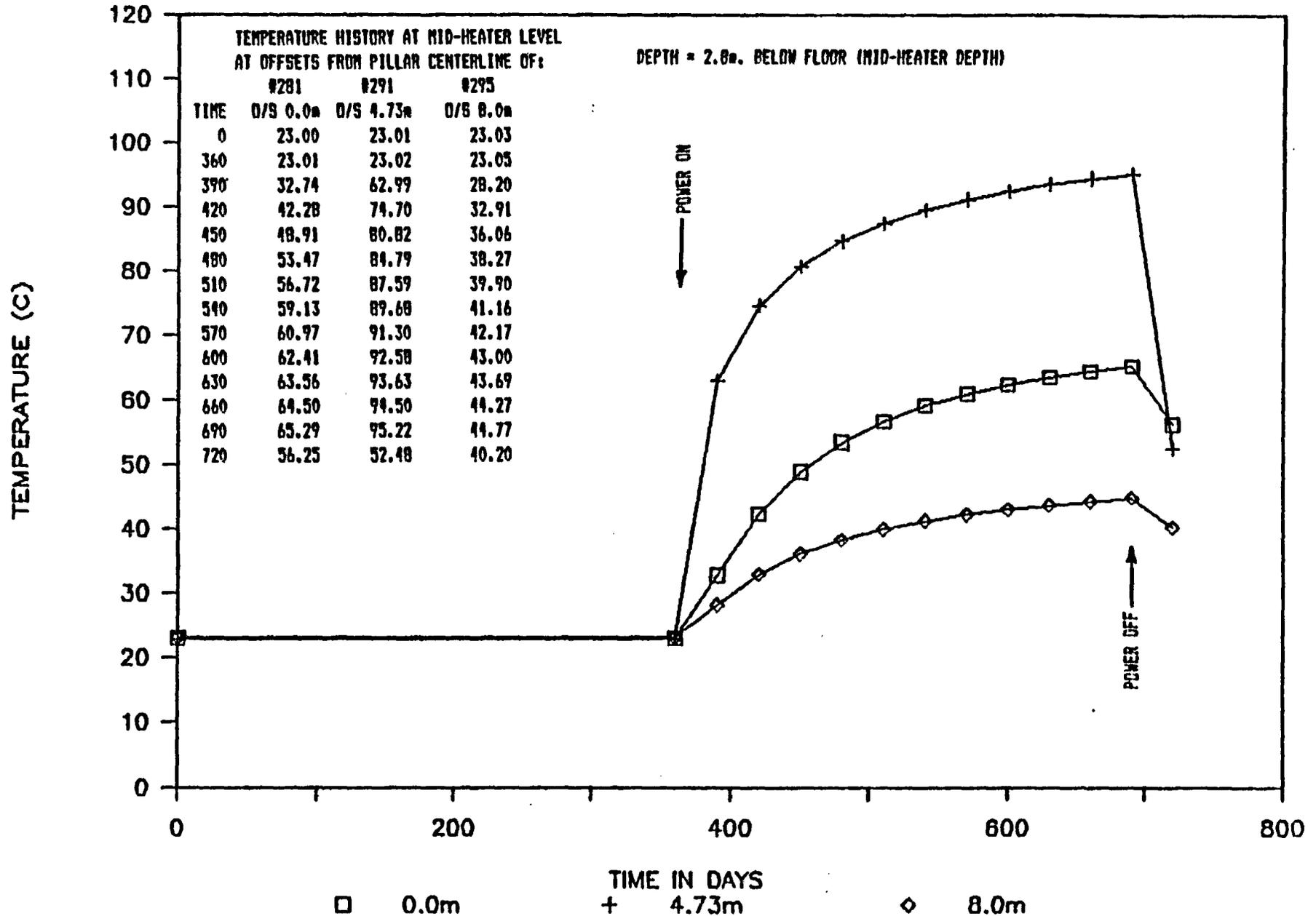
TEMPERATURE HISTORY @ MID-HEATER LEVEL



Problem 6.1P-Room 3
Temperature History at Various Offsets at Depths = 2.75m.
DOT Values

