ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois

1559/RE: A CODE TO COMPUTE
RESONANCE INTEGRALS IN MIXTURES

by

Charles N. Kelber

Reactor Engineering Division

May 1963

Operated by The University of Chicago
under
Contract W-31-109-eng-38
with the
U. S. Atomic Energy Commission

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SUMMARY

1559/RE is an experimental IBM-704 code in FORTRAN language to compute the resonance integrals of isotopes in mixtures in the presence of hydrogenic moderation. There may be up to four isotopes, each with no more than 75 resolved resonance levels. Doppler broadening and interference scattering are included. No estimate is made of contributions from unresolved resonances. Typical running times are 30 min (with no Doppler broadening) to 90 min (with Doppler broadening) for problems involving 67 levels and unit lethargy widths.

I. EQUATIONS SOLVED

The collision density is given by an integral equation involving scattering by atoms of all species.⁽¹⁾ In this report we assume all atoms are heavy or light (moderator) and in the moderator terms we use the narrow-resonance approximation; we replace the collision density by its asymptotic form. In using the code presented here, the moderator constants should be adjusted to give the correct asymptotic form.

1559/RE solves the equations

$$F(U) = \frac{1}{\alpha} \int_{U-\Delta}^U F(U') A(U') dU' + \frac{\Sigma_m}{E(U)} \quad (1)$$

and

$$\text{RESINT}(i,j) = N_i \int_{U(E_U)}^{U(E_L)} F(U) E(U) \frac{\sigma_{ji}}{\Sigma_t} du \quad (2)$$

The term RESINT is the resonance integral times the atomic density. Also,

$F(U)$ = the collision density at lethargy U , per unit energy

E_U = upper energy limit (ev)

E_L = lower energy limit (ev)

$E(U) = e^{-UE_U}$

Σ_m = "moderator" scattering cross section

α = heavy atom scattering term; $\alpha = 4A/(A+1)^2$

Δ = maximum logarithmic decrement in energy from heavy atom scattering, in units of lethargy.

N_i = number of atoms of isotope i per barn-cm

σ_{ji} = absorption ($j=a$) or fission ($j=f$) cross section of isotope i at energy $E(U)$

$A(U)$ = heavy atom scattering cross section divided by the total cross section.

For each isotope the cross sections are found from:

resonance scattering:

$$\sigma_s = \sum_{K=1}^J \left(\frac{\sigma_{oK} \Gamma_{nK}}{\Gamma_K} \psi_K(E) + \sqrt{\sigma_{pt} \sigma_{ok} g \Gamma_{nk} / \Gamma_K} \chi_K(E) \right) ; \quad (3)$$

absorption:

$$\sigma_a = \sum_{K=J}^J \left(\sqrt{\frac{|E_K|}{E}} \frac{(\Gamma_{\gamma K} + \Gamma_{fK})}{\Gamma_K} \sigma_{oK} \psi_K(E) \right) ; \quad (4)$$

fission:

$$\sigma_f = \sum_{K=1}^J \left(\sqrt{\frac{|E_K|}{E}} \frac{\Gamma_{fK}}{\Gamma_K} \sigma_{oK} \psi_K(E) \right) . \quad (5)$$

The various symbols have their usual meanings; in particular,

σ_{pt} = potential scattering of isotope i

$\sigma_{ok} = (2.62 \times 10^6) g \Gamma_{nK} / (|E_K| \Gamma_K)$

g = statistical weight (assumed constant for all levels of isotope i)

Γ_{nK} = neutron width of resonance K (ev)

E_K = energy of K^{th} resonance (ev)

Γ_K = total width of K^{th} resonance (ev)

Γ_{fK} = fission width of K^{th} resonance (ev)

$\Gamma_{\gamma K}$ = gamma width of K^{th} resonance (ev)

The functions $\psi_K(E)$ and $\chi_K(E)$ are the familiar Doppler-broadened line shapes:

$$\psi(\xi, x) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-\xi^2(x-y)^2/4}}{1+y^2} dy ; \quad (6)$$

$$\chi(\xi, x) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{\infty} 2y \frac{e^{-\xi^2 (x-y)^2/4} dy}{1+y^2} ; \quad (7)$$

$$\xi = \left(\frac{A_i \Gamma_K^2}{4EkT} \right)^{1/2} ; \quad x = \frac{2}{\Gamma_K} (E - E_K) ,$$

where

A_i = isotope mass (amu)

kT = material temperature, ev.

