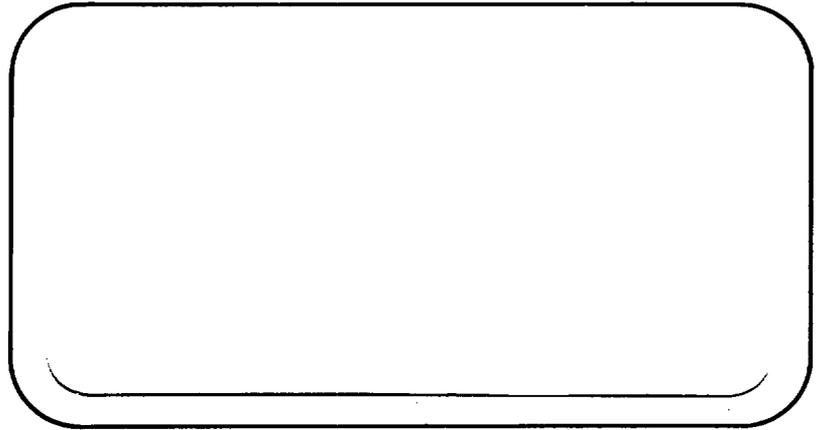


see 6/25/85 TO Coleman
From Vogt



8507120144 850625
PDR WMRES EECCORS
B-6985 PDR



**BENCHMARKING OF COMPUTER CODES
AND LICENSING ASSISTANCE**

**OPTIONAL TASK 6
TECHNOLOGY TRANSFER**

Submitted by:

CorSTAR Research, Inc.
2121 Allston Way
Berkeley, California 94704
(415) 548-4100

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

1. INTRODUCTION

CorSTAR Research, Inc., is under contract to the Nuclear Regulatory Commission to provide assistance in the evaluation of computer codes that may be used for the performance assessment of a high-level radioactive waste repository and to provide general licensing support. Our work for the NRC started in September 1981 and serves the following purposes:

- A review of available computer codes for the performance assessment of high-level radioactive waste repositories
- Development of benchmark or test problems for those computer codes
- Running the benchmark problems and assessing individual computer codes strengths and weaknesses
- Transfer computer codes and benchmarking technology to the NRC for their use
- Provide general licensing support

Our work is organized into four technical discipline areas:

- Repository Siting
- Radiological Assessment
- Repository Design
- Waste Package

A fifth code area, overall systems codes, has largely been covered in work on other code areas.

Work completed to date consists of reviews of the available computer software, development of a data set report describing typical input parameter values for those computer codes and the development of a benchmark problem specification report spelling out test problems to exercise various code features. This effort has been completed for all four of the above mentioned computer code areas. A second project phase involves running the benchmark problems for selected codes

and analyzing the results. Most of this effort has been completed for the code areas where the NRC has asked us to proceed with the work.

This proposal covers the transfer of computer codes and benchmarking technology to the NRC. CorSTAR views this technology transfer task as one of the most important under the contract. It will involve transferring information and skills that we have developed to the NRC so that they may be used by the NRC during the licensing process.

We believe that there are three key elements to the technology transfer process:

- Transfer of computer codes with instructional material making those codes easy to use
- Transfer of the technology surrounding the benchmarking procedures and solutions to benchmarking problems
- Summarizing our experiences on the need for benchmarking and software QA and the experiences of other organizations confronted with challenges similar to that of licensing a high-level waste repository.

Our approach to accomplishing this is discussed in more detail in the next section of the report entitled Technical Approach. Section 3 of this proposal discusses the schedule and level of effort and Section 4 contains our cost proposal.

2. TECHNOLOGY TRANSFER

Effective technology transfer must involve the transfer of three types of information gathered during this project: knowledge of computer codes, benchmarking procedures, and the need for benchmarking.

It is anticipated that during licensing of a repository the NRC will both review computer aided performance assessments performed by the Department of Energy and utilize computer programs to assess independently repository performance. In order to conduct effectively, these reviews and analyses, the NRC staff will need knowledge of the limitations and weaknesses of computer codes

as well as expertise in running individual codes. The code transfer task area is designed to document the information that we have gathered during the course of this project so that present and future NRC staff can review it and use codes or review code applications of others.