ADINAT - PROBLEM 6.1P - ROOM 3

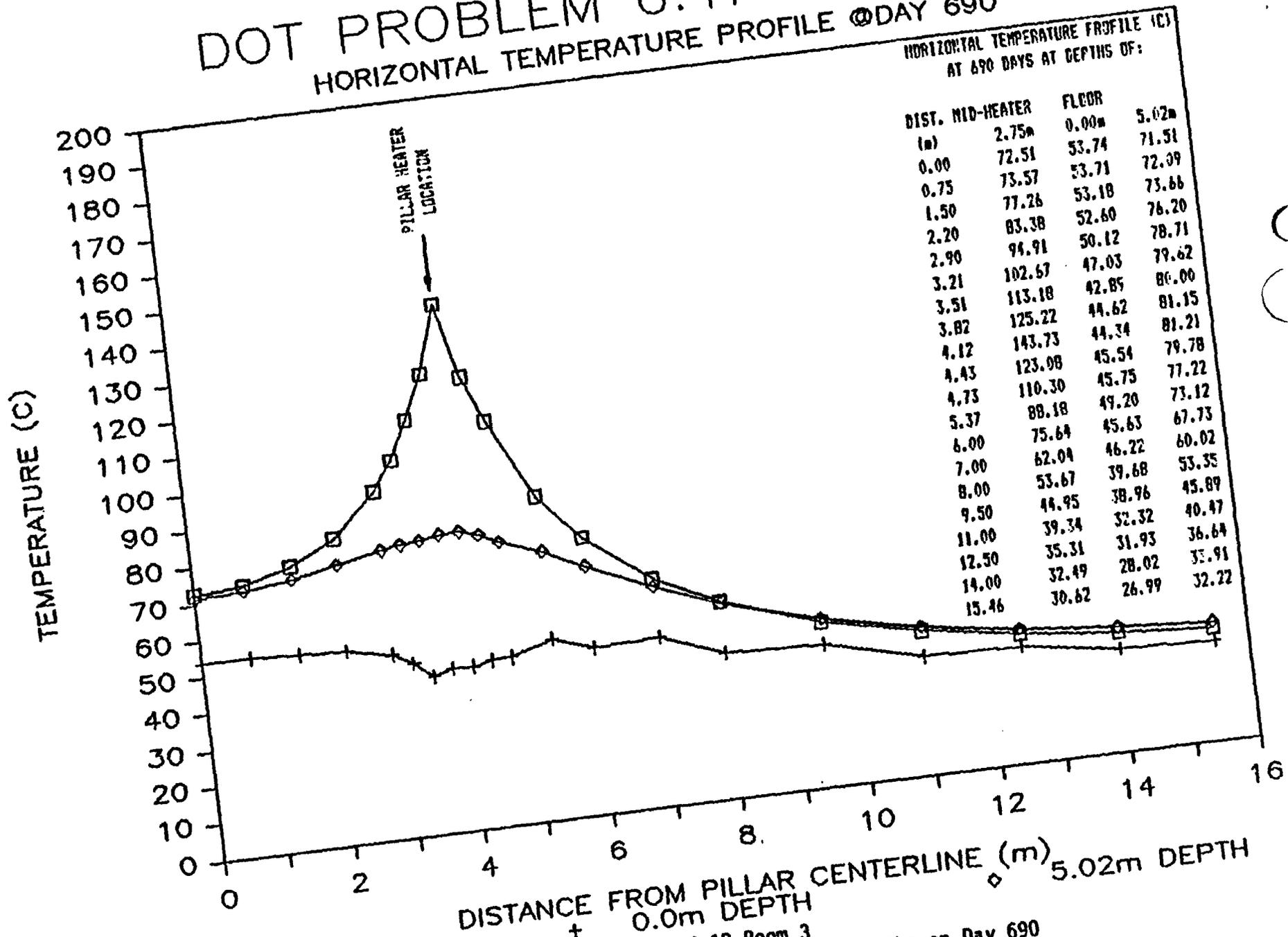
TEMPERATURE HISTORY AT VARIOUS OFFSETS



Problem 6.1P-Room 3
Temperature History at Various Offsets at Depth = 2.8m.
ADINAT Values

