CorSTAR

A TEKNEKRON INDUSTRIES AFFILIATE

September 20, 1984

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 August 1984

Dear Pauline:

This letter contains a management level summary of progress during the month of August. 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

By letter dated September 17, 1984, copies of the final data set report for the waste package codes were submitted. We apologize for the delay in submitting this report. It was caused by production problems and the time required to obtain permission to use all tables and figures. We have not as yet obtained permission for all tables and figures. The copy that we have transmitted to you should be considered an interim copy. Final copy and master for publication will be submitted once permission for use of all tables and figures has been obtained.

Task 3 - Benchmark Problem Report - Waste Package Codes

Because of concerns raised by the NRC during August, the draft waste package code benchmark problem report was edited and proofed. The report will be submitted to the NRC during September.

Tasks 4&5 - Siting Codes

In early September, we met with the NRC to review proposed changes to the benchmark analysis report. The results of the meeting with the NRC and a similar meeting with GeoTrans are documented in a memo enclosed with the technical status summary.

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Tasks 4&5 - Radiological Assessment Codes

During August effort concentrated on delivering and submitting ORIGEN runs at ORNL. By the end of August, approximately one-half of the ORIGEN runs were successfully completed. The remaining runs will be completed during September. During September we will begin writing the benchmark analysis report for the radiological assessment codes.

Tasks 4&5 - Repository Design Codes

During August, a CDC version of the code COYOTE was installed at the Brookhaven computer. Benchmark problems 2.6, 2.8 and 5.2 were successfully run using the code COYOTE. Preliminary results of these runs are contained in the technical status summary report.

General

The following items that were identified in the July monthly progress report have the potential to impact project schedule or budget. Their status is updated below:

- We have met with the NRC to review an approach for responding to comments on the Task 4&5 report for the siting codes. The results of that meeting are summarized in the technical status summary.

- Two options are being considered for using the codes ADINA and ADINAT. These are:

  - Using the code of the service bureaus
  - Using the code at Sandia National Laboratory

  By letter dated August 30, 1984 the NRC stated that it would make a decision on where to run the ADINA and ADINAT codes by the week of September 3, 1984.
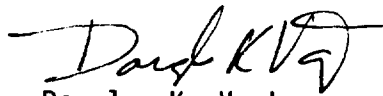
- Our recommendations on the benchmarking of the SPECTROM codes is included in the discussion of Tasks 4&5 of the repository design codes in the technical status summary.

- We understand that the NRC will obtain a charge number for use of the code STEALTH at the INEL computer facility by the end of September.

Our estimate of costs through the end of August (through August 19 for CorSTAR) is:

Actual costs this month:	47.5K
Actual costs this fiscal year:	719.5K
Actual costs to date:	2717.5K
Planned costs this month:	59K
Planned costs this fiscal year:	825K

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,

Douglas K. Vogt
Project Manager

cc: D. Fehringer

TECHNICAL STATUS SUMMARY

Technical Status - Tasks 4&5 - Radiological Assessment Codes

During the reporting period, we continued to document the results of the Radiological Assessment Code benchmarking effort. In addition to a comparison of code outputs, we are also providing an extensive evaluation of the codes with respect to their ease of use for high level waste assessment. From the point of view of eventual NRC users of the codes, we feel that this aspect of the report will be most helpful. For most of the codes, the greatest amount of effort was spent not in getting the code to run and analyzing the results, but in constructing the benchmark problem input files according to the requirements of the individual codes. The assumptions and compromises that were made during this input data file preparation are being thoroughly documented in the report. So far the most important conclusion of the benchmarking study is that, for the environmental transport and dose-to-man calculations, it is often easier to develop a special purpose code for the problem at hand rather than spend time trying to use a more general purpose code which is not well suited to the problem.

MEMORANDUM

TO: Peter Huyakorn, GeoTrans, Inc.   DATE: Sept. 13, 1984

FROM: Michael Mills

SUBJECT: Modifications to "Benchmarking of Flow and Transport
         Codes for Licensing Assistance" and "Revised Benchmark
         Problems for Repository Siting Models"

On Tuesday, September 11, Doug Vogt and I met with Peter Huyakorn and Dave
Ward at GeoTrans to discuss the QA and NRC comments concerning the two
reports referenced above. On the following day Doug Vogt and I met with Pauline
Brooks, Dick Codell, Jim McCartin and Mark Logson at NRC to discuss the
comments further. Based on these discussions the following conclusions were
reached regarding the modifications to the reports:

(1) The basic organization of the reports will not be changed.

