

US EPA ARCHIVE DOCUMENT

APPENDIX M  
CHAIN PROGRAM FILES

CHAIN Program Files  
CHAIN.FOR Program Listing

0            1            2            3            4            5            6            7  
12345678901234567890123456789012345678901234567890123456789012345678

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```
C... CALCULATE CONCENTRATIONS OF CHAIN MEMBERS GIVEN RELEASE
C... RATE OF PARENT. CALCULATIONS BASED ON ORNL/4992,
C... SECTIONS 3.1.1.1.2 AND 3.1.1.1.3.
C... C.B.NELSON 11 OCT 78
C... MODIFIED FOR SKRABLE'S METHOD AND ENVIRONMENTAL REMOVAL
C... C.B.NELSON 23 JAN 80
C
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```
    IMPLICIT REAL*8 (A-H,O-Z)
    DIMENSION A(20,20),AR(20,20),X(20,20),
$      Q(20),F(20),R(20),S(20),
$      TCON(5)
    REAL*8 LN2
    CHARACTER*72 TITLE
    CHARACTER*8 NAME(20),TUNIT
    CHARACTER*1 EUNIT,HUNIT,TCHAR(5)
    DATA A/400*0D0/,AR/400*0D0/,X/400*0D0/,
$      TCON/1D0,60D0,360D0,8640D0,31556925.5D0/,
$      TCHAR/'S','M','H','D','Y'/
    LN2=DLOG(2D0)
```

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C
C... SUPPRESS UNDERFLOW MESSAGES AND TRACE
C
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```
C    CALL ERRSET(208,0,-1,1)
C    OPEN FILES FOR INPUT AND OUTPUT
    OPEN(UNIT=5,FILE='FORT5')
    OPEN(UNIT=6,FILE='LPT1')
```

```
C
C... READ INPUT DATA
C
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```
    WRITE(6,1010)
1010 FORMAT(1X,'INPUT DATA:')
    READ(5,1012) TITLE
1012 FORMAT(A72)
    WRITE(6,1014) TITLE
1014 FORMAT(1X,'TITLE:',T9,A72)
    READ(5,1020) N,T,TUNIT
1020 FORMAT(I5,5X,F10.0,1X,A8)
    WRITE(6,1030) N,T,TUNIT
    DO 40 I=1,5
    IF(TUNIT(1:1).EQ.TCHAR(I)) GO TO 50
    40 CONTINUE
    STOP 1
    50 TC=TCON(I)
1030 FORMAT(1X,'N,T,TUNIT:',T13,I5,5X,F10.2,1X,A8)
    WRITE(6,1040)
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CHAIN Program Files  
CHAIN.FOR Program Listing  
(continued)

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1040 FORMAT(1X, 'NAME, H, HUNIT, F, E EUNIT: ')
      DO 80 I=1, N
        READ(5, 1050) NAME(I), H, HUNIT, F(I), E, EUNIT
1050  FORMAT(A8, 2X, F10.0, 1X, A1, 8X, F10.0, F10.0, 1X, A1)
        IF(EUNIT.EQ. ' ') EUNIT=TCHAR(1)
        WRITE(6, 1060) NAME(I), H, HUNIT, F(I), E, EUNIT
1060  FORMAT(1X, T13, A8, 2X, 1PE10.3, 1X, A1, 8X, 0PF10.5, 1PE10.3, 1X, A1)
      DO 60 J=1, 5
        IF(HUNIT.EQ.TCHAR(J)) GO TO 70
        60  CONTINUE
          STOP 2
        70  Q(I)=LN2*TC/(TCON(J)*H)
          DO 72 J=1, 5
            IF(EUNIT.EQ.TCHAR(J)) GO TO 74
            72  CONTINUE
              STOP 2
            74  R(I)=E*TC/TCON(J)
          80  CONTINUE
C
C... CALCULATE S VALUES
C
      S(N)=0.
      IF(N.EQ.1) GO TO 100
      I1=N-1
      DO 90 I=1, I1
        90  S(I)=F(I)*Q(I+1)
C
C... PRINT TABLE OF Q, R AND S VALUES
C
      100 WRITE(6, 1070) TUNIT
1070  FORMAT(1H1, 'CALCULATED VALUES FOR Q, R AND S (', A1, '**-1). '//)
      WRITE(6, 1080) (NAME(I), Q(I), R(I), S(I), I=1, N)
1080  FORMAT(1X, A8, 4X, 1PE12.3, 2E12.3)
C
C... CALCULATE ACCUMULATED CONCENTRATIONS OF MEMBERS OF CHAIN
C
      CALL ACON(A, Q, R, S, N, T)
C
C... CALCULATE RELATIVE ACCUMULATED CONCENTRATIONS
C
      DO 120 J=1, N
        AJJ=A(J, J)
        DO 120 I=J, N
