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Distribution:

x P. Brooks

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(Return to WM, 623-SS)

January 13, 1986

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 December 1985

Dear Pauline:

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

Task 3 - Benchmark Problem Report - Waste Package Codes

By letter dated December 30, 1985, a final copy of the Benchmark Problem Report for the Waste Package Code was submitted. This report is a revision of the draft report submitted to the NRC in September 1984. It incorporates responses to comments from NRC and outside reviewers, with your approval, a camera ready copy of this report will be submitted for publication.

Tasks 4 & 5 - Siting Codes

On December 11, 1985, CorSTAR met with GeoTrans to discuss completion of work on Tasks 4 & 5 of the siting codes. We believe that agreement was reached on the scope of work for GeoTrans and additional funding requirements but as of the date of this progress report we have not received an acceptable proposal from GeoTrans for this effort. Continued delays will impact the schedule for delivery of computer codes to the NRC and may impact our estimated costs to complete the project. We will keep you informed of developments.

Tasks 4 & 5 - Radiological Assessment Codes

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

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B-6985 PDR

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#### Tasks 4 & 5 - Repository Design Codes

On December 10, 1985, Bill Swanson (Acres), Bill Lamb (Acres) and Doug Vogt (CorSTAR) met with the NRC staff in Silver Spring to review technical progress on this task area. During the technical review meeting we summarized work completed to date, problems encountered and work to be completed. Following this meeting, Acres and CorSTAR met with Pauline Brooks and Seth Coplan to discuss a revised schedule and cost estimate for this work.

On December 11, 1985, Bill Swanson attended an NRC training session covering aspects of the changeover from the CDC 6600 (MFA) to the Cyber 180/830 (MFC) at BNL. Based on the details of the session, it appears that the changeover will have little significant impact on the status of project if all goes as planned.

During December, a backup copy of the code COYOTE that was stored on the MFA system was located, moved to the MFZ system and successfully compiled. All files on the MFA system were successfully copied to the MFZ system. Problems were encountered while copying these files due to delays for archive retrievals of files that had not been accessed recently. As a result, copying files from MFA to MFZ has taken longer than originally anticipated. It is expected that copying files from MFZ to MFC will not present significant problems, since all the files on MFZ were stored recently.

Problem 2.9 was set-up and run with COYOTECDC, once the code was compiled and installed on the MFZ machine. The analytical solution was refined using the BASIC program supplied by CorSTAR, and the results of the COYOTE and previously run ADINAT codes were compared. Plots showing the temperature histories using COYOTE and the differences between the analytical and code-computer temperatures are included later in this report.

The analytical solutions for both parts of Problem 3.5, using the Von Mises and Drucker-Prager failure criteria have been determined. The problem has been set up and run with ADINA, but the results have not yet been analyzed.

#### Task 6 - Technology Transfer

During December CorSTAR started the development of a QA plan and procedures. The new QA plan and procedures are based on the concepts presented in the QA plan used for this project with changes to make them easier to implement. During December we also began a literature search to locate information on software QA and benchmarking activities practiced by other government and private sector organizations and to locate information on major software errors. Development of Technology Transfer information for the trial code, ORIGEN, continued in December.

General

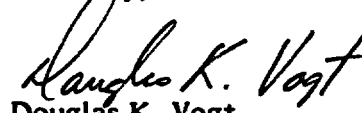
By letter dated December 12, 1985 CorSTAR notified the NRC that it had spent in excess of 75 percent of available funds. By letter dated December 31, 1985 CorSTAR provided the NRC with its current estimate of funds required to complete work on the project. Because of a number of uncertainties identified in our letter, CorSTAR will review the funds required to complete work again in 6 months. By letter dated December 27, 1985, CorSTAR submitted a letter proposal for completion of work on Tasks 4 & 5 of the repository design codes.

