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PC-BASED CALCULATION OF ACTIVATION ENERGY USING LINEAR REGRESSION

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INTRODUCTION

During a severe accident, various plant locations will be subjected to harsh environments - high temperature, high humidity, high radiation, etc. Equipment required for accident mitigation located in these areas must be capable of withstanding these conditions, i.e., environmentally qualified. Qualification is normally accomplished by type testing. The equipment undergoes accelerated aging to achieve a condition equivalent to the end-of-life condition. This aging consists of accelerated thermal aging and radiation aging. The aged equipment is then subjected to simulated seismic vibration and other vibration. After a radiation exposure simulating some maximum accident exposure, the equipment is then mounted in a test chamber and operated during a simulated design basis event (DBE) environment (high temperature, pressure, humidity, and possible submergence) and post-accident conditions. The Arrhenius equation is used to relate the test thermal aging and accident profiles to the expected plant conditions. The Arrhenius equation is as follows:

$$\ln (t_1/t_2) = (E_A/K)*(1/T_1 - 1/T_2)$$

where

t_1 = Duration of test conditions (hours)

T_1 = Test temperature (^oK)

t_2 = Actual/expected plant duration (hours)

T_2 = Plant temperature (^oK)

E_A = Activation energy (eV)

$K = 8.617 \times 10^{-5}$ ($eV/^oK$)

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* The information contained in this paper was developed during the course of work done under Contract DE-AC09--88SR18035 with the U. S. Department of Energy.

The test temperatures and times are given in the equipment test report. The expected plant conditions are often documented in the Final Safety Analysis Report (FSAR). Sometimes the activation energy is explicitly stated in the test report. More often than not, a table of aging data is the only information provided. This data can be used, with the linear regression method, to calculate the material activation energy.

This article describes two PC-based methods of applying the linear regression method to the thermal aging data to obtain an activation energy.

DISCUSSION

Linear Regression Method

Given a set of data points (x_1, y_1) through (x_m, y_m) that can be plotted on a straight line with the equation $y = a + bx$, the slope of the line (b) can be determined using the Linear Regression Method:

$$b = \sum_{i=1}^{m} (x_i - \bar{x})(y_i - \bar{y}) \Big/ \sum_{i=1}^{m} (x_i - \bar{x})^2$$

Where $$\bar{x} = \sum_{i=1}^{m} x_i \Big/ m$$

and $$\bar{y} = \sum_{i=1}^{m} y_i \Big/ m$$

Looking at the Arrhenius Equation:

$$\ln (t_1/t_2) = (E_A/K)*(1/T_1 - 1/T_2)$$

it can be seen that:

- o y corresponds to ln(t),
- o x corresponds to 1/T, and
- o $b = E_A/K$

Rearranging this last equation, the activation energy (E_A) is equal to bK.

Hand Calculation

The following activation energy hand calculation is based on thermal aging data for Dow-Corning Sylgard DC-170 given in Table 1.

$$\bar{x} = [(26.5 + 25.1 + 23.6 + 22.6 + 21.6 + 20.7)/6] \times 10^{-4}/6$$

$$\bar{x} = 23.3 \times 10^{-4} \quad 1/^{o}K$$

$$\bar{y} = (11.035 + 10.463 + 9.668 + 9.071 + 8.476 + 7.824)/6$$

$$\bar{y} = 9.423$$

$$b = [(25.5-23.3)(11.035-9.423) + (25.1-23.3)(10.463-9.423) + (23.6-23.3)(9.668-9.423) + (22.6-23.3)(9.071-9.423) + (21.6-23.3)(8.476-9.423) + (20.7-23.3)(7.824-9.423)] \times 10^{-4} / [(25.5-23.3)^2 + (25.1-23.3)^2 + (23.6-23.3)^2 + (22.6-23.3)^2 + (21.6-23.3)^2 + (20.7-23.3)^2] \times 10^{-8}$$

$$b = (11.506/18.31) \times 10^4$$

$$b = 6284 = \sim 6280$$

$$E_A = bK = (6280)(8.617 \times 10^{-5})$$

$$E_A = 0.54 \text{ eV}$$

As you can see, hand calculation of the activation energy is a time consuming process, with potential for error at each step. There is a simpler, faster, more accurate way of doing this. The calculations can be done using a PC-based spreadsheet (such as Lotus 1-2-3) or a FORTRAN language code.