During the course of this project, considerable information was developed concerning the procedures that should be used for benchmarking computer codes. For the most part this information was documented in our Quality Assurance procedures. These procedures and insights on their application will be transferred to the NRC so that in the future as the NRC maintains codes, makes changes to codes and applies computer codes, they will benefit from the formal record keeping requirements that were developed and applied during the course of this project. Over 20 of the more complex benchmark problems were solved using micro-computer software. This software will be documented and transferred to the NRC as a part of this effort. Transferring this information to the NRC will allow the NRC or the Department of Energy to benefit from the ready availability of the solutions.

A third key area of knowledge that we have built during the course of this project is a knowledge of the types of errors that frequently occur in computer software, their causes, ways to locate or avoid them and the requirements for record keeping in order to minimize the impact of an error once it is found. The purpose of work in this task area is to document our findings related to software quality assurance and benchmarking so that record-keeping requirements can be developed for the NRC, which the NRC at its discretion may require the Department of Energy to meet. Our approach to each of these task areas is discussed in more detail in the remainder of the discussion of technical approach.

2.1 Technology Transfer - Computer Codes

During the course of this task, CorSTAR will develop and transfer to the NRC selected computer programs, documentation, facility specific user's guides, and sample problems for selected computer programs. This information will encom

pass a complete package of the information required by an individual who is familiar with a given technical discipline to use a given computer program to perform meaningful engineering assessments of the type that the NRC's Waste Management Division may require in the course of repository performance assessments. For each computer code transferred to the NRC, CorSTAR will provide a magnetic tape containing the source code, object code, and executable module for the computer program. The computer codes transferred to the NRC will be the versions benchmarked by CorSTAR. The code version number, latest benchmarking date, and benchmark problems used will be noted in the first file on the tape. Inputs to relevant sample problems and benchmark problems will also be included on the computer tape. All tapes will be prepared in a format that will allow them to be interchanged between computer facilities. Tapes will be 9-track, 1600 BPI, unlabelled, ASCII characters with fixed block lengths. The computer codes will be installed and tested on a government computer facility.

Each computer code will also be provided with a user's manual consisting of the original code user's manual annotated to transfer information that we have gathered during the benchmarking process and supplemented with a how-to guide to allow a user to run the computer program at an individual facility. This facility-specific supplement will include all information including telephone numbers, job control language, appropriate commands, and so on required to access a computer program at specified computer facility. Also included will be a discussion of common pitfalls and user errors that we found as well as guidance on setting of optional parameters in the code. Guidance will also be provided for estimating computer run times, core usage, amount of printed output, etc. The original user's manuals will be transferred to the NRC in hard copy form. The additional items will be given to the NRC in both hard copy and IBM PC compatible disc form. The computer codes to be transferred to the NRC are summarized in Table 2.1-1.

Computer codes to be transferred to the NRC are:

- USGS3D
- FEMWATER

- FEMWASTE
- ORIGEN/S
- PATH1
- HEATING
- STEALTH
- ADINA (no magnetic tape required)
- ADINAT (no magnetic tape required)
- DOT (magnetic tape only)
- MATLOC (magnetic tape only)
- VISCOT (magnetic tape only)
- COYOTE (magnetic tape only)
- SALT4 (magnetic tape only)
- PORFLO (magnetic tape only)
- SWIFT (magnetic tape only)
- NWFT/DVM (magnetic tape only)

2.2 Technology Transfer - Benchmarking Procedures and Solutions

The purpose of this task area is to transfer to the NRC the benchmarking procedures used during code evaluation so that in the future they may benefit from the record keeping and software testing procedures that we have developed. We will also transfer the benchmark problem solutions used during this project.

The quality assurance procedures developed during the course of this project were based on two principles:

- Keeping thorough records of the computer programs and the benchmark problems used to test them and

- Developing benchmark problems with known solutions to serve as suitable tests of computer software.