Our estimate of costs through the end of December (January 4, 1986 for Corstar) is:

Actual costs this month:	51K
Actual costs this fiscal year:	110K
Actual costs to date:	3,305K
Planned costs this fiscal year:	110K
Planned costs this month:	40K

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:kg

Enclosures

**TECHNICAL STATUS SUMMARY**

TECHNICAL STATUS REPORT ATTACHMENT  
TO PROGRESS REPORT FOR DECEMBER 1985

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 most 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 was required. Finally, 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 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

A progress meeting between the NRC, CorSTAR, and Acres, was held at the NRC offices in Silver Spring, MD on December 10, 1985. Acres was represented at this meeting by Bill Lamb and Bill Swanson. During the meeting, a presentation given by Bill Swanson summarized Acres current project status including work completed to date, problems encountered, and work to be completed. The current status of CorSTAR's work was summarized by Doug Vogt. Several representatives of the NRC staff attended the presentations. A secondary meeting followed, during which CorSTAR and Acres presented revised time and cost schedules to the NRC, and the factors which led to schedule delays and overruns were discussed.

The NRC held a training session at their offices in Bethesda, MD on December 11, which covered the aspects of the changeover from the MFA (CDC 6600) machine to the MFC (CYBER 180/83) machine at Brookhaven National Laboratories. It was revealed at this session that the MFA machine would be permanently removed from the Brookhaven system on January 10, 1986. Acres was represented at this session by Bill Swanson.

CODES

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.

2.0 THERMAL ANALYSIS CASE PROBLEMS

- 2.6 Transient Temperature Analysis of an Infinite Rectangular Bar With Anisotropic Conductivity (Schneider, 1955, pp. 261)
- 2.8 Transient Temperature Response to the Quench of an Infinite Slab With a Temperature-Dependent Convection Coefficient (Kreith, 1958, pp. 161)
- 2.9 Transient Temperature Response of a Slab Exposed to a Uniform Radiative Environment (Rohsenow and Hartnett, 1973, pp. 3-49)

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
- 3.3 Thick-Walled Cylinder Subjected to Internal and/or External Pressure
  - c) Plane strain - creep
- 3.5 Plane Strain Compression of an Elastic-Plastic Material von Mises; Drucker, Prager

5.0 HYPOTHETICAL REPOSITORY DESIGN PROBLEMS

- 5.1 Hypothetical Very Near Field Problem
- 5.2 Hypothetical Near Field Problem
- 5.3 Hypothetical Far Field Problem

6.0 FIELD VALIDATION PROBLEMS

- 6.1 Project Salt Vault-Thermomechanical Response Simulation Problem
- 6.3 In Situ Heater Test-Basalt Waste Isolation Project

	ADINA - 3D	ADINAT - 3D	DOT	HEATING	MATLOC	SPECTRUM 11	SPECTRUM 41	VISCOT	COYOTE	SALT 4	STEALTH
2.6		■		0				■			0
2.8		■		0				■			0
2.9		■		0				■			0
3.2 a)	■				■			■			0
3.2 b)	■							■			0
3.3 c)	▲							▲			0
5.1	●	●	■	0	■			▲	▲	▲	0
5.2	●	●	■		■			▲	▲	▲	0
5.3	●	●								▲	0
6.1	●	●	■					▲		■	0
6.3	▲	■	■		■			■			0

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

- Problems completed
- Problem not attempted
- ▲ Problems attempted, difficulties encountered

Due to the configuration of the Brookhaven system, and the order in which the MFC machine components will be added, it is necessary to transfer files from the MFA to the MFC via MFZ. With the exception of the time required to transfer files and possible access queues during the changeover period, it now appears that the change to the MFC machine will have little impact on the status of the project.

An unsuccessful attempt was made in November to access the COYOTECDC code on the MFZ machine. An archive retrieval was requested, but the file could not be found. During December, a backup copy of the code, which had been stored on the MFA machine, was loaded and compiled on MFZ.

Acres received a floppy disk from CorSTAR containing:

- i) A BASIC program which calculates temperatures on the radiative and insulated faces for Problem 2.9 more accurately than can be obtained using the charts in figure 2.9-2 of the Benchmark Manual (NUREG/CR-3636).
- ii) A FORTRAN subroutine to estimate surface temperatures during convection, to be used with COYOTE to re-run problems 2.6 and 2.8.
- iii) A LOTUS-123 spreadsheet which contains the analytical solutions for the Von Mises and Drucker-Prager criteria for Problem 3.5. Acres encountered some errors in the spreadsheet and made the necessary corrections and modifications. The changes have been discussed with Doug Vogt and a copy of the revised spreadsheet will be sent to CorSTAR.