If the temperature kT is exactly 0, the subroutine which generates ψ and χ is not used; instead, $\psi = 1/(1+x^2)$, and $\chi = 2x/(1+x^2)$ are used. The parameters α and $\Delta = \ln [1/(1-\alpha)]$ were not made isotope dependent since 1559/RE is an experimental code designed largely to evaluate the interference effects between similar isotopes. Since we expect to investigate situations where the heavy atom scattering is largely from atoms of mass A , say, we usually take $\alpha = 4A/(A+1)^2$. It is not conceptually difficult to make α and Δ isotope dependent and remove this source of error; the additional programming complication, however, is sufficient to cause this change to be put off to the future.

II. METHOD OF SOLUTION - COLLISION DENSITY

Equations (1) and (2) are solved by trapezoidal integration, the asymptotic solution $F = (\Sigma_{pt} + \Sigma_m)/E$ being used to get started. This method has been frequently used before [see, for example, Nordheim⁽¹⁾].

A fixed lethargy interval is used during the entire integration scheme. The interval is given by $D = \Delta/N$ (see Eq. 2), where N is input information. Values of N between 25 and 100 are recommended. If N is greater than 100, storage allocations are exceeded and the program causes the machine to print the input error: "N OUT OF RANGE" and proceeds to the next problem.

The integration is carried out over $10N$ steps. Then the upper energy is reset and the integration resumed until the lower energy is less than EL (input). The actual equations solved for the collision density are*

$$AJ_i = AJ_{i-1} - \frac{0.5}{\alpha} (F_{i-N-1} \cdot A_{i-N-1} + F_{i-N} A_{i-N}) + F_{i-1} \frac{A_{i-1}}{\alpha} \quad (8)$$

and

$$F_i = [D AJ_i + (\Sigma_m/E_i)] / \left(1 - 0.5 D \frac{A_i}{\alpha} \right) , \quad (9)$$

as suggested by Nordheim.⁽¹⁾

* AJ is a variable, not A times J .

The $N+1$ values necessary to get the set (8,9) started are obtained initially from the asymptotic solution

$$F_i = (\Sigma_{pt} + \Sigma_m)/E_i \quad , \quad \text{for} \quad E_i = E_U e^{(N+1-i)D} \quad , \\ i=1, \dots, N+1 \quad . \quad (10)$$

After the completion of $10N$ lethargy steps, the last $N+1$ values of collision density and the auxiliary quantities AJ_i are stored (on tape 2) and the process restarted, with the information now on tape 2 used to get the set (8,9) going.

A quantity printed out under the misnomer "flux" and equal to $E_i F_i$ is also calculated and is used in getting the resonance integrals (Eq. 2) by trapezoidal integration, using the lethargy step, D . The actual flux per unit lethargy is equal to the printed quantity divided by the total cross section.

III. METHOD OF SOLUTION - CROSS SECTIONS

The sums 3, 4, and 5 are evaluated directly at each energy. At temperature 0, the analytic representations $\psi = 1/(1+x^2)$ and $\chi = 2x/(1+x^2)$ are used for the line shapes.

For temperatures greater than zero, the functions $\psi_K(E)$ and $\chi_K(E)$ are calculated by use of the W subroutine. The W subroutine was written by O'Shea and Thatcher⁽²⁾ for the express purpose of computing resonance line shapes.

The function actually computed is the complex probability integral $W(z)$ defined by

$$W(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z-t} dt \quad . \quad (11)$$

Setting

$$z = \frac{\xi x}{2} + i \frac{\xi}{2} \quad ,$$

we obtain

$$\psi(\xi, x) = \frac{\xi \sqrt{\pi}}{2} \operatorname{Re} W \quad ; \quad \chi(\xi, x) = \xi \sqrt{\pi} \operatorname{Im} W$$

(see Eq. 6 and 7). The probability integral $W(z)$ is computed by use of continued fractions:

$$W(z) = e^{-z^2} + \frac{2iz\nu}{\sqrt{\pi}} \left[\frac{1}{\nu - 1/3 +} \frac{2/45}{\nu + 1/21 +} \dots \frac{\frac{2r(2r-1)}{(4r-3)(4r+1)(4r-1)^2}}{\nu + \frac{1}{(4r-1)} \frac{1}{(4r+3)} +} \dots \right] \dots ;$$

$$\nu = -1/(2z^2) \quad (12a)$$

In the asymptotic form,

$$W(z) \sim \frac{2iz}{\sqrt{\pi}} \left[\frac{1}{\nu-1} - \frac{2}{\nu-5} - \dots \frac{2r(2r-1)}{(\nu-4r-1)} \dots \right] ; \quad \nu = 2z^2 \quad (12b)$$

Convergence profile mappings were used to determine the number of terms necessary to obtain accuracy to five decimal places. Ellipses were then fitted to these profiles to ensure that an adequate number of terms was retained in the expansion for a given argument.

