CorSTAR

A TEKNEKRON INDUSTRIES AFFILIATE

February 15, 1984

NRC FIN B6985

WM DOCKET CONTROL CENTER

WM Record File B6985

WM Project 10, 11, 16

Docket No.

PDR ✓

LPDR

84 FEB 17 P2:24

Distribution:

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P Hare

(Return to WM, 623-SS)

C2

Dr. Daniel Fehringer, 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 January 1984

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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BERKELEY WASHINGTON DC 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

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 enviornment 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

Table 1

	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	X	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	X	X	8.1, 8.3	N/A		Fully completed	
* NUTRAN	X	X	8.1, 8.2, 8.3, 8.4	No Conflict		Fully completed	
USGS3D	X	X	3.2, 3.4, 3.5, 3.3	Conflict with SWIFT resolved		Fully completed	
* SWIFT-II	X	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	X	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 groundwater 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}, SO_4^{-2} - S_2^- and NO_3^- - NH_4^+ utilizing several mine drainage studies that developed comprehenisve data sets.

- Mineral dissolution-precipitation reactions (reaction path) utilizing publsihed 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 CO_2 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

CorSTAR

Personnel Time Expenditures

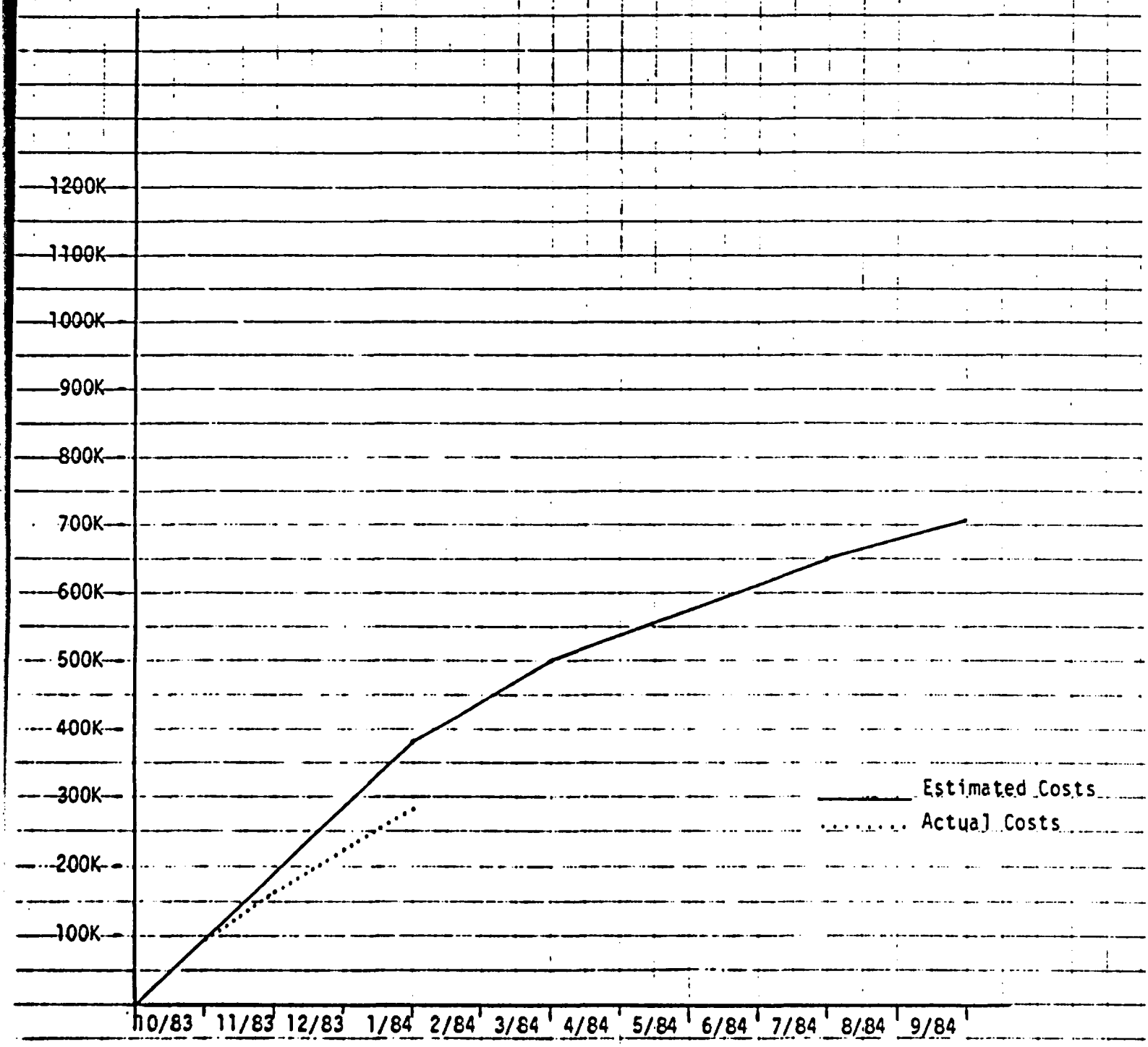
1/1/84 - 1/28/84

Name	Hours
CorSTAR	
Mills, M.	152
Rupert, P.	3
Silka, L.	72
Singer, M.	110
Vogt, D.	116
GeoTrans	
August, L.	16
Huyakorn, P.	40
Jones, B.	86
Kretschek, A	23
Lester, B.	14
Loxtercamp, M.	28.5
Ross, B.	25
Sherertz, C.	40

ESTIMATED vs ACTUAL COSTS
Tasks 1-3, Design, Waste Package
Tasks 4-5, Siting, Dosimetry
Tasks 7-8

Revised 11/15/83

Total Estimated Cost
through 9/84 - 707K



SUMMARY

COST MANAGEMENT REPORT

PAGE

1. Contract Identification: BENCHMARKING OF COMPUTER CODES AND LICENSING ASSISTANCE

2. Reporting Period: 1/1/84 through 1/28/84

3. Contract Number: NRC 02-81-026

4. Contractor (Name and address): Teknekron Research, Inc.
7315 Wisconsin Avenue, 702 North
Bethesda, MD 20814

5. Cost Plan Date: 10/83

6. Contract Start Date: 9/15/81

