CorSTAR

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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 July 1985

Dear Pauline:

This letter contains a management level summary of progress during the month of July. Attached to the report is a Technical Status Summary including further discussion of work performed during the period. Detailed Cost Summary Reports will not be available until CorSTAR completes a changeover in accounting system computers.

Task 3 - Benchmark Problem Report - Waste Package Codes

We are awaiting the receipt of the NRC's comments on this report.

WM DOCKET CONTROL CENTER
'85 SEP -9 A11:50

Tasks 4 & 5 - Siting Codes

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

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 July, the ADINAT code was compiled and used successfully to run sample problems supplied by ADINA Engineering. The ADINA-PLOT program was also compiled. However, no sample problems exist that would test its use. Compilation of the ADINA-IN code was attempted. However, due to FORTRAN errors debugging will be required if the code is to be used. Compilation of the ADINA code was attempted. However, due to the number of lines of FORTRAN this attempt was unsuccessful. We are trying another job stream that should result in ADINA being successfully compiled soon.

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In July, the NRC informed us that Brookhaven is phasing out both of its CDC 6600 machines. One has already been removed while the other is to be removed possibly by the end 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 should have little immediate impact on our work other than some accessing difficulties due to system congestion. However, it is recommended that we finish our current computer involvement with Brookhaven prior to the removal of the last CDC 6600 machine. Otherwise, schedule and cost changes may result.

During the month, Problem 2.6 was run using ADINAT. Results comparing the ADINAT and analytical solutions have been summarized and are included at the end of the report. Additionally, Problem 2.8 has been set up for use with ADINAT. However, this problem has not yet been run successfully. Problems 5.2 (Salt) and 5.3 (Salt) have both been run with SALT 4. Results for these problems, however, has not yet been reduced.

During July, the one-dimensional version of STEALTH was modified to incorporate temperature-dependent heat transfer boundary conditions. The modified code was used successfully to analyze benchmark problem 2.6. Preliminary results from this benchmark problem are presented in the technical status summary report. Problems 3.2 and 3.5 have been attempted unsuccessfully with STEALTH. These problems test static mechanical response analysis capabilities. The mathematical formulation of STEALTH is implicity dynamic. We have not yet been able to determine why correct solutions to these problems can't be obtained.

All of the STEALTH benchmark problems will require the development and testing of special user-supplied subroutines to model phenomena not addressed using the existing STEALTH code. These modifications will require more time than estimated in our proposal for this work. We will meet with you to discuss this in September.

The lengthly delay caused by the unavailability of the ADINA, ADINAT, and STEALTH codes have caused us to fall well behind schedule in meeting the proposed Draft Task Summary Report deadline date of March 15, 1985. Estimates of anticipated schedule and possible cost overrun will be reported when the problems with the programs have been resolved.

General

By letter dated June 25, CorSTAR submitted technical proposals for Optional Tasks 4 & 5 of the Waste Package Codes and Otional Task 6 — Technology Transfer. We understand that the proposals were technically acceptable and that they have been forwarded to the Division of Contracts.

We are changing accounting system computers. Cost information for this month will be provided when the new accounting computer system is available.

Sincerely,

Douglas K. Vogt

Douglas K. Vogt
Project Manager

TECHNICAL STATUS SUMMARY

TECHNICAL STATUS REPORT ATTACHMENT
TO PROGRESS REPORT FOR JULY 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 system used at Brookhaven and not necessarily due to computer code errors, further debugging is required. Compilation of the ADINA code was also attempted. However, because of the large size of this code, the initial attempt was unsuccessful. Other measures are currently being taken that should soon result in ADINA being successfully compiled.