(2) No additional codes or problems would be included in the study.

(3) Wherever appropriate, GeoTrans will provide more details concerning
    code input and output so as to facilitate a comparison of code
    results for a given problem and allow others to duplicate code runs.

(4) GeoTrans will prepare a new report section which
    summarizes the major findings of the study and shows
    the code comparisons which support these findings.

(5) GeoTrans will remove from the report any bias for or against
    particular codes and will make clear to the reader any "tricks"
    or special procedures that were invoked to solve the problems.

(6) GeoTrans will respond in writing to the questions and comments
    of the reviewers and make the appropriate changes to the reports.

(7) GeoTrans will standardize report notation, provide a discussion of
    general QA procedures and indicate which version of each code
    was used in the study.

(8) NRC will provide GeoTrans with more detailed outut to allow a
    better comparison with INTRACOIN results.

(9) CorSTAR will be responsible for integrating the CCC code results
    into the benchmarking report.

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(10) CorSTAR will be responsible for the technical editing of the two
    reports.

As we discussed, the NRC is preparing a contract modification to cover these
changes. We would appreciate your initial estimate of the cost for this effort by
September 21, 1984. This cost estimate should also include the additional funds
required to furnish NRC with magnetic tapes containing the codes and benchmark
problems as required by the contract. A more detailed cost proposal will be
required later.

ACRES

Mr. Douglas K. Vogt
Vice President
CorSTAR
7315 Wisconsin, North Tower 702
Bethesda, MD 20814

Dear Doug: Contract No. NRC-02-81-026
                                    Benchmarking of Computer Codes
                                    SPECTROM Codes

We received the list of codes that may be used in NNWSI performance assess-
ment. Among the codes are three applicable to repository design; COYOTE
(which we are currently benchmarking), JAC2D and SPECTROM. As discussed
previously, the SPECTROM-11 code which we had recommended for benchmarking
is not nor will it be available from ONWI.

Considering the widespread use of the SPECTROM codes, both by ONWI and
other DOE contractors, at least one thermal and geomechanical SPECTROM
code should be tested. At this time, we suggest the following course of
action:

1. Request formally through proper NRC-DOE-Sandia channels that documen-
    tation and the source code for the SPECTROM code(s) used at Sandia
    be provided for review and testing. It is noted that this·code is
    operational and therefore both documentation and the code should be
    available.

2. Obtain copies of SPECTROM-21 and SPECTROM-41 from ONWI when released
    (scheduled for September).

3. If documentation and the source code for an appropriate elastic-plastic
    code cannot be obtained from Sandia as requested in 1 above, the
    visco-elastic code SPECTROM-21 should be tested, together with the
    thermal code SPECTROM-41. This would result in both SPECTROM-21 and
    VISCOT being tested for visco-elastic problems and only ADINA (elastic-
    plastic) and MATLOC (bilinear) being tested for hard rock applications.
    To overcome this limitation in the testing program, VISCOT could be
    tested for elastic-plastic applications rather than visco-elastic
    applications.

Although the action outlined in 3 above may be the easiest solution
considering time constraints, we do not recommend its implementation
until all efforts to obtain the code to be used by NNWSI are exhausted.

If you have any questions, please call.

Yours very truly,

D. W. Lamb
Project Manager

RHC/jld

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TECHNICAL STATUS REPORT
ATTACHMENT TO PROGRESS REPORT FOR AUGUST

Repository Design Codes

Task 4 - Solve Benchmark Problems

Code Procurement

An earlier version (version 1.007) of COYOTE which was written specially
for CDC machines was obtained from Sandia. This was necessary due to
problems encountered in installing and running the more recent CRAY
version 1.10. Reasons for the necessity of using this version follow
under code installation.

Several discussions have been held relative to ADINA/ADINAT. Options
which the NRC are pursuing include:

- running the problems on an outside service bureau,
- running the problems at a national laboratory

                    or

- purchasing the code and installing at Brookhaven.

Access to these codes is required by the end of September to prevent a
delay in schedule.

A letter outlining our recommendations related to the SPECTROM codes was
prepared.