Spreadsheet Calculation

Figure 1 is a spreadsheet based on the DC-170 thermal aging data. Setting it up is a relatively straight-forward process. The main advantages are:

- Once the cell formulae are set up, you can use the spreadsheet for several materials. Just be careful converting the aging data temperature to degrees Kelvin:

$$K = C + 273 = (F + 460)/1.8.$$

- The round-off errors inherent in the hand calculation are eliminated.

It is a good practice, from a QA/QC standpoint, to print a listing of the cell formulae and making it part of your calculation.

FORTRAN Program

For you ambitious types, a FORTRAN program, written to run with the Ryan-MacFarland Professional Fortran Compiler is available. The code listing is shown in Figure 2.

CONCLUSION

An engineering professor once told me (longer ago than I like to remember) that a lazy engineer is a good engineer - he'll usually find the simplest, easiest way to solve a problem. This "lazy" engineer hopes you find this paper to be useful. You will be able to determine activation energies for EQ analyses more quickly and with fewer errors.

REFERENCES

1. NUREG-0588, Revision 1, "Interim Staff Position on Environmental Qualification of Safety-Related Electrical Equipment," July 1981.

2. 10CFR50.49, "Environmental Qualification of Electrical Equipment Important to Safety for Nuclear Power Plants."

3. IEEE 323-1974, "IEEE Standard for Qualifying Class 1E Equipment for Nuclear Power Generating Stations," February 1974.

4. EPRI NP-1558, "A Review of Equipment Aging Theory and Technology," September 1980.

5. Carnahan, Luther, and Wilkes, "Applied Numerical Methods," John Wiley & Sons, New York, NY, 1969.

6. Dow-Corning Report I-0340-13.

7. Lotus 1-2-3, Release 2.01, Lotus Development Corporation, 1987.

8. IBM Professional FORTRAN Compiler, Version 1.18, Ryan--McFarland Corporation, 1985, 1985.

TABLE 1

DC-170 THERMAL AGING DATA

RAW DATA		CONVERTED FOR LINEAR REGRESSION		
Temp (C)	Time (Hours)	Temp (K)	10^4 / Temp (1/K)	ln(t)
105	62000	378	26.5	11.035
125	35000	398	25.1	10.463
150	15800	423	23.6	9.668
170	8700	443	22.6	9.071
190	4800	463	21.6	8.476
210	2500	483	20.7	7.824

Source: Dow-Corning Report I-0340-13.

FIGURE 1

LOTUS 1-2-3 SPREADSHEET

MATERIAL: DC-170
REF: DOW-CORNING REPORT I-0340-13
NUMBER OF DATA PTS 6

TEMP (C)	TIME (H)	TEMP (K)	X=INV TEMP INV TEMP	Y=LN(TIME LN(TIME)
105	62,000	378	2.65E-03	11.035
125	35,000	398	2.51E-03	10.463
150	15,800	423	2.36E-03	9.668
170	8,700	443	2.26E-03	9.071
190	4,800	463	2.16E-03	8.476
210	2,500	483	2.07E-03	7.824
		SUM X =	1.40E-02	SUM Y = 56.537
		X BAR =	2.33E-03	Y BAR = 9.423

X-X BAR	(X-X BAR)* (X-X BAR)	Y-Y BAR	(X-X BAR)* (Y-Y BAR)
3.11E-04	9.64E-08	1.612	5.01E-04
1.78E-04	3.15E-08	1.040	1.85E-04
2.91E-05	8.48E-10	0.245	7.13E-06
-7.76E-05	6.02E-09	-0.352	2.73E-05
-1.75E-04	3.07E-08	-0.947	1.66E-04
-2.65E-04	7.00E-08	-1.599	4.23E-04
SUM =	2.36E-07	SUM =	1.31E-03