DOT PROBLEM 6.1P - ROOM 3

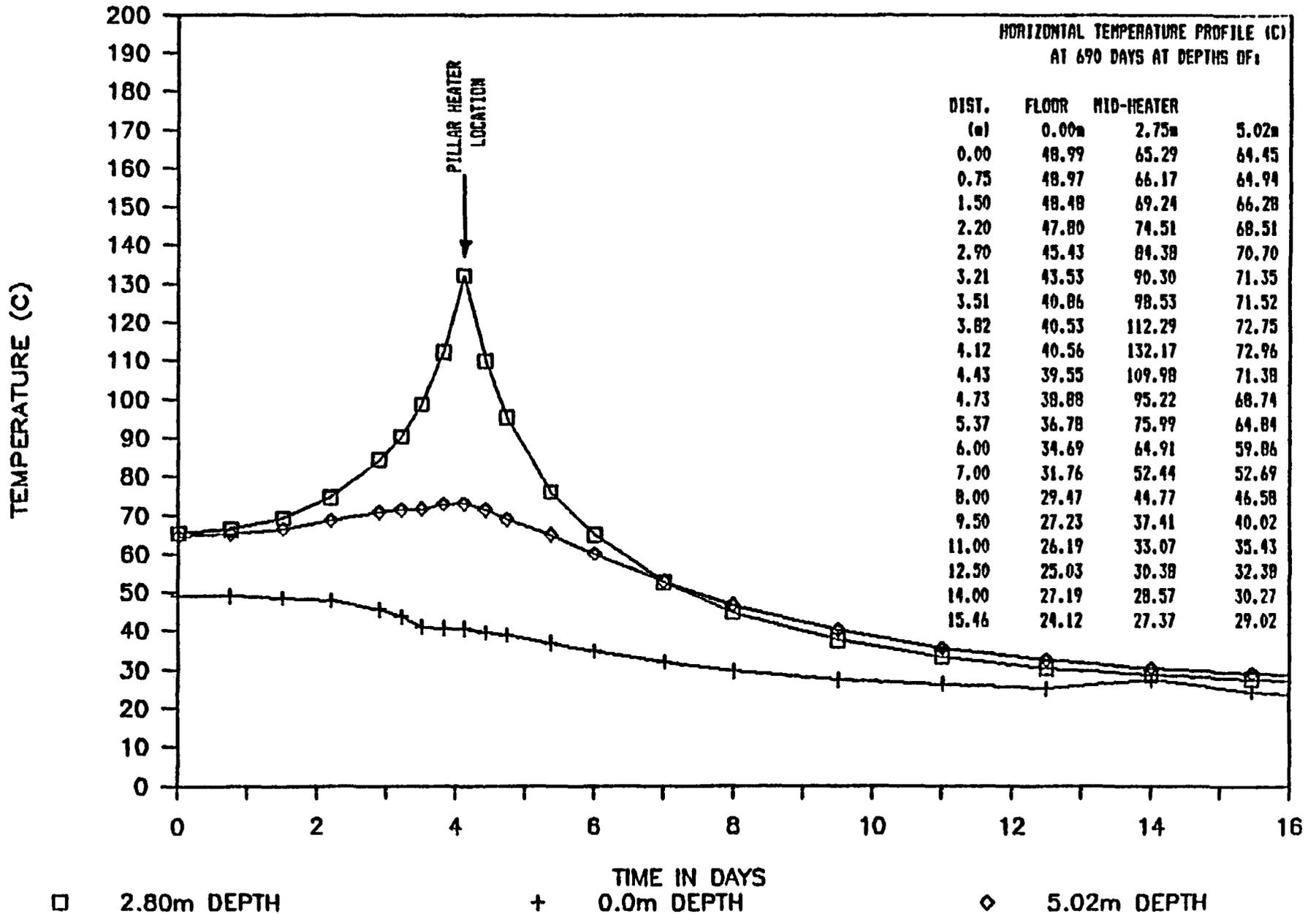
HORIZONTAL TEMPERATURE PROFILE @ DAY 690



□ 2.75m DEPTH
+ 0.0m DEPTH
◇ 5.02m DEPTH
 Problem 6.1P-Room 3
 Horizontal Temperature Profiles at Various Depths on Day 690
 DOT Values

ADINAT - PROBLEM 6.1P - ROOM 3

HORIZONTAL TEMPERATURE PROFILE @DAY 690



Problem 6.1P-Room 3
Horizontal Temperature Profiles at Various Depths on Day 690
ADINAT Values