PROPOSAL FOR PERFORMANCE ASSESSMENT BENCHMARKING WASTE PACKAGE CODES

Submitted by:

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Submitted to:

U.S. Nuclear Regulatory Commission
Division of Contracts
Attn: Mr. Ron Coleman, AR-2223
Washington, D.C. 20555

June 25, 1985

RK-81-3009

CorSTAR

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1. Introduction

CorSTAR Research, Inc. is pleased to submit this proposal to the NRC for Tasks 4 and 5 under Contract No. NRC 02-81-026. This work involves the solution of benchmark problems and an analysis of results for waste package performance assessment computer codes. Our proposed approach to code benchmarking will be described in Section 2. The codes to be benchmarked and the associated benchmark problems will be identified in Section 3. The project schedule and list of deliverables will be given in Section 4 followed in Section 5 by the Cost Proposal. In this proposal, Task 4, "Solve Benchmark Problems," and Task 5, "Analyze and Describe Results," are not treated separately because the two tasks are interrelated and cannot be performed sequentially.

2. Technical Approach

CorSTAR will benchmark the following waste package performance assessment computer codes: ADINA, ADINAT, HEATING, COVE, WAPPA and ANISN. The necessary documentation for these codes is already in-house. With the exception of COVE, which will be run at the BNL computer facility, the codes are already available at Brookhaven National Laboratory or Oak Ridge National Laboratory. All computer runs will be performed at the Brookhaven National Laboratory Computer Center or ORNL under an NRC account.

CorSTAR will copy the source code onto a project tape and a listing of each code will be delivered to CorSTAR. It is anticipated that minor modifications will have to be made to some of the codes to allow successful compilation and running of the benchmark problems. CorSTAR will keep a detailed account in a log book of the problems encountered in the compilation of the computer codes. Modifications required for code compilations will be documented both externally and within the source code by use of the UPDATE facility. These modified source codes will be saved on the project tape. CorSTAR will responsible for

maintaining a log for the project source code tapes. When codes are modified, both the original and modified versions of the source code will be assigned unique identifiers.

Once all code compilations have been successfully carried out, the benchmark problem inputs will be coded, entered and verified. The codes will then be run using the appropriate benchmark problems. For those codes such as ADINA and ADINAT that can require relatively large amounts of computer time for simulation of a benchmark problem, the code will first be run for a relatively short time to ensure the code is working properly before the full simulation is attempted. The output of each successful benchmark problem run will be placed on the project tape. To minimize the time and resources associated with storage and editing of source codes and input data files on a large mainframe computer, a microcomputer will be used for this project. The microcomputer allows input and full screen editing of data as opposed to the use of more cumbersome line editors. Also, the response time for file editing on the microcomputer is much faster than is possible over a phone line to the mainframe computer.

During the running of the benchmark problems a number of difficulties could arise. These could range from relatively simple problems such as array dimensioning to more serious obstacles which could prevent the code from successfully running the benchmark problem without extensive code modifications. Problems which might be encountered include:

- Program READ and FORMAT statements not consistent with the user's manual input instructions
- Benchmark problem calculations which use faulty portions of the code which have not been previously tested (specific problems include dividing by zero, taking logarithm of a negative number, and exceeding array dimensions.)
- Benchmarking problem input coding errors due to misleading code documentation
- Improper choice of time steps
- Input values overridden by values "wired" into the code

CorSTAR will make minor modifications to the computer codes and input files so that the benchmark problems can be run successfully. These changes will be recorded both in the code log book and internally within the source code by means of the update facility. Our estimated level of effort is sufficient for minor code modifications. If code modifications requiring more than a few man-days of effort are required we will bring the problem to the attention of the NRC and outline the options available for dealing with it.

When all benchmark problems for a particular code have been run successfully, the final source code will be written to the project tape. The final version of a code will be capable of running all the benchmark problems associated with that code. If a code requires modification to run a particular benchmark problem, the modified code will be rerun for previous benchmark problems to ensure that the modification did not introduce any new problems in the code. After a particular benchmark problem has been run, the final input files will be written to a project tape. When this process has been completed for all of the benchmark problems, Teknekron will prepare an expanded version of the earlier "Benchmark Problem Report." In addition to the material contained in this earlier report, the expanded version will include the following additional items:

- All input data expressed both in tabular form and in the code input format
- An analysis of the benchmark problem results
- A listing of the final benchmark problem results on microfiche

CorSTAR will also prepare a letter report which will deal with each of the codes which were benchmarked. The report will follow the same outline as the earlier "Code Summary Report," but will contain more information regarding code operating characteristics, applicability and limitations.