          120 AR(I, J)=A(I, J)/AJJ
C

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CHAIN Program Files  
CHAIN.FOR Program Listing  
(continued)

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C... CALCULATE EFFECTIVE INPUT RATES FOR CHAIN
C
      DO 130 I=1,N
      AII=A(I,I)
      DO 130 J=1,I
130  X(I,J)=A(I,J)/AII
C
C... OUTPUT INGROWTH FACTORS (EFFECTIVE INPUT RATES)
C   FOR USE IN AIRDOSE-EPA.
C
      WRITE(6,2000) TITLE
2000 FORMAT(1H1,A72)
      WRITE(6,2010) T,TUNIT
2010 FORMAT(1H0,'AIRDOS-EPA INGROWTH FACTORS CALCULATED FOR',/
$       1H , 'TIME=',F10.2,1X,A8//)
      WRITE(6,2020)
2020 FORMAT(1H0,'NUCLIDE',T24,'INGROWTH FACTOR FOR PARENT NUCLIDE'/)
      WRITE(6,2030) (NAME(I-1),I=2,N)
2030 FORMAT(1H ,T14,6(A8,2X):/(1H ,T15,6(A8,2X)))
      DO 140 I=2,N
      JJ=I-1
140  WRITE(6,2040) NAME(I),(X(I,J),J=1,JJ)
2040 FORMAT(1H0,A8,2X,T12,1P,6E10.2:/(1H ,T13,6E10.2))
      WRITE(6,2050)
2050 FORMAT(1H1)
C   CALL EXIT
      STOP
      END
      SUBROUTINE ACON(A,Q,R,S,N,T)
C
C... CALCULATE ACCUMULATED CONCENTRATIONS FOR MEMBERS OF CHAIN
C... CALCULATIONS IN DOUBLE PRECISION TO MINIMIZE TRUNCATION ERRORS.
C
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Q8(20),A0(420),A(20,20),Q(1),R(1),S(1)
C
      DO 10 I=1,N
10  Q8(I)=Q(I)+R(I)
      CALL H1(A0,N,Q8,S,T)
      DO 20 I=1,N
      DO 20 J=1,N
      AIJ=0.
      IF(I.GE.J) AIJ=A0(I+(J-1)*(2*N-J)/2)
20  A(I,J)=AIJ
      RETURN

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      END
      REAL*8 FUNCTION DEXP1(XX)
C
C... EVALUATE EXP1(X)=(EXP(X)-1.0)/X
C
      IMPLICIT REAL*8 (A-H,O-Z)
      DATA XL/-.69314718D0/,XU/.40546511D0/
C
      X2=1.D0
      IF(XX.EQ.0.) GO TO 30
C
C... USE SERIES EXPANSION WHEN 0.5.LE.EXP(X).LT.1.5
C
      IF(XL.LE.XX.AND.XX.LT.XU) GO TO 10
      X2=(DEXP(XX)-1.D0)/XX
      GO TO 30
C
10  X1=1.0D0
      DO 20 I=2,100
      X1=XX*X1/I
      IF(DABS(X1).LT.1.D-17) GO TO 30
      X2=X2+X1
20  CONTINUE
30  DEXP1=X2
      RETURN
      END
      SUBROUTINE H1(H,N,Q,S,T)
C
C... CALCULATE THE TRANSFER MATRIX FOR THE UNIT STEP FORCING FUNCTION
C      SOLUTION OF THE LINEAR CHAIN EQUATIONS. THE METHOD IS BASED ON
C      HEALTH PHYSICS, VOL 27, PP 155-157 (1974). Q AND S ARE THE
C      REMOVAL RATES AND TRANSFER RATES TO THE SUCCEEDING COMPARTMENT.
C      THE TRANSFER MATRIX, H, IS THE LOWER TRIANGLE OF A N*N MATRIX
C      STORED BY COLUMN IN N*(N+1)/2 LOCATIONS. H IS CALCULATED BY
C      COLUMN WITH COMPUTATIONALLY INSIGNIFICANT VALUES SET TO 0. Q
C      IS A DOUBLE PRECISION VARIABLE TO ALLOW NEARLY IDENTICAL VALUES
C      FOR ANY OF ITS ELEMENTS. CALCULATIONS ARE PERFORMED IN DOUBLE
C      PRECISION TO REDUCE THE EFFECT OF TRUNCATION ERRORS.
C      C.B.NELSON 3/20/80
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION H(1),Q(1),S(1),F(20),X(20)
C
      DO 10 I=1,N
10  F(I)=T*DEXP1(-Q(I)*T)

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C

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      DO 70 J=1,N
      HL=F(J)*1.D-15
      IO=(J-1)*(2*N-J)/2
      DO 20 I=J,N
20    X(I)=F(I)
      DO 40 I=J,N
      QI=Q(I)
      SI=S(I)
      HI=0.D0
      DO 30 K=J,N
      IF(K.NE.I) X(K)=X(K)/(QI-Q(K))
      IF(K.LE.I) HI=HI+X(K)
30    X(K)=X(K)*SI
