PDR-1
LPDR-Wm-10 (2)
Wm-11 (2)
Wm-16 (2)

WM DOCKET CONTROL CENTER

January 2, 1987

Mr. K. C. Chang
Mail Stop 623-SS
US Nuclear Regulatory Commission
Washinton DC 20555

'87 JAN -7 A11:14

Dear Kien:

SUMMARY OF EFFORT, DECEMBER 22, 1986 - JANUARY 2, 1987

This letter describes the tasks which have been addressed during the time period indicated.

1. Continued coding a user-friendly version of CONVO for use on a PC.

2. Performed some mathematical analysis on low-frequency external events in conjuction with R. Moler.

Enclosed is a Voucher for Professional Services for the subject time period.

Tasks planned for the next work period are:

1. Continuation of CONVO modelling.

2. Further analysis of hydrogen concentration around the canister surface.

Please call me if you have any questions. Please note the change in phone number.

Very Truly Yours,

Gary

Gerald H. Fuller
10024 Colvin Run Road
Great Falls VA 22066
703-759-9527

87166323
WM Project: WM-10,11,16
PDR w/encl
(Return to WM, 623-SS)

H

WM Record File: A4165
LPDR w/encl

WM-RES
WM Record File
A4165
A35D

WM Project 10, 11, 16
Docket No.
PDR ✓
X LPDR ✓ (B, N, S)

Distribution:
Chang
(Return to WM, 623-SS)
Sac

8708110216 870102
PDR WMRES EECFLLER
A-4165 PDR

3880

To: Kien Chang

From: Loren Zaremba LZ

Date: January 5, 1987

Subject: Activity Report, December 22, 1986 - January 4, 1987

In the two week period from December 22, 1986 through January 4, 1987 I performed the following consulting services for the NRC. The designated weeks below refer to the number of weeks since I began this contract.

Week 11

Dec. 22

Morning - Prepare biweekly report for NRC and complete vouchers.

Afternoon - Prepare memo on TEMPH and HEATING5 comparison.

Dec. 23

Continue attempting to debug program QFIT2 for determining a fit to a decay heat curve. Still unable to determine the problem with the IMSL subroutine IFLSQ which performs the least squares fits.

Week 12

Dec. 30

Finally determine problem with the IMSL subroutine IFLSQ. The IMSL library contains both a single and double precision version of IFLSQ. In order to obtain the single precision version, which I assumed I was getting, you must specify:

```
//        LIBNAME='ZABCRUN.IMSL.SLIB'
```

in the JCL.

Dec. 31

Prepare travel expense report. Begin to test alternative search routines in QFIT2 to determine a set of decay rates which minimizes the square error.

Jan. 2

Complete test of alternative search routines. The most efficient method appears to be one in which five or six initial values are input by the user, along with a search increment value for each and the number of increments to be made. A listing of the program, along with a sample input data set and output are attached. The JCL needed to run the program through WYLBUR on the NIH IBM 370 computer is also provided.