3. Benchmarking Considerations for Individual Codes

A. ADINA

ADINA is a one-, two-, and three-dimensional finite element mechanical analysis computer code. ADINA is a tool suitable for engineering design analysis of radioactive waste package mechanical stresses and displacements. By using temperature profiles calculated by the code ADINAT, the code ADINA can be used to estimate thermally induced stresses. The code ADINA has been widely used for elastic and plastic analysis of static and dynamic structures. We believe that these features of the code have been well tested, though code errors may still remain.

One of the areas of concern in waste package performance assessment is the potential for creep of the waste package over long loading times. The high in situ pressures may also give rise to elastic or creep buckling of cylindrical waste packages. We do not know how well ADINA analyzes creep, elastic buckling or creep buckling. Benchmark problems to test these features of the code are included in this task.

B. ADINAT

ADINAT is a one-, two-, and three-dimensional finite element thermal analysis code. ADINAT can be used for engineering design analysis of the temperatures and heat fluxes in a radioactive waste package. The code is particularly well suited for analysis of conduction heat transfer. From the code documentation, apparent weaknesses include the analysis of convection and radiation heat transfer at points other than the finite element model boundary. It is not clear how well the code ADINAT handles problems in which a phase change will occur. In selecting benchmark problems for the code ADINAT, problems were selected that would test the potential weaknesses of the code.

C. HEATING

HEATING is a one-, two-, or three-dimensional finite difference thermal analysis code. HEATING can be used for engineering design analysis of waste package temperatures and heat fluxes. The code has been widely used for analysis of conduction heat transfer. Apparent weaknesses include the analysis of convection and radiation heat transfer at points other than model boundaries. We do not know how well the code HEATING handles problems dealing with phase change. The selection of benchmark problems for HEATING took into consideration these potential weaknesses.

D. COVE1

COVE1 is a special purpose creep buckling code. It is a one-dimensional finite difference computer program with the capability to estimate the deformation and time to geometric buckling for a finite length hollow tube experiencing creep. The code has not been widely used but appears to be a good tool to address the creep buckling phenomenon. The benchmark problem selected for this code were designed to provide a test of the code's ability to predict the time of onset of creep buckling.

E. WAPPA

WAPPA is a special purpose waste package performance assessment computer code. The code has submodels for thermal, mechanical, radiation, corrosion, and leaching phenomena. The code has not been widely used outside the waste management community. Based on our preliminary review of computer program documentation, a major weakness of the code appears to be the need for a large data base, some of which is empirical (particularly in the corrosion and leaching areas) and the use of fairly simple models for predicting the thermal and mechanical effects. Thermal and mechanical analysis benchmark problems were selected that will allow a comparison of predictions by the code WAPPA with predictions from the codes ADINA, ADINAT, HEATING, and ANISN.

F. ANISN

ANISN is a one-dimensional discrete ordinants transport theory radiation schielding code. The code has been widely used by the nuclear community over a period of some 15 years. However, we know of few test problems using measured data in conditions that are similar to those that would be expected in and around a high level radioactive waste package. In selecting benchmark problems for this code, problems dealing specifically with measured data for spent fuel assemblies and hypothetical waste package designs were included.

The benchmark problems recommended for each of the computer codes is summarized in Table 1.

4. Schedule and List of Deliverables

The list of project deliverables and due dates, assuming a August 15, 1985, start date, is given below:

1. Letter-reports on benchmark results (one per code/problem combination) to be submitted with the monthly progress reports

2. Tape and microfiche of codes, input, and output - September 1, 1986

3. Letter report describing recommended changes in input parameters for problems 3.9, 4.4, and 4.5 based on input from NRC - March 15, 1986.