      IF(HI.LT.HL) GO TO 50
40    H(I+IO)=HI
      GO TO 70
50    II=I
      DO 60 I=II,N
60    H(I+IO)=0.
70    CONTINUE
      RETURN
      END

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CHAIN Program Files  
 TH100Y02.DAT Listing  
 Input Data for Thorium Decay Chain Factor Calculations

THORIUM SERIES (TH-232 AND PRINCIPAL PROGENY TO THALLIUM-208)

	10	100. YEARS		
TH-232	1.405E10 Y		1.0	.02 Y
RA-228	5.75 Y		1.0	.02 Y
AC-228	6.13 H		1.0	.02 Y
TH-228	1.9131 Y		1.0	.02 Y
RA-224	3.66 D		1.0	.02 Y
RN-220	55.6 S		1.0	4.532E-2 D
PO-216	0.15 S		1.0	.02 Y
PB-212	10.64 H		1.0	.02 Y
BI-212	60.55 M		.3593	.02 Y
TL-208	3.07 M		1.0	.02 Y



CHAIN Program Files  
 U100Y02.DAT Listing  
 Input Data for Uranium Decay Chain Factor Calculations

URANIUM SERIES (URANIUM-238 AND PRINCIPAL PROGENY)			
14	100. YEARS		
U-238	4.468E9 Y	1.0	.02 Y
TH-234	24.10 D	1.0	.02 Y
PA-234	1.17 M	.9987	.02 Y
U-234	2.445E5 Y	1.0	.02 Y
TH-230	7.7E4 Y	1.0	.02 Y
RA-226	1600. Y	1.0	.02 Y
RN-222	3.8235 D	1.0	.04532 D
PO-218	3.05 M	.99980	.02 Y
PB-214	26.8 M	1.0	.02 Y
BI-214	19.9 M	.99979	.02 Y
PO-214	1.637E-4 S	1.0	.02 Y
PB-210	22.26 Y	1.0	.02 Y
BI-210	5.013 D	1.0	.02 Y
PO-210	138.378 D	1.0	.02 Y

Thorium Series (Thorium-232 and Principal Progeny)

Nuclide	Ingrowth Factor for Parent Nuclide							
	TH-232	RA-228	AC-228	TH-228	RA-224	RN-220	PO-216	PB-212
RA-228	5.076E+00							
AC-228	3.580E+04	7.052E+03						
TH-228	1.295E+01	2.578E+00	3.655E-04					
RA-224	2.343E+03	4.664E+02	6.613E-02	1.809E+02				
RN-220	1.332E+07	2.652E+06	3.760E+02	1.029E+06	5.686E+03			
PO-216	4.938E+09	9.829E+08	1.394E+05	3.813E+08	2.107E+06	3.707E+02		
PB-212	1.934E+04	3.849E+03	5.458E-01	1.493E+03	8.253E+00	1.451E-03	3.916E-06	
BI-212	2.039E+05	4.058E+04	5.754E+04	1.574E+04	8.701E+01	1.530E-02	4.129E-05	1.054E+01
TL-208	1.445E+06	2.876E+05	4.078E+01	1.116E+05	6.166E+02	1.084E-01	2.926E-04	7.471E+01
								7.086E+00

## Uranium Series (Uranium-238 and Principal Progeny)

Nuclide	Ingrowth Factor for Parent Nuclide												
	U-238	TH-234	PA-234	U-234	TH-230	RA-226	RN-222	PO-218	PB-214	BI-214	PO-214	PB-210	BI-210
TH-234	4.540E+02												
PA-234	1.344E+07	2.961E+04											
U-234	9.698E-05	2.689E-07	9.087E-12										
TH-230	2.374E-08	8.310E-11	2.810E-15	3.092E-04									
RA-226	2.286E-10	9.841E-13	3.329E-17	3.664E-06	1.492E-02								
RN-222	6.446E-07	2.775E-09	9.388E-14	1.033E-02	4.208E+01	2.820E+03							
PO-218	9.308E-04	4.008E-06	1.356E-10	1.492E+01	6.078E+04	4.073E+06	1.444E+03						
PB-214	1.059E-04	4.560E-07	1.543E-11	1.698E+00	6.915E+03	4.635E+05	1.643E+02	1.138E-01					
BI-214	1.426E-04	6.141E-07	2.078E-11	2.286E+00	9.313E+03	6.241E+05	2.213E+02	1.532E-01	1.347E+00				
PO-214	1.040E+03	4.478E+00	1.515E-04	1.667E+07	6.791E+10	4.551E+12	1.614E+09	1.117E+06	9.821E+06	7.292E+06			
PB-210	1.515E-10	7.355E-13	2.490E-17	2.740E-06	1.268E-02	9.644E-01	3.754E-04	2.599E-07	2.285E-06	1.696E-06	2.326E-13		
BI-210	1.488E-07	7.226E-10	2.446E-14	2.692E-03	1.246E+01	9.477E+02	3.690E-01	2.555E-04	2.245E-03	1.667E-03	2.286E-10	9.828E+02	
PO-210	5.297E-09	2.586E-11	8.752E-16	9.632E-05	4.481E-01	3.421E-01	1.336E-02	9.248E-06	8.128E-05	6.035E-05	8.276E-12	3.558E+01	3.621E-02

CHAIN Program Files  
Ingrowth Factors for Uranium Decay Series