Code Installation

The installation of COYOTE has been a major problem. Originally
version 1.1 was obtained from Sandia. Before a successful compilation,
the following changes were made:

- The program structure was modified using overlays due to the small core memory limitation on the CDC machine;

- Large arrays were stored in large core memory with the necessary programming changes;

- Subroutine calls to plot data were eliminated since several of the required system subroutines were not available; and

- The number of bits per character had to be changed for compatibility with CDC.

With these changes, difficulties were still encountered in running the code. For this reason, Sandia was contacted and an earlier version written specifically for a CDC was obtained. This version (1.007, referred to as COYOTECDC) was successfully compiled and has been used for the execution of several problems this month. The author of COYOTE indicates that there are no major differences between the versions other than the size problems which can be handled.
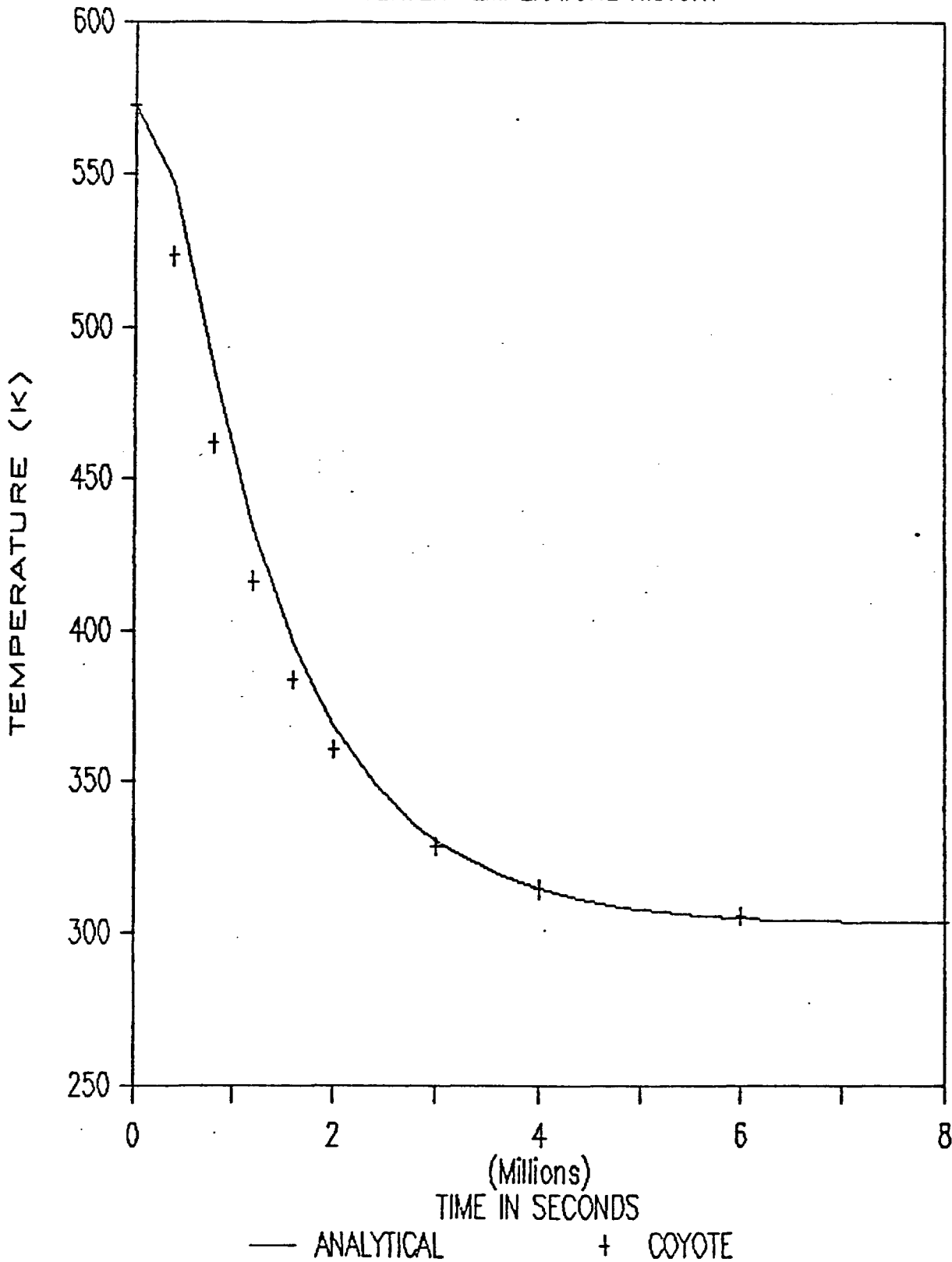
Run Benchmark Problems