4. Revised benchmark problem report (draft Task 4 & 5 report) - June 30, 1986

5. Revised benchmark problem report (final Task 4 & 5 report) - August 31, 1986

6. Summary report on code characteristics (draft) - August 31, 1986

7. Summary report on code characteristics (final) - October 30, 1986

Table 1

Recommended Benchmark Problems

	Benchmark Problem	ADINA/ ADINAT	HEATING	WAPPA	COVE	ANISN
2.3	Transient temperature response of a solid cylinder	X	X	X		
2.4	One-dimensional temperature response with phase change	X	X			
2.6	Heat transfer analysis at a PWR fuel assembly in a vertical canister	X	X	X		
2.7	Temperature distribution in a canister filled with hot molten glass	X	X			
3.1	Thermal stresses in a thick-walled cylinder	X	X			
3.3	Elastic-Plastic deformation of a thin rod	X				
3.6	Stress relaxation due to creep of a pretensioned body	X				
3.7	Elastic stability of an infinite length cylindrical tube	X				
3.8	Creep deformation of a finite length cylindrical tube	X			X	

Table 1

Recommended Benchmark Problems
(continued)

	Benchmark Problem	ADINA/ ADINAT	HEATING	WAPPA	COVE	ANISN
3.9	Deformation (including creep) of a hypothetical waste package	X		X	X	
3.11	Stress analysis of a canister filled with hot molten glass	X				
4.2	PWR Fuel Assembly Radiation Levels			X		X
4.4	Shielding analysis of a "thin-walled" waste package			X		X
4.5	Shielding analysis at a "thick-walled" waste package			X		X
5.1	Corrosion and leaching concepts used in WAPPA			X		
5.2	Solute transport by diffusion across an infinitely long cylindrical segment			X		

5. Estimated Level of Effort

Level of effort estimates are given below.

Level of Effort by Labor Category

	Hours
Project Manager/Task Leader	1,000
Mechanical Engineer	1,000
Administrative/Clerical Support	400
QA Director	100
EQAT	50

6. Estimated Costs

Our cost estimate follows.

CONTRACT PRICING PROPOSAL
(RESEARCH AND DEVELOPMENT)

Office of Management and Budget Approval No. 29-R0184

This form is for use when *(i)* submission of cost or pricing data (see FPR 1-3.807-3) is required and *(ii)* substitution for the Optional Form 59 is authorized by the contracting officer.

PAGE NO 1 | NO. OF PAGES 2

NAME OF OFFEROR: CorSTAR Research, Inc.

HOME OFFICE ADDRESS: 2121 Allston Way, Berkeley, CA 94704

SUPPLIES AND/OR SERVICES TO BE FURNISHED: Solve Benchmark Problems and Analyze and Describe Results (Tasks 4 and 5) for the Radiological Assessment Codes under NRC Contract No. 02-81-026

DIVISION(S) AND LOCATION(S) WHERE WORK IS TO BE PERFORMED: Berkeley, CA

TOTAL AMOUNT OF PROPOSAL: $224,639

GOV'T SOLICITATION NO.: 02-81-026

DETAIL DESCRIPTION OF COST ELEMENTS

			EST COST ($)	TOTAL EST COST[1]	REFERENCE[2]
1 DIRECT MATERIAL *(Itemize on Exhibit A)*					
a. PURCHASED PARTS					
b. SUBCONTRACTED ITEMS					
c. OTHER—(1) RAW MATERIAL					
(2) YOUR STANDARD COMMERCIAL ITEMS					
(3) INTERDIVISIONAL TRANSFERS *(At other than cost)*					
TOTAL DIRECT MATERIAL					
2 MATERIAL OVERHEAD[1] *(Rate %X$ base=)*					
3 DIRECT LABOR *(Specify)*	ESTIMATED HOURS	RATE/HOUR	EST COST ($)		
See Exhibit A	2,550		108,097		
TOTAL DIRECT LABOR				108,097	
4 LABOR OVERHEAD *(Specify Department or Cost Center)*[1]	O.H. RATE	X BASE=	EST COST ($)		
	57.20	108,097	61,831		
TOTAL LABOR OVERHEAD				61,831	
5 SPECIAL TESTING *(Including field work at Government installations)*			EST COST ($)		
TOTAL SPECIAL TESTING					
6 SPECIAL EQUIPMENT *(If direct charge) (Itemize on Exhibit A)*					
7 TRAVEL *(If direct charge) (Give details on attached Schedule)*			EST COST ($)		
a. TRANSPORTATION					
b. PER DIEM OR SUBSISTENCE					
See Exhibit A — TOTAL TRAVEL				3,924	
8 CONSULTANTS *(Identify—purpose—rate)*			EST COST ($)		
TOTAL CONSULTANTS					
9 OTHER DIRECT COSTS *(Itemize on Exhibit A)*				4,600	
10 TOTAL DIRECT COST AND OVERHEAD				178,452	
11 GENERAL AND ADMINISTRATIVE EXPENSE *(Rate 13 % of cost element Nos. 3,7,9)*[1]				23,199	
12 ROYALTIES[1]					
13 TOTAL ESTIMATED COST				201,651	
14 FEE OR PROFIT				18,149	
15 TOTAL ESTIMATED COST AND FEE OR PROFIT				219,800	