Plans for Weeks 13 and 14

Now that I have transferred and tested all of my programs relating to thermal analysis, I can begin to write the User's Manual for this suite of programs. I estimate that 3 to 4 weeks will be required for this task. The manual will contain instructions for using QFIT2, TEMP and TEMPH with examples. A discussion of a method which can be used for generating a thermal response surface will also be provided.

```
C*****************************************************************
C
C          PROGRAM QFIT2 TO DETERMINE A LEAST SQUARES FIT
C          TO A TABLE OF WASTEFORM RELATIVE DECAY HEAT VS.
C          TIME USING A SET OF EXPONENTIAL DECAY FUNCTIONS.
C          THIS VERSION (2) INCLUDES A SEARCH ROUTINE TO
C          DETERMINE A SET OF DECAY RATES WHICH MINIMIZES
C          THE SQUARE ERROR.  THE MAIN PROGRAM DIRECTS THE
C          SEARCH. THE SUBROUTINE QFIT CALLS THE IMSL
C          SUBROUTINE IFLSQ TO DO THE LEAST SQUARES FIT.
C          IT THEN COMPUTES THE SQUARE ERROR FOR THAT SET
C          OF DECAY RATES. THE EXTERNAL FUNCTION F COMPUTES
C          THE VALUES OF THE EXPONENTIAL DECAY FUNCTIONS AT
C          THE TABLE TIMES.
C
C*****************************************************************
C
      REAL T(20),Q(20),WK(500),EST(20),OLAM(10),DLAM(10),ALAM(10),
     .     BLAM(10),BEST(20)
      INTEGER NLAM(10)
      EXTERNAL F
      COMMON /EX/ ALAMI(10),A(10)
C
C   T=TABLE TIMES
C   Q=TABLE RELATIVE DECAY HEATS
C   A=COEFFICIENTS OF DECAY FUNCTIONS DETERMINED BY LEAST SQUARES
C   WK=WORKSPACE FOR IMSL SUBROUTINE IFLSQ
C   EST=ESTIMATES OF DECAY HEATS USING EXPONENTIAL DECAY FUNCTIONS
C   BEST=BEST EST. OF DECAY HEATS USING EXPONENTIAL DECAY FUNCTIONS
C   F=FUNCTION WHICH DETERMINES VALUES OF USER SUPPLIED EXPONENTIAL
C     DECAY FUNCTIONS AT TABLE TIMES
C   M=NUMBER OF DATA POINTS IN TABLE (MAX=20)
C   N=NUMBER OF EXPONENTIAL DECAY FUNCTIONS (MAX=10)
C   ERR=LEAST SQUARES ERROR
C   OLAM=INITIAL VALUES OF EXPONENTIAL DECAY RATES(YRS)
C   DLAM=SEARCH INCREMENTS FOR EXPONENTIAL DECAY RATES(YRS)
C   NLAM(I)=NUMBER OF SEARCH INCREMENTS FOR I-TH DECAY RATE
C   ALAM=DECAY RATES USED IN SEARCH(YRS)
C   ALAMI=INVERSES OF SEARCH DECAY RATES(1/YRS)
C   BLAM=BEST FIT DECAY RATES(YRS)
C
C   READ AND WRITE TABLE OF TIMES AND DECAY HEATS, INITIAL
C   VALUES OF DECAY RATES AND INCREMENTS
C
      READ(1,1001) M,N
1001  FORMAT(2I5)
      READ(1,1002) (T(I),Q(I),I=1,M)
1002  FORMAT(2F10.3)
      READ(1,1003) (OLAM(I),DLAM(I),NLAM(I),I=1,N)
1003  FORMAT(2F10.3,I10)
```

```
      WRITE(9,2001)
2001  FORMAT(' PROGRAM QFIT TO DETERMINE A LEAST SQUARES FIT',/,
     .       ' TO A TABLE OF WASTEFORM RELATIVE DECAY HEAT VS',/,
     .       ' TIME USING A SET OF EXPONENTIAL DECAY FUNCTIONS.',/,
     .       ' THIS VERSION (2) INCLUDES A SEARCH ROUTINE TO',/,
     .       ' DETERMINE A SET OF DECAY RATES WHICH MINIMIZES',/,
     .       ' THE SQUARE ERROR. THE MAIN PROGRAM DIRECTS THE',/,
     .       ' SEARCH. THE SUBROUTINE QFIT CALLS THE IMSL',/,
     .       ' SUBROUTINE IFLSQ TO DO THE LEAST SQUARES FIT.',/,
     .       ' IT THEN COMPUTES THE SQUARE ERROR FOR THAT SET',/,
     .       ' OF DECAY RATES. THE EXTERNAL FUNCTION F COMPUTES',/,
     .       ' THE VALUES OF THE EXPONENTIAL DECAY FUNCTIONS AT',/,
     .       ' THE TABLE TIMES.',///)
      WRITE(9,2002)
2002  FORMAT(' TABLE OF TIMES AND RELATIVE DECAY HEATS',/,
     .       ' TIME(YRS)',5X,' REL. HEAT',/)
      WRITE(9,2003) (T(I),Q(I),I=1,M)
2003  FORMAT(E12.5,5X,E12.5)
      WRITE(9,2004)
2004  FORMAT(//,' INITIAL DECAY RATES AND SEARCH INCREMENTS',/,
     .          ' RATE(YRS)',5X,' INCREMENT(YRS)',
     .          ' NO. OF INCREMENTS ',/)
      WRITE(9,2005) (OLAM(I),DLAM(I),NLAM(I),I=1,N)
2005  FORMAT(E12.5,5X,E12.5,5X,I10)
C
C   SET INITIAL SEARCH DECAY RATES
C
      DO 10 I=1,N
      ALAM(I)=OLAM(I)
      ALAMI(I)=1.0/OLAM(I)
10    CONTINUE
C
C   BEGIN SEARCH FOR BEST FIT DECAY RATES
C
      DO 100 I=1,N
      BLAM(I)=ALAM(I)
C
C   FIND BEST I-TH RATE
C
      DO 200 J=1,NLAM(I)
      ALAM(I)=OLAM(I)+DLAM(I)*(J-1)
      ALAMI(I)=1./ALAM(I)
      CALL QFIT(T,Q,M,N,EST,ERR)
      IF((I .EQ. 1) .AND. (J .EQ.1))
     .   GO TO 115
      IF(ERR .GT. ERRO) GO TO 200
115   BLAM(I)=ALAM(I)
      DO 20 K=1,M
      BEST(K)=EST(K)
20    CONTINUE
      ERRO=ERR
200   CONTINUE
```

```
C
C   SEARCH OF I-TH RATE COMPLETE--RESET TO BEST FIT
C
      ALAM(I)=BLAM(I)
      ALAMI(I)=1./BLAM(I)
      WRITE(9,2009) I
2009  FORMAT(/,' BEST FIT FOR RATE NO.',I2,//)
      WRITE(9,2007) (ALAM(K),K=1,N)
2007  FORMAT(' RATES(YRS)= ',/,10(E10.3,3X))
      WRITE(9,2008) ERRO
2008  FORMAT(' ERR= ',E12.5,/)
100   CONTINUE
      WRITE(9,2010)
2010  FORMAT(///,' BEST OVERALL FIT ',/)
      WRITE(9,2007) (ALAM(I),I=1,N)
      WRITE(9,2008) ERRO
      WRITE(9,2011)
2011  FORMAT(//,' TIME(YRS)',5X,' REL.HEAT',10X,' FIT',/)
      WRITE(9,2012) (T(I),Q(I),BEST(I),I=1,M)
2012  FORMAT(F10.1,5X,F10.5,5X,F10.5)
      STOP
      END
C
C*****************************************************************
C
C          SUBROUTINE QFIT TO COMPUTE THE LEAST SQUARES FIT
C          TO A TABLE OF WASTEFORM RELATIVE DECAY HEAT VS TIME
C          USING A SET OF EXPONENTIAL DECAY FUNCTIONS WITH
C          DECAY RATES SUPPLIED BY THE MAIN PROGRAM QFIT2.
C
C*****************************************************************
C
      SUBROUTINE QFIT(T,Q,M,N,EST,ERR)
      REAL T(20),Q(20),WK(500),EST(20)
      EXTERNAL F
      COMMON /EX/ ALAMI(10),A(10)
C
C   CALL IMSL SUBROUTINE IFLSQ TO COMPUTE LEAST SQUARES FIT
C
      CALL IFLSQ(F,T,Q,M,A,N,WK,IER)
C
C   COMPUTE SQUARED ERROR
C
      ERR=0.
      DO 10 I=1,M
      EST(I)=0.
      TI=T(I)
      DO 20 J=1,N
      FUN=F(J,TI)
      EST(I)=EST(I)+A(J)*FUN
20    CONTINUE
      ERR=ERR+(Q(I)-EST(I))*(Q(I)-EST(I))/Q(I)**2
10    CONTINUE
      RETURN
      END
```

```
C
C*********************************************************************
C
C          EXTERNAL FUNCTION TO DETERMINE THE VALUES OF THE
C          EXPONENTIAL DECAY FUNCTIONS AT THE TABLE TIMES
C
C*********************************************************************
C
      REAL FUNCTION F(K,T)
      COMMON /EX/ ALAMI(10),A(10)
      AX=ALAMI(K)*T
      IF(AX .GT. 20.) F=0.
      IF(AX .GT. 20.) GO TO 10
      F=EXP(-AX)
10    CONTINUE
      RETURN
      END
```