The procedures developed during the course of this project require that the benchmark problems for a computer code be specified prior to code modification. When the code is modified, the benchmark problems are run and the results compared with expectations. If these benchmark problem results indicate a problem with the computer code, the code is modified until adequate agreement is obtained. The results of the last benchmark problem run and the computer program source code are then baselined and written to tape. The baseline version of the code is used for future analyses.

Under this task, CorSTAR will provide the NRC with the QA procedures used during software benchmarking and a letter report with recommendations for implementing these procedures at NRC. These procedures will be described in a way that will facilitate their automation. These record keeping requirements will provide the NRC with traceability. If problems are encountered in the future with a version of a given code, it will be easy to determine which version of the code had those errors and which analyses performed by the NRC (or DOE) may be in error.

The second part of this task is the transfer of methods for solving individual benchmark problems. Small computer programs were used to solve a large number of the benchmark problems in order to provide reproducibility of results and speed solution of these problems. The benchmark problems for which solutions were developed are listed in Table 1. The computer programs containing these solutions will be documented during the course of this task and transferred to the NRC in a form suitable for execution on an IBM personal computer using FORTRAN, BASIC, or spread sheet programs.

2.3 Benchmarking and Software Quality Assurance

The purpose of this task area is to transfer to the NRC the information that we have gained on software quality assurance and computer code benchmarking.

Table I
Microcomputer-Based Benchmark Problem Solutions

Code Area	Problem Number	Language	Comments
Radiological Assessment	2.1, 2.2, 2.3	FORTRAN	ANSIDECH-estimates decay heat
	2.1, 2.2, 2.3	FORTRAN	BURNUP-estimates fission by isotope
	3.1, 3.2	FORTRAN	CELLTRAN-environmental transport
	3.1, 3.2	FORTRAN	DOSEFAC-dose factors
	3.1, 3.2	FORTRAN	CELLPOST-post-processor
Repository Design	3.2a	LOTUS	
	3.2b	LOTUS	
	3.2c	LOTUS	
	2.6	BASIC	
	3.5	BASIC	
	5.2, 5.3, 6.1, 6.3	BASIC	Grid generator for STEALTH
Waste Package	2.3	BASIC	
	2.4	BASIC	
	3.1	BASIC	
	3.3	LOTUS	
	3.4	LOTUS	
	3.6	LOTUS	
	4.1	LOTUS	
	5.1	FORTRAN	
	5.2	FORTRAN	

This information can be used by the NRC to evaluate the effectiveness of programs now being used by the Department of Energy. The purpose of this task area is to review the technical basis for benchmarking and software quality assurance drawing on the experience of our organization and subcontractor organizations during the course of this work and the experience of other government agencies. The effort would include a review of the QA program used by CorSTAR as well as a review of the efforts by NASA, and selected private sector firms, including A/E firms, aerospace companies and electric utilities. The software quality assurance and benchmarking requirements of computer code centers that have large numbers of programs used during repository performance assessment would also be reviewed. In particular, the National Energy Software Center at Argonne National Laboratory has been a storage and release center for many of the computer programs used by the Department of Energy.

In addition, several relevant software errors will be studied to determine why those errors occurred and what steps could have been taken to have located those errors and minimize the impacts of those errors. For example, several years ago, an error was discovered in a small computer program developed by Stone & Webster to estimate the stress in nuclear powerplant pipe supports. Although the error could have been detected by code benchmarking, it was not discovered until after the design of several powerplants. Stone & Webster did not have adequate records of the nuclear powerplants at which the computer program was used or within a given plant, which pipehangers were analyzed using the code. To make certain that the pipehangers in the suspect plants were adequately designed, it was necessary to reanalyze essentially all of the hangers in the potentially affected powerplants. Widely used computer programs will be reviewed to determine their typical frequency of updating, the types of changes normally made and the number and severity of errors found during a typical update.