OPTIONAL FORM 60
October 1971
General Services Administration
FPR 1-16.806
5060-101

This proposal is submitted for use in connection with and in response to *(Describe RFP, etc.)*
Solve Benchmark Problems and Analyze and Describe Results (Tasks 4 and 5) for the Radiological Assessment Codes under NRC Contract No. 02-81-026

and reflects our best estimates as of this date, in accordance with the Instructions to Offerors and the Footnotes which follow.

TYPED NAME AND TITLE	SIGNATURE
Douglas K. Vogt Vice President	

NAME OF FIRM	DATE OF SUBMISSION
CorSTAR Research, Inc.	June 18, 1985

EXHIBIT A—SUPPORTING SCHEDULE *(Specify. If more space is needed, use reverse)*

COST EL NO.	ITEM DESCRIPTION *(See footnote 5)*				EST COST *($)*
3	DIRECT LABOR				
		Hours	Rate	Amount	
	Project Manager	1000	33.66	$ 33,660.00	
	QA Director	100	36.06	3,606.00	
	Admin./Clerical Support	400	11.30	4,520.00	
			Subtotal	41,786.00	
			Labor Add. 51%	21,310.86	
	Mechanical Eng. (Assoc)	1000	42.50	42,500.00	
	External Quality (Assoc)	50	50.00	2,500.00	
	Assurance Reviewers				
	TOTAL LABOR				108,096.86
7	TRAVEL				
	4 round-trips to Washington, DC (3 days ea.) with auto rental:				
	One round-trip @ $636			2,544.00	
	$75/per diem			900.00	
	3-day auto rental @ $120			480.00	
					3,924.00
9	OTHER DIRECT COSTS				
	Reproduction - 20,000 @ $.10/copy			2,000.00	
	Miscellaneous Office Expense @ $200/13 mo.			2,600.00	
					4,600.00

I. HAS ANY EXECUTIVE AGENCY OF THE UNITED STATES GOVERNMENT PERFORMED ANY REVIEW OF YOUR ACCOUNTS OR RECORDS IN CONNECTION WITH ANY OTHER GOVERNMENT PRIME CONTRACT OR SUBCONTRACT WITHIN THE PAST TWELVE MONTHS?

[XX] YES [ ] NO *(If yes, identify below.)*

NAME AND ADDRESS OF REVIEWING OFFICE AND INDIVIDUAL	TELEPHONE NUMBER/EXTENSION
DCAA, Oakland Army Base-Bldg. 1, Oakland, CA 94626	(415)466-3043

II. WILL YOU REQUIRE THE USE OF ANY GOVERNMENT PROPERTY IN THE PERFORMANCE OF THIS PROPOSED CONTRACT?

[ ] YES [XX] NO *(If yes, identify on reverse or separate page)*

III. DO YOU REQUIRE GOVERNMENT CONTRACT FINANCING TO PERFORM THIS PROPOSED CONTRACT?

[ ] YES [XX] NO *(If yes, identify.)*: [ ] ADVANCE PAYMENTS [ ] PROGRESS PAYMENTS OR [ ] GUARANTEED LOANS

IV. DO YOU NOW HOLD ANY CONTRACT *(Or, do you have any independently financed (IR&D) projects)* FOR THE SAME OR SIMILAR WORK CALLED FOR BY THIS PROPOSED CONTRACT?

[XX] YES [ ] NO *(If yes, identify.)*: Contract No. 02-81-026

V. DOES THIS COST SUMMARY CONFORM WITH THE COST PRINCIPLES SET FORTH IN AGENCY REGULATIONS?

[XX] YES [ ] NO *(If no, explain on reverse or separate page)*

See Reverse for Instructions and Footnotes

OPTIONAL FORM 60 (10-71)