Problems 2.6, 2.8 and 5.2 were run using COYOTECDC. Attached are figures showing a comparison of COYOTECDC results with the analytical solution for problem 2.6. Also are temperature vs. time curves for COYOTECDC and DOT results of problem 5.2 with salt and basalt repository materials, respectively.
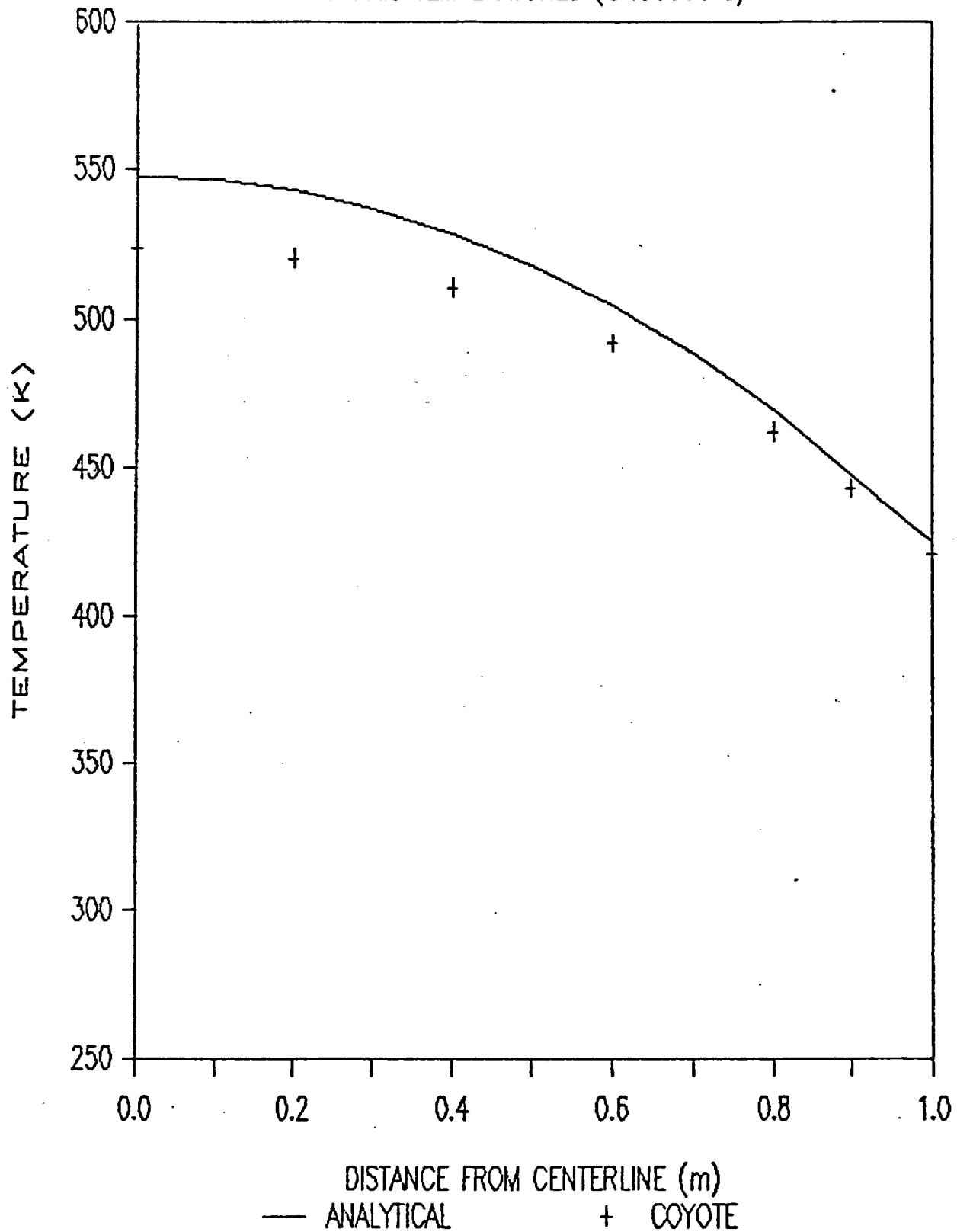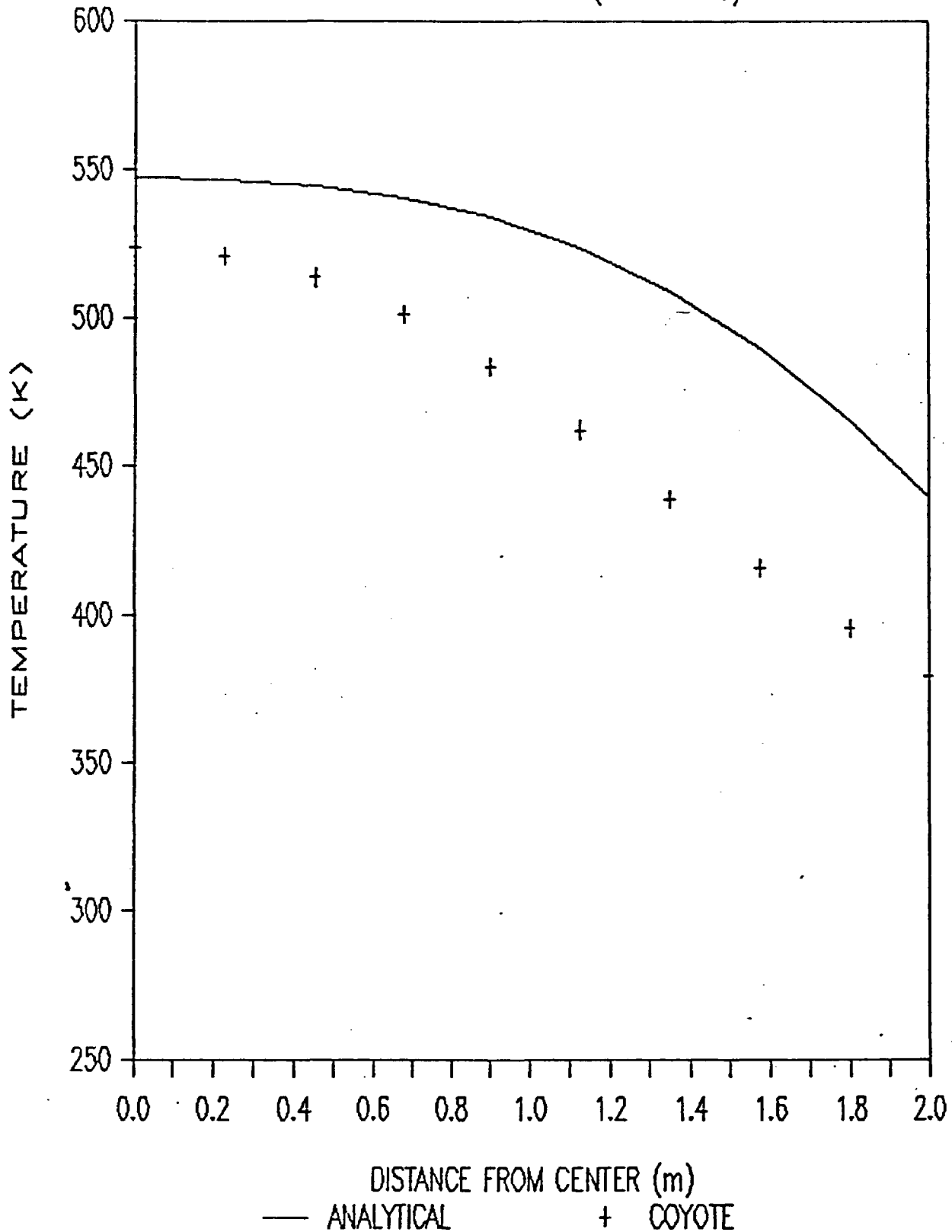
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COYOTE PROBLEM 2.6

