

A TEKNEKRON INDUSTRIES AFFILIATE

February 15, 1984

NRC FIN B6985 WM DOCKET CONTROL CENTER

Division	l Fehringer, Project Officer of Waste Management	WM Record File 126985	Docket No PDR LPDR
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Subject:	Contract No. NRC 02-81-026	(Return to WM, 623-SS)	Cz
· ·	Benchmarking of Computer Coo Monthly Letter Progress Repo	des and Licensing A	ssistance 4

Dear Dan:

This letter contains a management level summary of progress during January. Also enclosed are a Technical Status Report and a Cost Summary Report.

Task 1 - Literature Search - Waste Package Codes

By letter dated January 18, 1984, we received Brookhaven National Laboratory's comments on the Draft Data Set Report. Because of the late date of receipt of these comments, they were not incorporated into the Draft Report now being finalized for the NRC.

Task 3 - Benchmark Problem Report - Waste Package Codes

As of the end of January, approximately 90 percent of the benchmark problems have been described in draft form. Based on comments received from the NRC, we are developing benchmark problems for geochemistry codes. The attached Technical Status Report contains a brief summary of our plan in this area.

Tasks 4 & 5 - Siting Codes

The following items were accomplished during January:

- All remaining problems were run and results were analyzed
- All remaining chapters of the draft of the task summary report were completed
- Input and output files for various codes were transferred from the computer to magnetic tapes

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CORPORATE SYSTEMS TECHNOLOGIES AND RESOURCES
7315 WISCONSIN NORTH TOWER #702 • BETHESDA MARYLAND 20814 • (301) 654-8096

BERKELEY

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INCLINE VILLAGE

Revision of the benchmark problem report was commenced

Tasks 4 & 5 - Radiological Assessment Codes

During January, sample problems were successfully run for all of the radiological assessment codes except ORIGEN. Minor code changes were required to correct small errors in the versions of the codes that we obtained. Overall progress on this portion of the project is summarized in the Technical Status Summary Report.

Task 8 - Earth Sciences Data Base

During January, there was no significant effort on the data base.

General

On February 9, we met with the NRC to discuss the status of work on the waste package codes and our proposal dealing with Tasks 4&5 of the Repository Design Codes. We understand that the NRC has completed its initial evaluation of the repository design code benchmarking proposal and will provide us with written questions soon.

Our estimate of costs through January 31 (through January 28 for CorSTAR) is:

Actual costs this month:	\$ 55,580
Actual costs this fiscal year:	281,333
Actual costs to date:	2,279,111
Planned costs this month:	88,000
Planned costs this fiscal year:	384,000

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: Pauline Brooks

TECHNICAL STATUS SUMMARY

Technical Status - Tasks 4 & 5 - Siting Codes

The status of the benchmark problem runs and code documentation is summarized in Table 1.

Technical Status - Tasks 4 & 5 - Radiological Assessment Codes

During the past reporting period the following Radiological Assessment Codes were converted to compile under VS FORTRAN at NIH and tested with sample input problems: BIODOSE, LADTAP and PABLM. A test run of the PATH1 code was made at Brookhaven. Benchmark problem inputs for these codes are currently being prepared. The final checkout of a program which provides an independent solution of the pathways/dose-to-man problems was also completed. Arrangements are in progress which will allow CorSTAR to indirectly access the SCALE System at Oak Ridge National Laboratory for the purpose of running the heat generation and isotope inventory benchmark problems.

Technical Status - Tasks 1-3 - Waste Package Codes

Geochemical Code Benchmark Problem Design

In order to design benchmark problems that will fully test the codes for simulating the geochemical environment in the near field, we have assessed the processes that will be considered. Two major processes identified are equilibrium and non-equilibrium (kinetics) processes. Although the previous work has focused on the well understood equilibrium thermodynamic processes, kinetically controlled processes may be very important to the assessment of the very near field, especially in a region undergoing temperature changes.