7. Contract Completion Date: 9/15/86

8. Government Funding: 2,500,000*

9. Contractor Funding: $

10. Number of Invoices Billed: 34

11. Frequency: 4 week periods

12. Number of Invoices Paid: 34

13. Total Invoice Amounts Billed: 2,137,477.93

14. Total Payment Received: 2,130,099.44

15. Subcontractor Number	16. Reporting Category (e.g., contract line item or work breakdown structure element)	17. Accrued Costs: During Reporting Period a. Actual	b. Planned	Cumulative to Date c. Actual	d. Planned	18. Estimated Accrued Costs: a. Subsequent Reporting Period	b. Balance of Fiscal Year	c. Total Contract	Remarks
TASKS									
	COMPLETED PRIOR FISCAL YEARS								*Incremental Funding
1-3	Siting Codes								
1-3	Dosimetry Codes								
7	BWIP								
	TOTAL	--	--	867,557	834K	--	--	834K	
1-3	Repository Design	--	--	368,309	369K	--	--	369K	
1-3	Waste Package	19,503	20K	207,501	238K	9K	8K	255K	
8	Earth Sciences Data Base	1,347	26K	446,850	470K	26K	67K	627K	
4 & 5	Siting Codes	21,295	28K	367,143	341K	20K	81K	442K	
4 & 5	Rad. Assmnt. Codes	13,435	14K	21,751	40K	14K	99K	152K	
	Total	55,580	88K	227,911	2292K	69K	254K	2679K	

SUMMARY

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7315 Wisconsin Avenue, 702 North
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9. Contractor Funding: 0

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15. Subsystem Number Or Tasks	16. Reporting Category (e.g., contract line item or work breakdown structure element)	17. Accrued Costs: During Reporting Period a. Actual	b. Planned	Cumulative to Date c. Actual	d. Planned	18. Estimated Accrued Costs: a. Subsequent Reporting Period	b. Balance of Fiscal Year	c. Total Contract
	COMPLETED PRIOR FISCAL YEARS							
1-3	Siting Codes							
1-3	Dosimetry Codes							
7	BWIP							
	TOTAL	--	--	867,557	834K	--	--	834K
1-3	Repository Design	--	--	368,309	369K	--	--	369K
1-3	Waste Package	19,503	20K	207,501	238K	9K	8K	255K
8	Earth Sciences Data Base	1,347	26K	446,850	470K	26K	67K	627K
4 & 5	Siting Codes	21,295	28K	367,143	341K	20K	81K	442K
4 & 5	Rad. Assmnt. Codes	13,435	14K	21,751	40K	14K	99K	152K
	Total	55,580	88K	227,911	2292K	69K	254K	2679K

Remarks: *Incremental Funding

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9. Contractor Funding: 0

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13. Total Invoice Amounts Billed:

14. Total Payment Received:

15. Subcontractor Number	16. Reporting Category (e.g., contract line item or work breakdown structure element)	17. Accrued Costs: During Reporting Period a. Actual	b. Planned	Cumulative to Date c. Actual	d. Planned	18. Estimated Accrued Costs: a. Subsequent Reporting Period	b. Balance of Fiscal Year	c. Total Contract
TASKS								
	COMPLETED PRIOR FISCAL YEARS							
1-3	Siting Codes							
1-3	Dosimetry Codes							
7	BWIP							
	TOTAL							
1-3	Repository Design	--	--	211,545	191K	--	--	191K
1-3	Waste Package							
8	Earth Sciences Data Base							
4 & 5	Siting Codes							
4 & 5	Rad. Assmnt. Codes							
	Total	--	--	211,545	191K	--	--	191K

Remarks

*Incremental Funding

CONTROL DATA CORP.

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9. Contractor Funding: 0

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12. Number of Invoices Paid:

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14. Total Payment Received:

15. Sub-activity Number	16. Reporting Category (e.g., contract line item or work breakdown structure element)	17. Accrued Costs: During Reporting Period a. Actual	b. Planned	Cumulative to Date c. Actual	d. Planned	18. Estimated Accrued Costs: a. Subsequent Reporting Period	b. Balance of Fiscal Year	c. Total Contract	Remarks
TASKS									
	COMPLETED PRIOR FISCAL YEARS								*Incremental Funding
1-3	Siting Codes								
1-3	Dosimetry Codes								
7	DWIP								
	TOTAL								
1-3	Repository Design								
1-3	Waste Package								
8	Earth Sciences Data Base	--	--	86,612	96K	--	--	96K	
4 & 5	Siting Codes								
4 & 5	Rad. Assmnt. Codes								
	Total	--	--	86,612	96K	--	--	96K	

CorSTAR Research, Inc.

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14. Total Payment Received:

15. Subcontractor Number	16. Reporting Category (e.g., contract line item or work breakdown structure element)	17. Accrued Costs: During Reporting Period a. Actual	b. Planned	Cumulative to Date c. Actual	d. Planned	18. Estimated Accrued Costs: a. Subsequent Reporting Period	b. Balance of Fiscal Year	c. Total Contract
TASKS								
	COMPLETED PRIOR FISCAL YEARS							
1-3	Siting Codes							
1-3	Dosimetry Codes							
7	BWIP							
	TOTAL	--	--	462,036	401K	--	--	401K
1-3	Repository Design	--	--	149,210	166K	--	--	166K
1-3	Waste Package	19,503	20K	207,501	238K	9K	8K	255K
8	Earth Sciences Data Base	1,122	16K	252,452	235K	16K	50K	365K
4 & 5	Siting Codes	4,761	11K	102,062	124K	11K	46K	181K
4 & 5	Rad. Assmnt. Codes	13,435	14K	21,751	40K	14K	98K	182K
	Total	38,821	61K	1,195,012	1204K	50K	202K	1520K

Remarks: *Incremental Funding

GEOTRANS

COST MANAGEMENT REPORT

PAGE

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3. Contract Number: NRC 02-81-026

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6. Contract Start Date: 9/15/81

7. Contract Completion Date: 9/15/86

8. Contract Funding: 2,500,000*

9. Contractor Funding: 0

10. Number of Invoices Billed:

11. Frequency: 4 week periods

12. Number of Invoices Paid:

13. Total Invoice Amounts Billed:

14. Total Payments Received:

15. Subcontractor Number	16. Reporting Category (e.g., contract line item or work breakdown structure element)	17. Accrued Costs: During Reporting Period a. Actual	b. Planned	Cumulative to Date c. Actual	d. Planned	18. Estimated Accrued Costs: a. Subsequent Reporting Period	b. Balance of Fiscal Year	c. Total Contract
TASKS								
	COMPLETED PRIOR FISCAL YEARS							
1-3	Siting Codes							
1-3	Dosimetry Codes							
7	BWIP							
	TOTAL	--	--	405,521	433K	--	--	433K
1-3	Repository Design	--	--	6,168	12K	--	--	12K
1-3	Waste Package	--	--	--	--	--	--	--
8	Earth Sciences Data Base	225	10K	107,786	139K	10K	17K	166K
4 & 5	Siting Codes	16,534	17K	265,081	217K	9K	27K	261K
4 & 5	Rad. Assmnt. Codes	--	--	--	--	--	--	--
	Total	16,759	27K	784,556	801K	19K	44K	872K

Remarks: *Incremental Funding