CENTER TEMPERATURE HISTORY

COYOTE PROBLEM 2.6

Y-AXIS TEMPERATURES (@400000 s)

DISTANCE FROM CENTERLINE (m)

— ANALYTICAL   +   COYOTE

COYOTE PROBLEM 2.6

X-AXIS TEMPERATURES (@400000 s)

TEMPERATURE (K)

DISTANCE FROM CENTER (m)

—— ANALYTICAL   +   COYOTE

COYOTE PROBLEM 5.2–SALT

TEMPERATURE HISTORY

Chart: TEMPERATURE (C) vs TIME IN YEARS

□ MID–WALL   + MID–HEATER O/S 2.5m
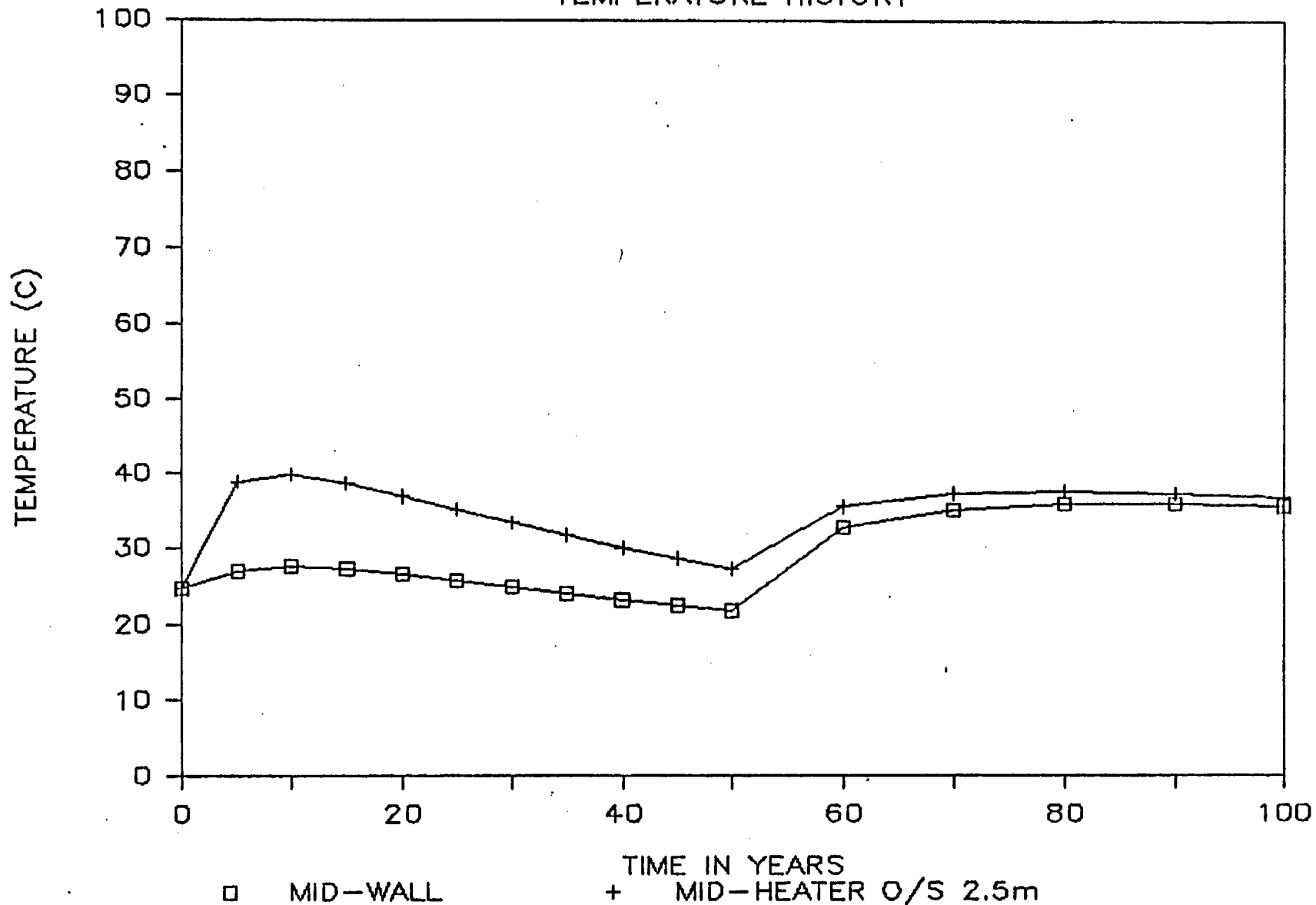
DOT PROBLEM 5.2—BASALT

TEMPERATURE HISTORY

MID—WALL   MID—HEATER O/S 2.5M