All files contained on the MFA machine have been successfully copied to the MFZ machine. Several problems were encountered while copying these files, mainly related to delays due to archival retrievals of files that have not been accessed for quite some time. As a result, copying files from MFA to MFZ has taken longer than originally anticipated. It is expected that copying files from MFZ to MFC will not present any problem, since all the files on MFZ were recently stored.

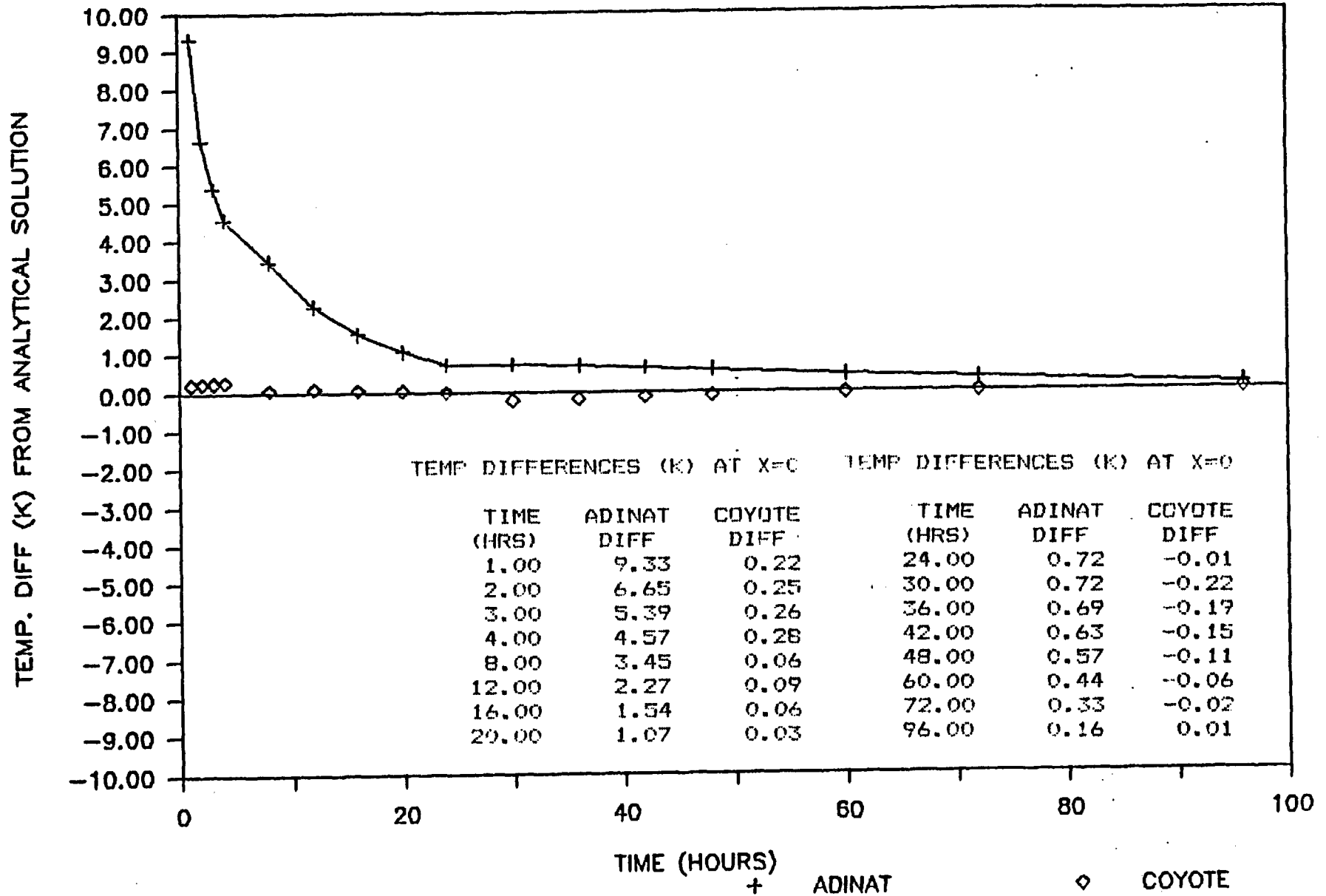
#### Run Benchmark Problems

Problem 2.9 was set-up and run with COYOTECDC, after the code was compiled and installed on the MFZ machine. The analytical solution was refined using a BASIC program supplied by CorSTAR, and the results of the COYOTE and previously run ADINAT codes were compared. Plots showing the temperature histories from COYOTE and the differences between the analytical and code-computed temperatures are included later in this report.

