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March 17, 1986

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WM-RES
WM Record File
B6985
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WM Project 10,11,16
Docket No.
PDR ✓
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Distribution:
*P. Brooks
(Return to WM, 623-SS)

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 February 1986

Dear Pauline:

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

Task 3 - Benchmark Problem Report - Waste Package Codes

CorSTAR is awaiting an NRC decision on whether to delete the geochemistry problems from this report.

Tasks 4 & 5 - Siting Codes

During February GeoTrans started revising the report "Benchmarking of Flow and Transport Codes for Licensing Assistance." On February 27, Dr. Large of CorSTAR conducted a QA audit at GeoTrans. Results of that audit are summarized in a letter dated March 4, 1986, a copy of which is included in the technical status summary.

Tasks 4 & 5 - Radiological Assessment Codes

A draft copy of this report is scheduled to be submitted in March.

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CORPORATE SYSTEMS, TECHNOLOGIES, AND RESOURCES
2121 ALLSTON WAY • BERKELEY, CALIFORNIA 94704 • (415) 548-4100

BERKELEY WASHINGTON, D.C. INCLINE VILLAGE

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## Tasks 4 & 5 - Repository Design Codes

Acres has encountered difficulties running the structural analysis of Problem 6.1 — Axisymentric using the code ADINA. The ADINA code creep law does not include a temperature variable. The creep rates predicted for this benchmark problem are highly dependent on temperature. These difficulties encountered are discussed in more detail in the Technical Status Summary.

Acres has set up the thermal analysis for Problem 5.1 using the ADINAT code. See the Technical Status Summary Report for a more detailed discussion of the work performed to date.

By the end of February, the inputs for all the STEALTH problems had been prepared and forwarded to Krishan Wahi for debugging and running.

During February, we submitted an application for computer time at ORNL. The documentation for HEATING was reviewed and the inputs for problems 2.6, 2.8, 2.9, and 5.1 were prepared. These problems will be run when we can access the ORNL computer.

## Tasks 4 & 5 - Waste Package Codes

At the end of the reporting period, all the waste package computer codes except WAPPA had been acquired. DOE may release a new version of WAPPA in the next 1-2 months. If a new version of WAPPA is received by April 30, it probably can be run without significantly affecting project schedule. We expect to run WAPPA at the BNL or INEL computer facility. The other codes and their expected computer facilities are given below.

| Code | Computer Facility |
|---|---|
| ADINA/ADINAT | BNL |
| XSDRNPM (ANISN) | ORNL |
| HEATING 6 | ORNL |
| COVE | IBM/PC |

The Technical Status Summary contains a discussion or our progress with the code COVE during the month.

## Task 6 - Technology Transfer

Work continued at a relatively low level of effort on the technology transfer task. Because of delays in completing work on Tasks 4 & 5 of the siting codes and repository design codes, our original schedule for delivery of computer codes to the NRC will be revised. Over the next 3 to 6 weeks, a revised schedule will be developed.

# TECHNICAL STATUS SUMMARY

TECHNICAL STATUS REPORT ATTACHMENT
TO PROGRESS REPORT FOR FEBRUARY 1986

## Repository Design Codes

### General Information

On January 9, 1986, Dr. David Large of CorSTAR visited Acres office in Buffalo to perform a Quality Assurance Audit of the files related to this project. In his letter of January 17, 1986 to Acres, Dr. Large reported that he found Acres' files to be in order with two exceptions:

1. Backup copies of the project tapes to which additions or changes have been made were not stored on premises different from the primary tapes.

   Acres has copied the most recently used versions of the COYOTE, DOT, MATLOC, SALT4 and VISCOT codes on nine-track tape. The tape is currently stored at Acres' offices in Buffalo, New York, and will be turned over to CorSTAR at the completion of this project. Back-up copies of the ADINA and ADINAT codes have not been made by Acres since the responsibility of maintaining back-up copies of these proprietary codes lies with the Repository Projects Branch of the NRC, as stated in Dr. Large's letter.

2. The file P6678.573-COYOTE-"Code Listings & Updates" which contains the original source code and documents changes to the program, was empty during Dr. Large's visit. The reason for this is explained below.

   Two versions of the COYOTE code were obtained from the author at Sandia National Laboratories. The first version attempted, (V 01.10C) had been written for a CRAY computer. An initial attempt to use this version of COYOTE was unsuccessful due to the numerous changes necessary to adapt the code for the CDC System at Brookhaven National Laboratories.

   Subsequently, version V 01.007 of the COYOTE code was obtained from the author. This earlier version had been written for use with a CDC computer and has run on the BNL system without changes. Discussions with the codes author indicate that the only significant change in the CRAY version from the CDC version was the size of problem that could be solved. Since none of the Benchmark Problems run with the COYOTE CDC code have been limited by the BNL storage capacity, the differences between the CRAY and CDC versions of COYOTE have had no impact on this project.

### ADINA

The structural analysis of the Axisymmetric model of Problem 6.1 (PSV) has been set up for use with the ADINA code. Several runs have been attempted, but the program has terminated at various places due to a lack of convergence while integrating the stress or strain of the elements. The input includes the temperature results from the ADINAT run, a vertical load on the top of the model equal to the weight of the overburden, and a material creep law. The creep law specified in the Benchmark Manual (NUREG/CR-3636) could not be used directly by ADINA. The problem specifies a creep law with the stress,

temperature and time each raised to a power. The power creep law provided by ADINA considers the stress and time only. Thus, the multiplier of the entire expression was modified to account for an average temperature. Since this type of approximation would over-estimate the creep at lower temperatures, it may be the cause of the computational divergence. Problem 6.1 will be run with the ADINA code without the creep law and without temperature data. When the source of the divergence is isolated, the model will be adjusted accordingly.