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 phone conversation on July 29, 1985, John Voglewede of the NRC informed us that Brookhaven is phasing out both of its CDC 6600 machines. One has already been removed while the other is to be removed possibly by the end 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 effect on our work. However, accessing difficulties, as a result of system congestion, has already been experienced. Additionally, it is recommended that we finish our current computer involvement with Brookhaven prior to the removal of the last CDC 6600 machine. Otherwise, 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 2.6 was run using ADINAT. Results comparing the ADINAT and analytical solutions have been summarized and are included at the end of this report. Two ADINAT runs were made using time step increments of 100,000 sec. and 10,000 sec. As expected, while both ADINAT runs show good agreement with analytical results, the 10,000 sec. time increment run compared much better to the analytical solution than did the 100,000 sec. time increment run. However, the 10,000 sec. time increment run required many more iterations to complete the analysis and as a result, was more expensive to run.

Problem 2.8 has also been set up for use with ADINAT. However, this problem has not yet been run successfully.

Finally, Problems 5.2 (Salt) and 5.3 (Salt) have both been run with SALT 4. While both these problems have run successfully, the required output specification for each problem has not yet been determined.

Attachments

JAB:sd
8/7/85
P6678.250

PROJECT STATUS

TABLE 3

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

Legend:

x Benchmark Problems by Acres.
O 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)		(3)	x	0					x		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)		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					[illegible]						
b) Unlined in plastic medium (Tresca) von Mises	(2)							[illegible]			0
3.3 Thick-Walled Cylinder Subjected to Internal and/or External Pressure											
c) Plane strain - creep	(2)							[illegible]			
3.5 Plane Strain Compression of an Elastic-Plastic Material von Mises; Drucker, Prager	(2)							[illegible]			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 (3)		B [illegible]			S,B (4)	S x	S x	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)	x					[illegible]		x	0
6.3 In Situ Heater Test-Basalt Waste Isolation Project	(2)	(2)	(1)		x			x	x		0

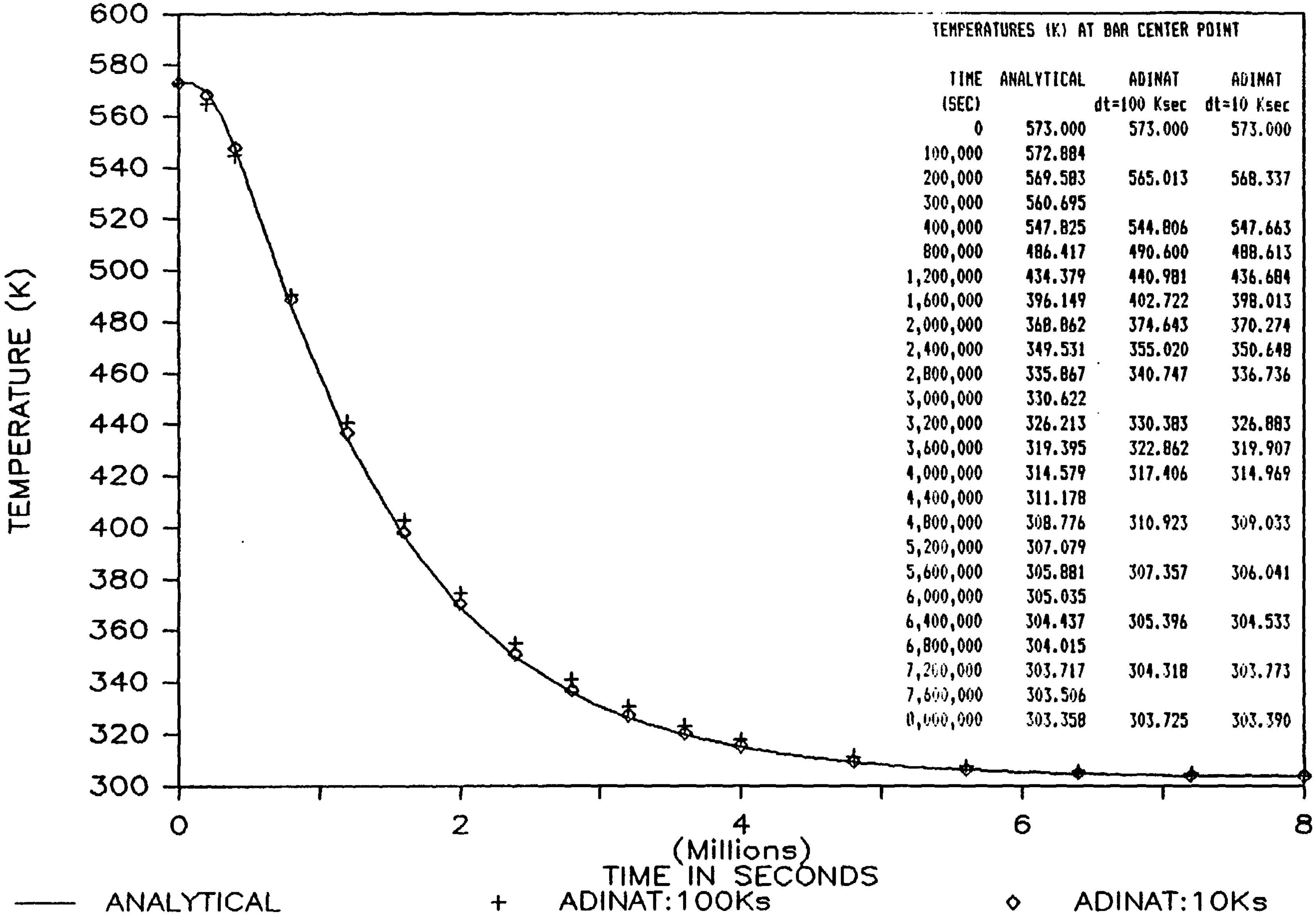
* From NUREG/CR-3636, Benchmark Problems for Repository Design Models, February 1984.