SLOPE = 5556.00
ACTIVATION ENERGY = 0.48 ev

FIGURE 2

FORTRAN CODE LISTING

```
C ************************  EMILY  ***************************
C
C THIS PROGRAM WILL CALCULATE THE ACTIVATION
C ENERGY OF A MATERIAL, GIVEN TABULATED
C AGING DATA, USING LINEAR REGRESSION
C
C                          BUTCH BORNT
C                          JANUARY 1989
C
C ********************** MAIN ********************************
      IMPLICIT REAL*8 (A-H,O-Z)
      CHARACTER*8 IFILE,OFILE
      COMMON /INOUT/ INP,IOU,ICASE,MATL
      COMMON /DATA/ X(10),Y(10),RN
      COMMON /NNNNN/ N,IT
      DIMENSION TEMP(10)
      DIMENSION TIME(10)
      INP = 2
      IOU = 4
      OPEN(INP,FILE='INP.DAT',STATUS='OLD')
      OPEN(IOU,FILE='OUT.DAT',STATUS='UNKNOWN')
C READ ICASE - STACKED CASES; ICASE = 0 END OF CASES
    1 READ(INP,*) ICASE
      IF(IMATL.EQ.0) STOP
C
C     READ MATERIAL NAME
C
      READ(INP,50) MATL
   50 FORMAT(A10)
C
C     READ MATERIAL THERMAL AGING DATA
C
C  N = NUMBER OF AGING DATA POINTS
      READ(INP,*) N
C  IT = FLAG INDICATING UNITS OF AGING DATA TEMPERATURE
C       IT = 1 --> TEMP IN DEG F
C       IT = 2 --> TEMP IN DEG C
C       IT = 3 --> TEMP IN DEG K
      READ(INP,*) IT
C  TEMP = TEMPERATURE (DEG F, DEG C, OR DEG K)
C  TIME = TIME (HOURS)
      DO 100 I=1,N
      READ(INP,*) TEMP(I),TIME(I)
  100 CONTINUE
      WRITE(IOU,110) MATL
  110 FORMAT(10X,'MATERIAL: ',A10//)
```

FIGURE 2

FORTRAN CODE LISTING

```
      WRITE(IOU,120)
  120 FORMAT(10X,10('*'),' INPUT AGING DATA ',10('*')//)
      WRITE(IOU,*) '          TEMPERATURE          TIME'
      IF (IT.EQ.1) WRITE(IOU,*) '              (F)              (HR)'
      IF (IT.EQ.2) WRITE(IOU,*) '              (C)              (HR)'
      IF (IT.EQ.3) WRITE(IOU,*) '              (K)              (HR)'
      DO 130 I=1,N
      WRITE(IOU,140) TEMP(I),TIME(I)
  140 FORMAT(12X,F5.1,9X,F8.1)
  130 CONTINUE
C
      CALL LINREG(TEMP,TIME,DELXX,DELXY,SLOPE,ACTNRG)
C
      CALL OUTDT(DELXX,DELXY,SLOPE,ACTNRG)
      GOTO 1
      END
C ------------------------------------------------------------------
      SUBROUTINE OUTDT(DELXX,DELXY,SLOPE,ACTNRG)
      IMPLICIT REAL*8 (A-H,O-Z)
      CHARACTER*8 IFILE,OFILE
      COMMON /INOUT/ INP,IOU,ICASE,MATL
      COMMON /DATA/ X(10),Y(10),RN
      COMMON /NNNNN/ N,IT
      DIMENSION TEMP(10)
      DIMENSION TIME(10)
      WRITE(IOU,100)
  100 FORMAT(10X,10('*'),' OUTPUT DATA ',10('*')//)
      WRITE(IOU,110)
  110 FORMAT(10X,'SLOPE = SUM (X-XAVG)*(Y-YAVG)/SUM(X-XAVG)*(X-XAVG)')
      WRITE(IOU,120) DELXY,DELXX,SLOPE
  120 FORMAT(10X,'SLOPE = ',E8.2,'/',E8.2,' = ',F8.2)
      WRITE(IOU,130)
  130 FORMAT(10X,'ACTIVATION ENERGY (EV) =  SLOPE   * 8.617E-5')
      WRITE(IOU,140) SLOPE
  140 FORMAT(10X,'ACTIVATION ENERGY (EV) = ',F8.2,' * 8.617E-5')
      WRITE(IOU,150) ACTNRG
  150 FORMAT(10X,'ACTIVATION ENERGY (EV) = ',F4.2)
      RETURN
      END
```