?

JOB CONTROL LANGUAGE TO RUN QFIT2 ON
NIH IBM 370 COMPUTER THROUGH WYLBUR

```
//EBBQFIT  JOB  (WDC9,701,E,60),ZAREMBA
//*
//*  COMPILE STEP
//*
//STEP1  EXEC FORVCOMP
//*
//*  DEFINE FORTRAN SOURCE
//*
//COMP.SYSIN  DD  DSN=WDC9EBB.QFIT2.FRT,DISP=SHR,UNIT=FILE,
//            VOL=SER=FILE44
//*
//*  LOAD AND GO
//*
//STEP2  EXEC FORVLKGO,LIBDISK=MSTAT1,
//           LIBNAME='ZABCRUN.IMSL.SLIB'
//*
//*  DEFINE INPUT DATA FILE
//*
//GO.FT01F001  DD  DSN=WDC9EBB.QFIT2.DTA,DISP=SHR,UNIT=FILE,
//           VOL=SER=FILE44
//*
//*  DEFINE OUTPUT FILE
//*
//GO.FT09F001  DD DSN=WDC9EBB.OUTPUT.DTA,DISP=(NEW,KEEP),UNIT=FILE,
//           VOL=SER=FILE44,SPACE=(TRK,(2,2),RLSE),
//           DCB=(RECFM=VB,LRECL=137,BLKSIZE=274)
//*
//*  END
//*
```