▢ Problems completed

◯ Problems attempted, results not analyzed

ADINAT PROBLEM 2.6

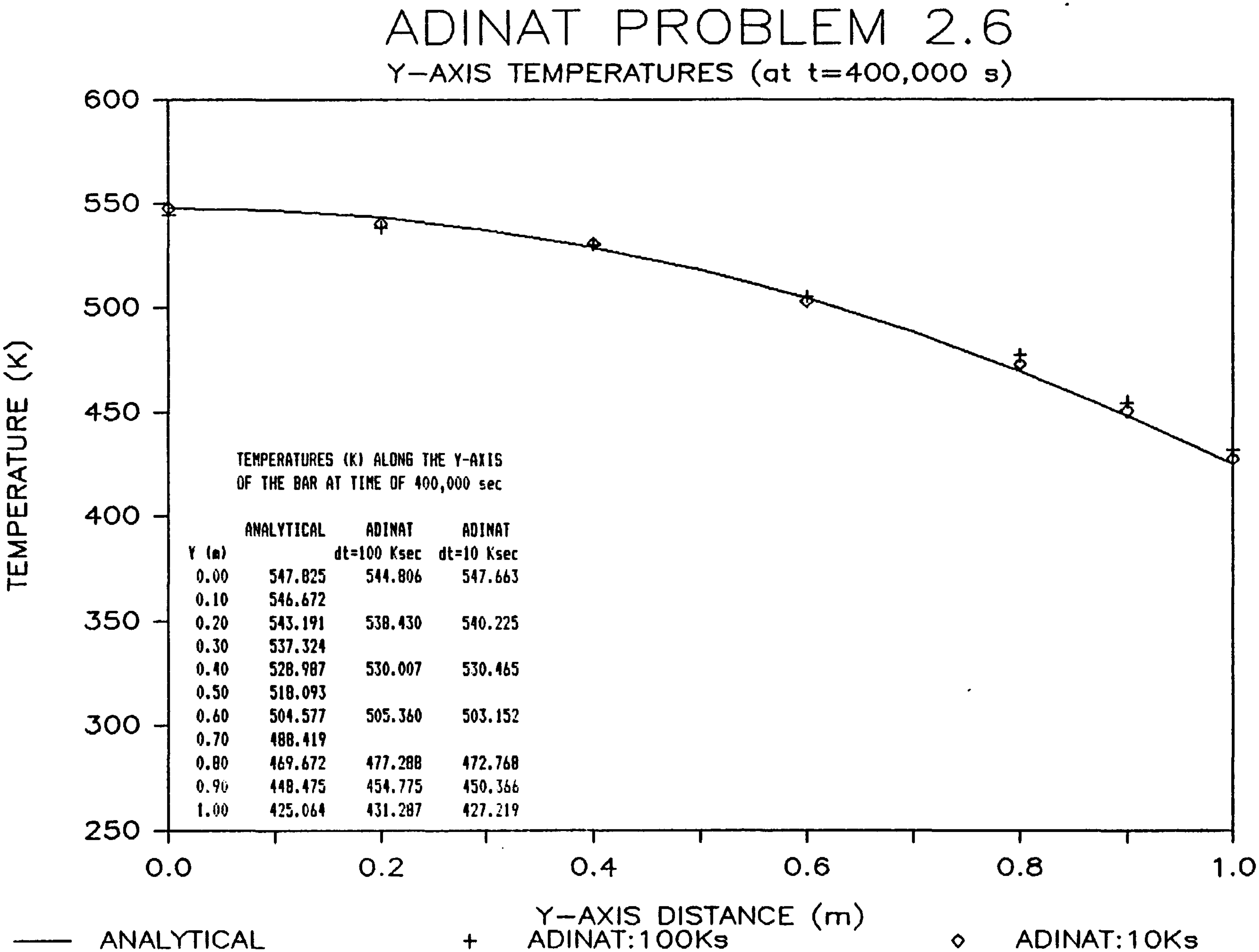
CENTER POINT TEMPERATURE HISTORY



TEMPERATURES (K) AT BAR CENTER POINT

TIME (SEC)	ANALYTICAL	ADINAT dt=100 Ksec	ADINAT dt=10 Ksec
0	573.000	573.000	573.000
100,000	572.884		
200,000	569.583	565.013	568.337
300,000	560.695		
400,000	547.825	544.806	547.663
800,000	486.417	490.600	488.613
1,200,000	434.379	440.981	436.684
1,600,000	396.149	402.722	398.013
2,000,000	368.862	374.643	370.274
2,400,000	349.531	355.020	350.648
2,800,000	335.867	340.747	336.736
3,000,000	330.622		
3,200,000	326.213	330.383	326.883
3,600,000	319.395	322.862	319.907
4,000,000	314.579	317.406	314.969
4,400,000	311.178		
4,800,000	308.776	310.923	309.033
5,200,000	307.079		
5,600,000	305.881	307.357	306.041
6,000,000	305.035		
6,400,000	304.437	305.396	304.533
6,800,000	304.015		
7,200,000	303.717	304.318	303.773
7,600,000	303.506		
8,000,000	303.358	303.725	303.390