FIGURE 2

FORTRAN CODE LISTING

```
C ***************************************************************
      SUBROUTINE LINREG(TEMP,TIME,DELXX,DELXY,SLOPE,ACTNRG)
C
C     LINEAR REGRESSION ALGORITHM
C
      IMPLICIT REAL*8 (A-H,O-Z)
      CHARACTER*8 IFILE,OFILE
      COMMON /INOUT/ INP,IOU,ICASE,MATL
      COMMON /DATA/ X(10),Y(10),RN
      COMMON /NNNNN/ N,IT
      DIMENSION TEMP(10)
      DIMENSION TIME(10)
      WRITE(IOU,100)
  100 FORMAT(10X,10('*'),' LINEAR REGRESSION ',10('*')//)
      WRITE(IOU,101)
  101 FORMAT(10X,5('*'),' X = 1/TEMPERATURE (1/K) ',5('*'))
      WRITE(IOU,102)
  102 FORMAT(10X,5('*'),'        Y = LN(TIME)        ',5('*')//)
      WRITE(IOU,*) '          1/TEMPERATURE   LN(TIME)'
      WRITE(IOU,*) '              (1/K)'
      DO 120 I=1,N
      IF (IT.EQ.1) TEMP(I) = (TEMP(I)+460.0)/1.8
      IF (IT.EQ.2) TEMP(I) = TEMP(I)+273.0
      IF (IT.EQ.1) TEMP(I) = TEMP(I)
      X(I) = 1/TEMP(I)
      Y(I) = DLOG(TIME(I))
      WRITE(IOU,121) X(I),Y(I)
  121 FORMAT(11X,E9.3,5X,F6.3)
  120 CONTINUE
      WRITE(IOU,130)
  130 FORMAT(10X//)
      XSUM = 0.0
      YSUM = 0.0
      RN = 0.0
      DO 140 I=1,N
      XSUM = XSUM + X(I)
      YSUM = YSUM + Y(I)
      RN = RN + 1.0
  140 CONTINUE
      XAVG = XSUM/RN
      YAVG = YSUM/RN
      WRITE(IOU,150)
  150 FORMAT(10X,5('*'),' AVERAGE X AND Y ',5('*')//)
```

FIGURE 2

FORTRAN CODE LISTING

```
      WRITE(IOU,151) XSUM,RN,XAVG
151   FORMAT(10X,'AVG X = ',E9.3,'/',F4.1,' = ',E9.3)
      WRITE(IOU,153) YSUM,RN,YAVG
153   FORMAT(10X,'AVG Y = ',F6.3,'/',F4.1,' = ',F6.3)
      WRITE(IOU,154)
154   FORMAT(10X//)
      DELXY = 0.0
      DELXX = 0.0
      DO 160 I=1,N
      DELXY = DELXY + (X(I)-XAVG)*(Y(I)-YAVG)
      DELXX = DELXX + (X(I)-XAVG)*(X(I)-XAVG)
160   CONTINUE
      SLOPE = DELXY/DELXX
C
C CALCULATE ACTIVATION ENERGY
C
      ACTNRG = SLOPE*8.617E-5
      RETURN
      END
```