SAMPLE DATA SET FOR PROGRAM QFIT2

```
19    6
     0.0      1.000
     5.0      0.838
    10.0      0.750
    15.0      0.681
    20.0      0.622
    30.0      0.525
    40.0      0.449
    50.0      0.387
    70.0      0.301
    90.0      0.243
   100.0      0.238
   190.0      0.137
   290.0      0.108
   390.0     0.0919
   490.0     0.0806
   990.0     0.0466
  1990.0     0.0247
  5990.0     0.0148
  9990.0     0.0144
     1.0        1.0         20
    20.0        2.0         15
    50.0       50.0         10
   500.0      100.0         15
  2000.0      500.0         16
 10000.0     1000.0         40
```

PROGRAM QFIT TO DETERMINE A LEAST SQUARES FIT
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DETERMINE A SET OF DECAY RATES WHICH MINIMIZES
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SEARCH. THE SUBROUTINE QFIT CALLS THE IMSL
SUBROUTINE IFLSQ TO DO THE LEAST SQUARES FIT.
IT THEN COMPUTES THE SQUARE ERROR FOR THAT SET
OF DECAY RATES. THE EXTERNAL FUNCTION F COMPUTES
THE VALUES OF THE EXPONENTIAL DECAY FUNCTIONS AT
THE TABLE TIMES.

TABLE OF TIMES AND RELATIVE DECAY HEATS

TIME(YRS)	REL. HEAT
0.00000E+00	0.10000E+01
0.50000E+01	0.83800E+00
0.10000E+02	0.75000E+00
0.15000E+02	0.68100E+00
0.20000E+02	0.62200E+00
0.30000E+02	0.52500E+00
0.40000E+02	0.44900E+00
0.50000E+02	0.38700E+00
0.70000E+02	0.30100E+00
0.90000E+02	0.24300E+00
0.10000E+03	0.23800E+00
0.19000E+03	0.13700E+00
0.29000E+03	0.10800E+00
0.39000E+03	0.91900E-01
0.49000E+03	0.80600E-01
0.99000E+03	0.46600E-01
0.19900E+04	0.24700E-01
0.59900E+04	0.14800E-01
0.99900E+04	0.14400E-01

INITIAL DECAY RATES AND SEARCH INCREMENTS

RATE(YRS)	INCREMENT(YRS)	NO. OF INCREMENTS
0.10000E+01	0.10000E+01	20
0.20000E+02	0.20000E+01	15
0.50000E+02	0.50000E+02	10
0.50000E+03	0.10000E+03	15
0.20000E+04	0.50000E+03	16
0.10000E+05	0.10000E+04	40

BEST FIT FOR RATE NO. 1

RATES(YRS)=
0.100E+01 0.200E+02 0.500E+02 0.500E+03 0.200E+04 0.100E+05
ERR= 0.65991E-01

BEST FIT FOR RATE NO. 2

RATES(YRS)=
0.100E+01 0.220E+02 0.500E+02 0.500E+03 0.200E+04 0.100E+05
ERR= 0.65866E-01

BEST FIT FOR RATE NO. 3

RATES(YRS)=
0.100E+01 0.220E+02 0.500E+02 0.500E+03 0.200E+04 0.100E+05
ERR= 0.65866E-01

BEST FIT FOR RATE NO. 4

RATES(YRS)=
0.100E+01 0.220E+02 0.500E+02 0.500E+03 0.200E+04 0.100E+05
ERR= 0.65866E-01

BEST FIT FOR RATE NO. 5

RATES(YRS)=
0.100E+01 0.220E+02 0.500E+02 0.500E+03 0.850E+04 0.100E+05
ERR= 0.39899E-01

BEST FIT FOR RATE NO. 6

RATES(YRS)=
0.100E+01 0.220E+02 0.500E+02 0.500E+03 0.850E+04 0.490E+05
ERR= 0.28574E-01

?

BEST OVERALL FIT

RATES(YRS)=
0.100E+01 0.220E+02 0.500E+02 0.500E+03 0.850E+04 0.490E+05
ERR= 0.28574E-01

TIME(YRS)	REL.HEAT	FIT
0.0	1.00000	1.00003
5.0	0.83800	0.83399
10.0	0.75000	0.75307
15.0	0.68100	0.68345
20.0	0.62200	0.62295
30.0	0.52500	0.52398
40.0	0.44900	0.44757
50.0	0.38700	0.38779
70.0	0.30100	0.30255
90.0	0.24300	0.24694
100.0	0.23800	0.22640
190.0	0.13700	0.14033
290.0	0.10800	0.11051
390.0	0.09190	0.09354
490.0	0.08060	0.08063
990.0	0.04660	0.04394
1990.0	0.02470	0.02435
5990.0	0.01480	0.01664
9990.0	0.01440	0.01333