ADINAT Problem 2.6
CENTER POINT TEMPERATURE HISTORY



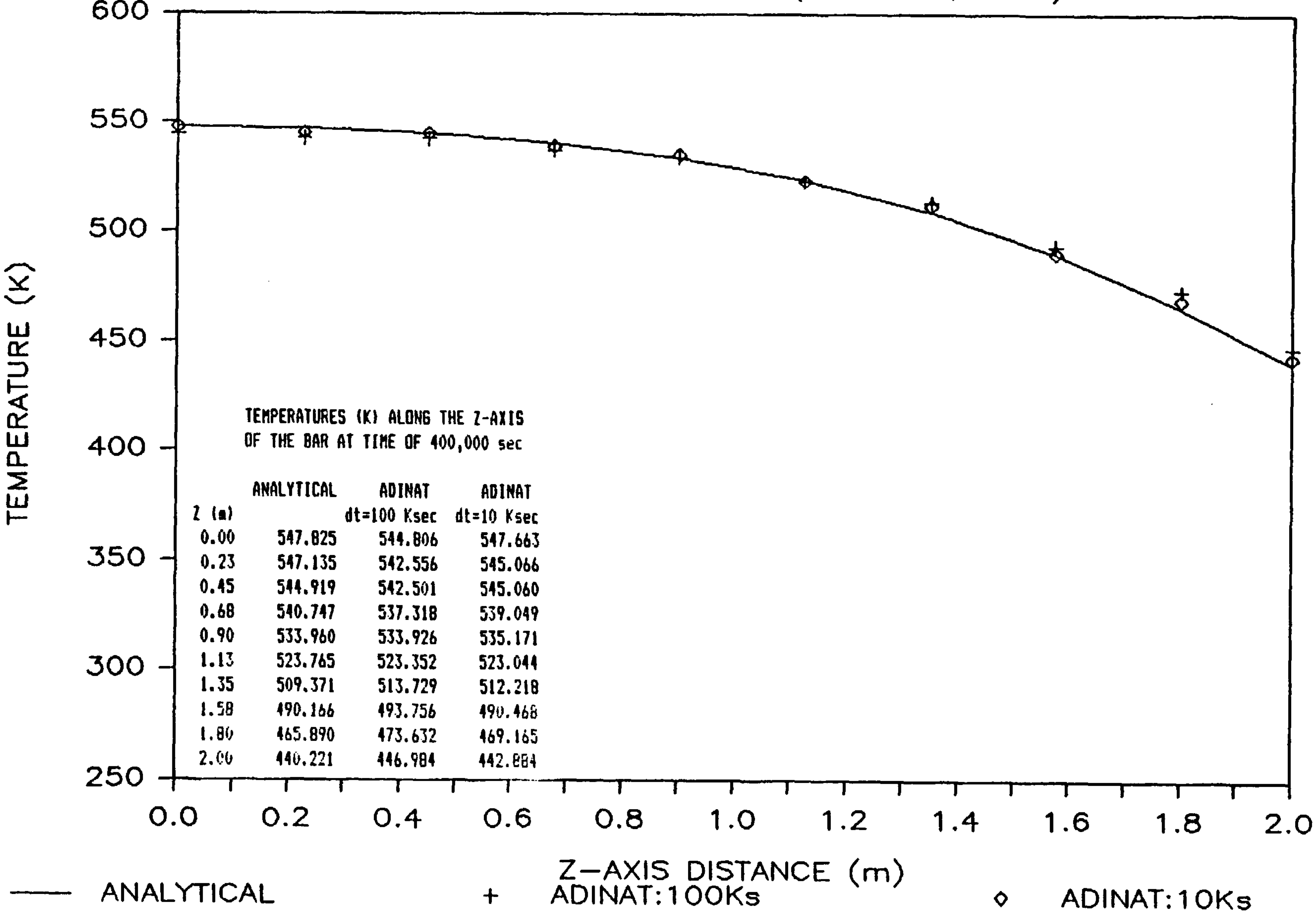
TEMPERATURES (K) ALONG THE Y-AXIS
OF THE BAR AT TIME OF 400,000 sec

Y (m)	ANALYTICAL	ADINAT dt=100 Ksec	ADINAT dt=10 Ksec
0.00	547.825	544.806	547.663
0.10	546.672		
0.20	543.191	538.430	540.225
0.30	537.324		
0.40	528.987	530.007	530.465
0.50	518.093		
0.60	504.577	505.360	503.152
0.70	488.419		
0.80	469.672	477.288	472.768
0.90	448.475	454.775	450.366
1.00	425.064	431.287	427.219

ADINAT PROBLEM 2.6
Y - Axis Temperature Distribution
at Time = 400,000 sec.