The design of geochemical benchmark problems will necessitate an approach different than that utilized for the saturated-unsaturated flow codes. For example, in the flow code benchmarl problems, exact solutions to problems can be defined such as the Theis equation. For the



	Code received	Code compiled	Benchmark problems completed*	Hypothetical problems rerun (only if answers conflict between codes)	Microfiche code version(s) used, final input files, and final output files	Chapter completed for draft summary report	Chapter completed for final summary report
SWIFT-1	х	x	3.4, 3.5, 3.6, 7.1, 3.2, 5.3, 8.2, 5.2, 8.4	No Conflict		Fully completed	
NWFT/DVM	х	X	8.1, 8.3	N/A		Fully completed	
NUTRAN	Х	X	8.1, 8.2, 8.3, 8.4	No Conflict		Fully completed	
USGS3D	Х	X	3.2, 3.4, 3.5, 3.3	Conflict with SWIFT resolved		Fully completed	
SWIFT-II	х	X	9.1, 9.2, 9.3, 6.1	No Conflict		Fully completed	
PORFLO	x	x	3.2, 5.1, 3.3, 9.1, 8.1, 8.3, 5.2, 8.2	No Conflict		Fully completed	
FEMWATER FEMWASTE	χ	x	4.1, 4.2, 4.3, 10.1, 10.2	No Conflict		Fully completed	

^{*} This column indicates problem runs before comparison with results using other codes.

geochemical problems, exact solutions are not available to easily solve the interactions of complexation, redox and chemical reactions and other processes that affect the geochemical regime. Therefore, the geochemical benchmark problems will be more qualitative. For example, the benchmark problem may test a code for predictions of precipitation—dissolution by input of the actual chemical characteristics of a ground—water and comparing predicted saturation indices for minerals to known minerals present. This test is qualitative in that the rates or masses of precipitated or dissolved minerals are not known, i.e., only the direction of the reaction is known.

Benchmark test data proposed for geochemical codes include the following:

- Verification of code algorithm by comparison to hand calculated solutions. This approach is considered impracticable to carry out due to the necessary iterative nature of the problem and the large number of calculations required. Comparison of code results to published calculations is possible though.
- Validation of code utility through published documenation of code use. The degree of application of the codes varies from WATEQ that has been used by many investigators to the less frequently used EQ3/6.
- Verification and validation of codes by comparison to results of controlled laboratory experiments.
 There are several candidate laboratory studies reported in the literature.
- Validation of geochemical codes by comparison to field studies with confirmatory minerologic data. A number of candidate data sets have been identified.

These approaches to the design of the benchmark problems are capable of providing the necessary tests of the geochemical codes.

The geochemical codes are based on chemical processes, which leads to the design of problems along process lines. The following general benchmark problem areas are based on those controlling processes.

- Aqueous speciation problem utilizing the seawater solution of Garrels and Thompson (1962) for high ionic strength and a not yet identified data set for low ionic strength water.
- Redox equilibrium considering couples such as FE+2 Fe+3, SO₄-2 S₂- and NO₃- NH₄+ utilizing several mine drainage studies that developed comprehenisve data sets.
- Mineral dissolution-precipitation reactions (reaction path) utilizing published studies such as Bock et al. (1983).
- Adsorption-Ion Exchange (reactor path)
 utilizing published studies such as Los
 Alamos National Laboratory (1982) and
 Chapells and Knobel (1983).
- Phase equilibria in high temperature systems utilizing considerable work on CO₂ in caronate and geothermal systems.
- Biological metabolism (not defined yet).

In designing these benchmark problems, we anticipate, that as many as twelve problem sets will be required for the equilibrium processes. A like number would be required for kenetically controlled processes (if the data exists).

The geothermal codes are important to the illucidation of the chemical environment, as well as providing input to waste package corrosion models, radionuclide transport models and backfill performance models. Although at this time, the kinetics are poorly understood, the equilibrium thermodynamic based models have considerable potential use because many of the processes controlling the chemical reactions will be equilibrium controlled. Therefore it may be important to develop kinetics benchmark problems for eventual benchmarking of the code.

Because of the number of benchmark problems being considered, our schedule for the benchmark problem report may require revision. We will discuss the schedule with you in the next two weeks.

COST MANAGEMENT REPORT

Period 1/1/84 - 1/28/84

Personnel Time Expenditures 1/1/84 - 1/28/84

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1 8	Waste Package Earth Sciences Data Base	225	10K	107,786	139K		-		}		
4 8 5	Siting Codes	16,534	- - 	265,081	- 139K - 217K	10K 9K	17K	166K 261K			
4 8 5	Rad. Assmit. Codes	10,001	- 								
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	Total	16,759	27K	784,556	801K	19K	44K	0724			
l		10,733	<u> </u>		1 0015	417/\	1 441	872K			