The three-dimensional thermal model of Problem 5.1 (Very Near Field Problem) has been set-up for ADINAT. In order to increase the size of the smallest element, an axisymmetric model of the canister emplacement hold was run first. This model included the steel block above the canister, the steel sleeve and backfill along the walls of the emplacement hold, and the rock on the hold bottom. The temperature profiles along the interior surfaces of the emplacement hold were compared to the temperature profiles along the outer boundaries of the model.

The thermal model for Problem 5.1 simulates the canister emplacement hole as a cylindrical cutout in the rock and applies the heat directly to the rock boundaries. Since the Benchmark Manual does not provide thermal data for concrete, the concrete block above the canister emplacement hold is modeled as rock.

Heating

Documentation for the HEATING 6 "A Multidimensional Heat Conduction Analysis with the Finite-Difference Formulation" code contained in the SCALE-1 package was reviewed in preparation for running the repository design benchmark problems. Also, efforts were initiated to gain access to the HEATING code at the ORNL computing center.

Input data decks were prepared for the following repository design benchmark problems:

| | |
|---|---|
| **Problem 2.6** | Transient Temperature Analysis of an Infinite Rectangular Bar with Anisotropic Conductivity |
| **Problem 2.8** | Transient Temperature Response to the Quench of an Inifinite Slab with a Temperature-Dependent Convection Coefficient |
| **Problem 2.9** | Transient Temperature Response of a Slab Exposed to a Uniform Radiative Environment |
| **Problem 5.1** | Hypothetical Very Near Field Problem |

Since Acres is also getting ready to run Problem 5.1, we have coordinated our efforts with them to assure that, so far as possible, we both use the same simplifying assumptions to define the problem.

We have decided to simulate the problem in two dimensional axisymetry through the canister/tunnel centerline. Detailed simulation of conduction, convection, and radiation heat transfer between the canister and the steel sleeve (canister and the host rock on the bottom) will be modeled since hand calculations indicate

that all three mechanisms are involved to a significant extent in transferring heat away from the canister. We also plan, at this time, to consider all three heat transfer mechanisms in the tunnel. Temperature as a function of time at elevations of -400 & -600 Meters (+/- 100 Meters from the canister centerline) developed by Acres in Problem 5.2, will be imposed as boundary conditions on Problem 5.1.

## TECHNICAL STATUS SUMMARY - TASK 4 & 5 WASTE PACKAGE CODES

### COVE

The COVE-1 "A Finite Difference Creep Collapse Code for Oval Fuel Pin Cladding Material" code, received on a magnatic tape from the Argonne Code Center was copied to an IBM-PC floppy disk and placed in the Quality Assurance file. The code was then modified to run on an IBM-PC. A preliminary check-out run has indicated that changes made to the code by Battelle PNL in 1979 (the PNL creep model January 1978 version replaced the original creep model in SUBROUTINE RATE) significantly increases the fuel pin ovality compared to that reported in a test case accompanying the original COVE-1 documentation. We have talked to Wendy Bennett at PNL who made the 1979 code changes and were referred to Chuck Mohr, the code author, to find out if he has a sample case that we can use to make sure that hte code runs properly on the IBM-PC.

Computer runs with the original COVE-1 test case took about 65 minutes using single precision arithmetic and about 70 minutes using double precision. The results were the same in both cases, indicating that double precision arithmetic will probably not be required for the benchmark runs. We plan to compile the program to run on a PC that has an 8087 chip to see if run times can be improved.

## TECHNICAL STATUS - TASK 6

### LITERATURE SEARCH

A literature search was performed to gather information related to costs and impacts of computer code errors. A computerized search of 12 databases in the DIALOG system related to computer and to engineering subjects produced 510 citations when searched for: computer(s) and (code(s) or software) and (error(s) or mistake(s)) and (cost(s) or safety). A review of these citations yielded 20 relevant reports. An expanded search for reports by specific author or title produced 10 additional relevant reports. Most of these reports have been acquired and reviewed; a few are still on order. Additional relevant articles on this subject were found in various IEEE publications at the University of California engineering library.

Most of the literature on this subject does not include specific dollar amounts that can be attributed to computer code errors. Instead, it focuses on studies related to the number and types of errors contained in various size software packages. The recent literature is concerned with methods of producing error-free software and the development of software engineering standards.

The Technical Status Summary includes a brief description of accomplishments to date on our review of the benchmarking and software quality assurance program of other organizations.

General

Our estimate of costs through the end of February (March 1, 1986, for CorSTAR) is:

| | |
|---|---|
| Actual costs this month: | 55K |
| Actual costs this fiscal year: | 214K |
| Actual costs to date: | 3,408K |
| Planned costs this fiscal year: | 210K |
| Planned costs this month: | 50K |

Estimated costs include labor, labor additive, overhead, subcontractor costs, G&A and fee. These costs have not been confirmed by our accounting department.

Sincerely,

Douglas K. Vogt

Douglas K. Vogt
Project Manager

DKV:kg

Enclosures