ADINAT PROBLEM 2.6

Z–AXIS TEMPERATURES (at t=400,000 s)



TEMPERATURES (K) ALONG THE Z-AXIS OF THE BAR AT TIME OF 400,000 sec

Z (m)	ANALYTICAL	ADINAT dt=100 Ksec	ADINAT dt=10 Ksec
0.00	547.825	544.806	547.663
0.23	547.135	542.556	545.066
0.45	544.919	542.501	545.060
0.68	540.747	537.318	539.049
0.90	533.960	533.926	535.171
1.13	523.765	523.352	523.044
1.35	509.371	513.729	512.218
1.58	490.166	493.756	490.468
1.80	465.890	473.632	469.165
2.00	440.221	446.984	442.884

ADINAT PROBLEM 2.6
Z - Axis Temperature Distribution
at Time = 400,000 sec

Problem 2.8 Transient Temperature Response to the Quench of an Infinite Slab with a Temperature-Dependent Convection Coefficient

Input Data

An infinite slab was modeled using a one-dimensional finite element grid. Input data for the problem was obtained from the benchmark problem report (3) and included the following code-specific data:

Mesh Geometry	
Slab thickness	0.203 m
Number of mesh points	11
Spacing between mesh points	0.0203 m

Run Problem

Solution of problem 2.6 required the development of a method to estimate the temperature of a grid point from the temperature of the neighboring zone.

STEALTH calcuates heat fluxes at grid points. Temperatures are calculated for material "zones" located between grid points. By assuming that temperature varies slowly with time ($\partial T/\partial t \ll 1$), a very good assumption for most repository-scale waste management thermal analyses, a heat flux balance can be performed at a boundary grid point.

The heat being conducted from the mid-point of a zone to the grid point is

$$Q = K \frac{(\theta_i - \theta_s)}{\Delta x/2}$$

Where:
- Q = Heat flux
- θ_i = Temperature at zone midpoint
- θ_s = Temperature at grid point (surface temperature)
- $\Delta x/2$ = Distance from zone midpoint to grid point

The heat being convected from the wall is

$$Q = h(\theta_s - \theta_b) \qquad (2)$$

where:
- h = surface heat transfer coefficient
- θ_b = Temperature of heat sink at boundary

Equating conduction and convection heat fluxes yields:

$$\frac{K\ (\theta_i - \theta_s)}{(\Delta x/2)} = h\ (\theta_s - \theta_b) \qquad (3)$$

Solving for Θ_s yields

$$\Theta_s = \frac{2K\ \Theta_i/\Delta x + h\ \Theta_b}{2K/\Delta x + h} \tag{4}$$

If h = $h(\Theta_s - \Theta_b)$ as in problem 2.8, equation (4) may be solved by iteration.

Assuming that $h = (A + B\,\Delta T)\ \Delta T^C$

where: $\Delta T = \Theta_s - \Theta_b$
A, B, C are constants

one can rewrite equation (4) in terms of ΔT as

$$T = \frac{2K/\Delta x \cdot (\Theta_i - \Theta_b)}{2K/\Delta x + (A + B\ \Delta T) \cdot \Delta T^C} \tag{5}$$

expanding equation (5) and setting it equal to 0, we have

$$(2K/\Delta x) \cdot \Delta T + A\Delta T^{C+1} + B\Delta T^{C+2} - (2K/\Delta x) \cdot (\Theta_i - \Theta_b) = 0 = f(\Delta T) \tag{6}$$

This equation can be differentiated to yield

$$F'(\Delta T) = (2K/\Delta x) + A(C+1)\ \Delta T^C + B(C+2)\ \Delta T^{C+1} \tag{7}$$

Equation (6) can be solved by Newton-Raphson iteration

$$\Delta T_{n+1} = \Delta T_n - \frac{f(\Delta T)}{f(\Delta T)}$$

Results

The results of the analysis are tabulated in Table 1. The STEALTH solution compares favorably with the solution presented in Krieth. The large temperature difference between the STEALTH prediction and Krieth's solution is due to the treatment of specific heat in the user-defined STEALTH model ($C\,\partial T/\partial t = 0$). This effect is only important at relatively short times. At a time of 2.3 hours into the transient, the STEALTH-predicted temperatire is within 2°c of that presented in Krieth.

Table 1. Problem 2.6 Results STEALTH vs. Krieth

Time (hours)	Temperature	
	STEALTH	Krieth
2.3	176.04	174
4.6	155.63	154
7.0	142.37	141