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# PROBLEM 2.9 - COMPARISON OF CODES

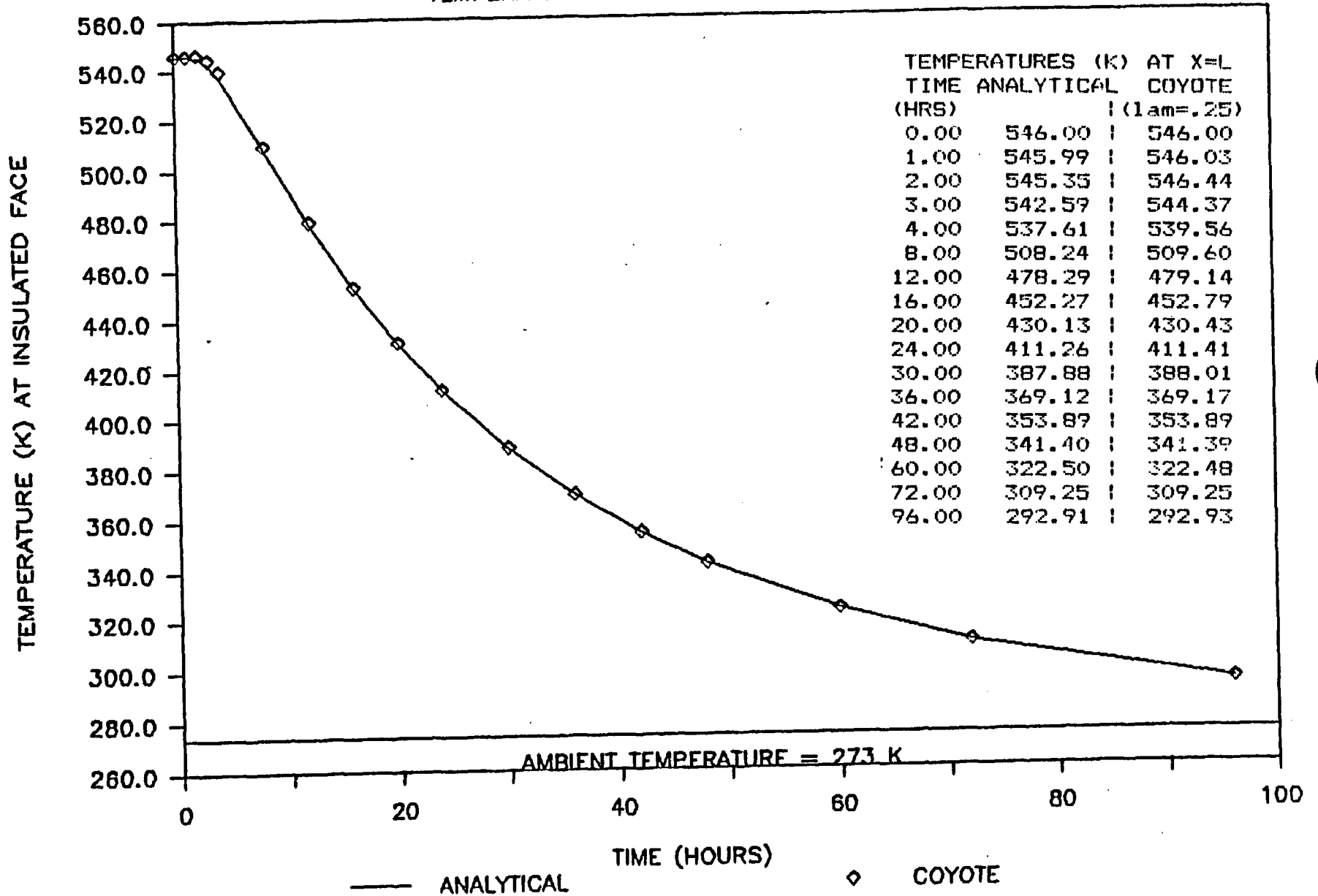
TEMPERATURE ERRORS AT RADIATIVE FACE





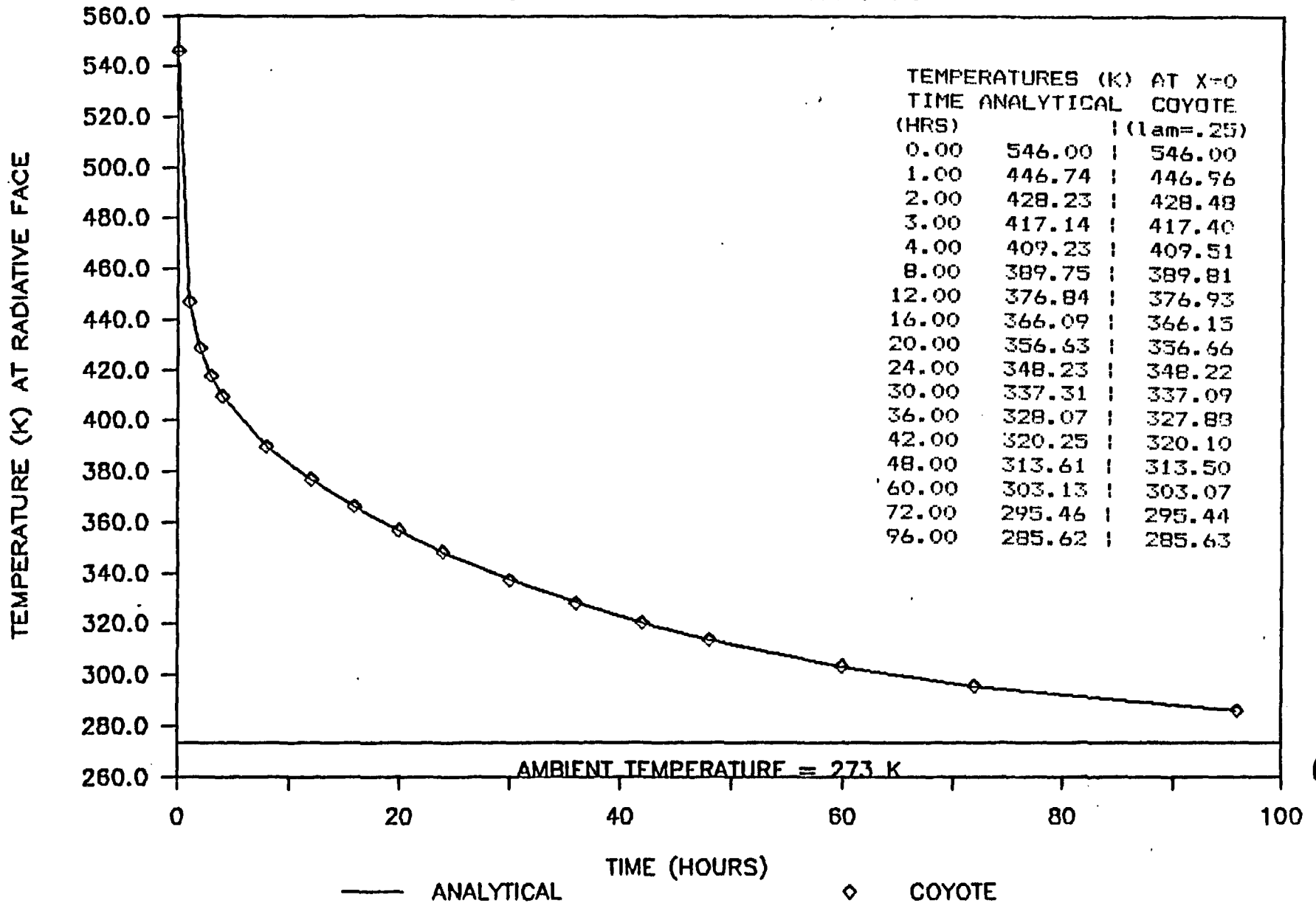
# PROBLEM 2.9 - COYOTE

TEMPERATURE HISTORY AT INSULATED FACE



# PROBLEM 2.9 - COYOTE

TEMPERATURE HISTORY AT RADIATIVE FACE



# PROBLEM 2.9 - COMPARISON OF CODES

TEMPERATURE ERRORS AT INSULATED FACE