3. SCHEDULE AND LEVEL OF EFFORT

Our schedule for these tasks is predicated on July 15, 1985 start of work. The schedule for major deliverable items is:

- Kickoff meeting to establish delivery schedule for specific codes week of July 15, 1985
- Trial Code Computer Magnetic Tape with annotated user's manual and facility specific running instructions September 15, 1985
- Seven computer code magnetic tapes with annotated user's manuals and facility-specific running instructions (order determined by NRC in kickoff meeting) One per month November 1, 1985 through May 1, 1986
- Remaining Computer Magnetic Tapes with annotated user's manuals and facility-specific running instructions as required June 1, 1986
- Benchmarking Procedures and Solutions
 - QA manual with letter report December 1, 1985
 - Benchmark problem solutions April 1, 1986
- Draft letter report on Software QA and Benchmarking July 1, 1986
- Final letter report on software QA and Benchmarking September 1, 1986

Our estimated level of effort is:

<u>Labor Category</u>	<u>Hours</u>
Project Manager/Task Leader	600
Computer Specialist	1,600
Secretarial/Clerical Support	450
QA Director	100
External QA review	100

4. COST PROPOSAL

Our cost proposal for this effort follows.

CONTRACT PRICING PROPOSAL
(RESEARCH AND DEVELOPMENT)

Office of Management and Budget
Approval No. 29-RO184

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 39 is authorized by the contracting officer.

PAGE NO

NO OF PAGES

NAME OF OFFEROR

CorSTAR Research, Inc.

SUPPLIES AND/OR SERVICES TO BE FURNISHED Task 6
Technology Transfer

HOME OFFICE ADDRESS

2121 Allston Way
Berkeley, CA 94704

DIVISION(S) AND LOCATION(S) WHERE WORK IS TO BE PERFORMED

Berkeley, CA 94704

TOTAL AMOUNT OF PROPOSAL

\$196,485

GOV'T SOLICITATION NO

Contract No. 02-81-026

DETAIL DESCRIPTION OF COST ELEMENTS

1 DIRECT MATERIAL (Itemize on Exhibit A)	EST COST (\$)	TOTAL EST COST	REFERENCE
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 (Rate % X \$ base =)			
3 DIRECT LABOR (Specify)	ESTIMATED HOURS	RATE/HOUR	EST COST (\$)
See Exhibit A	2,850		\$92,619
TOTAL DIRECT LABOR			92,619
4 LABOR OVERHEAD (Specify Department or Cost Center)	O.H. RATE	X BASE =	EST COST (\$)
	57.20	92,619	52,978
TOTAL LABOR OVERHEAD			52,978
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		154,121
11 GENERAL AND ADMINISTRATIVE EXPENSE (Rate 13% of cost element Nos. 3,7,9)			20,036
12 ROYALTIES			174,157
13	TOTAL ESTIMATED COST		174,157
14 FEE OR PROFIT 9%			15,674
15	TOTAL ESTIMATED COST AND FEE OR PROFIT		189,831

This proposal is submitted for use in connection with and in response to (Describe RFP, etc.)
Task 6- Technology Transfer

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 Douglas K. Vogt Vice President	SIGNATURE <i>Douglas K. Vogt</i>
NAME OF FIRM CorSTAR Research, Inc.	DATE OF SUBMISSION June 18, 1985

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

COST EL NO.	ITEM DESCRIPTION (See footnote 5)	Hours	Rate	Amount	EST COST (\$)
3	DIRECT LABOR				
	Project Manager/Task Leader	600	33.66	20,196.00	
	Secretarial	450	11.30	5,085.00	
	Quality Assurance	100	36.06	3,606.00	
	Subtotal			28,887.00	
	Labor Add 51%			14,732.00	
	Associates:				
	Vernon, V. (Computer Specialist)	100	27.50	2,750.00	
	External Quality Assurance	100	50.00	5,000.00	
	TOTAL LABOR				92,619.00
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?
 YES NO (If yes, identify below.)

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

II. WILL YOU REQUIRE THE USE OF ANY GOVERNMENT PROPERTY IN THE PERFORMANCE OF THIS PROPOSED CONTRACT?
 YES NO (If yes, identify on reverse or separate page)

III. DO YOU REQUIRE GOVERNMENT CONTRACT FINANCING TO PERFORM THIS PROPOSED CONTRACT?
 YES 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?
 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?
 YES NO (If no, explain on reverse or separate page)

See Reverse for Instructions and Footnotes

OPTIONAL FORM 60 (10-71)