IV. INPUT PREPARATION

The first two cards contain 119 Alpha numeric characters in columns 2-72 (card 1) and 1-47 (card 2). Column 1, card 1 is left blank. Even if all the columns on card 1 or card 2 are blank, both cards must be present. In the program all isotopes with fission cross sections are to be listed first, and then the remainder. If this procedure is not followed, the absorption resonance integrals will be printed correctly but fission integrals will not. There are no other restrictions on the ordering of isotopic data.

The input is then:

card 1 }
card 2 } See above.

card 3: N, the number of subintervals per logarithmic decrement Δ .
 $0 < N \leq 100$. FORMAT, I3.

IP, the number of heavy isotopes. $0 < I \leq 4$. FORMAT, I3.

IFP, the number of fissionable isotopes, $0 < IFP \leq 4$. FORMAT, I3.

ICO, the number of subintervals per output statement,
 $0 < ICO \leq 1000$. FORMAT, I3.

EU, upper energy limit (ev). $0 < EU$. FORMAT, E12.6

EL, lower energy limit (ev). $0 < EL$. FORMAT, E12.6

AO, $4A/(A+1)^2$, A = heavy atom scattering mass (see text).
 $0 < AO$. FORMAT, E12.6

TEMP, heavy atom temperature, ev. $0 \leq T$. FORMAT, E12.6

SMOD, moderator scattering cross section (cm^{-1}). $0 < S \text{ MOD}$.
 FORMAT, E12.6

card 4: $J(1), \dots, J(IP)$ the number of resonance levels for isotopes 1, $\dots$,
 IP . $0 < J \leq 75$. FORMAT, I12

card 5 to card 4 + IP; on each card:

AMAS, the atomic mass (amu) of isotope i

SW, the statistical weight $\left[\frac{2J+1}{2(2I+1)} \right]$ of isotope i

SIGPT, the potential scattering cross section (barns) of isotope i

ABUN, the density of nuclei of isotope i (per barn-cm), FORMAT,
 4E12.6

Card 4 + IP + 1 to card 4 + IP + $\sum_{L=1}^{IP} J(L)$ on each and for the K^{th} resonance
 of isotope L :

$ER(K, L)$, energy (ev)

$\Gamma_{\gamma}(K, L)$, gamma width (ev)

$\Gamma_n(K, L)$, neutron width (ev)

$\Gamma_f(K, L)$, fission width (ev)

FORMAT 3E12.6

(N.B.: The data on each card obviously must refer to the same level;
 and the first $J(1)$ cards must refer to isotope 1, the next $J(2)$
 to isotope 2, etc)

For use with the Argonne Monitor system, all input is put on tape
 (logical tape 7). To run problems sequentially, simply stack the data cards
 for the various problems in sequence. Each set of data must be complete
 in itself, and there should be no extra cards between data decks. Avoid the
 use of resonances at $E_R(K, L) = 0$. This will cause a divide check; should
 there be an inaccurate level count, this can occur.

Table I

RESONANCE PARAMETERS (For problems discussed in text)

<u>Level Energy</u>	<u>Gamma Gamma</u>	<u>Gamma N</u>	<u>Gamma F</u>
<u>U²³⁵</u>			
-0.140000E-01	0.330000E-01	0.282000E-02	0.194000E-00
-0.200000E-01	0.330000E-01	0.340000E-06	0.860000E-01
0.273000E-00	0.290000E-01	0.290000E-05	0.990000E-01
0.420000E-00	0.270000E-01	0.120000E-05	0.213000E-00
0.910000E+00	0.300000E-01	0.137000E-04	0.330000E-00
0.114000E+01	0.440000E-01	0.172000E-04	0.125000E-00
0.203500E+01	0.350000E-01	0.770000E-05	0.120000E-01
0.282000E+01	0.300000E-01	0.300000E-05	0.700000E-01
0.316000E+01	0.310000E-01	0.323000E-04	0.155000E-00
0.360000E+01	0.370000E-01	0.460000E-04	0.450000E-01
0.484000E+01	0.250000E-01	0.520000E-04	0.400000E-02
0.545000E+01	0.330000E-01	0.220000E-04	0.375000E-01
0.580000E+01	0.330000E-01	0.160000E-04	0.375000E-01
0.620000E+01	0.330000E-01	0.270000E-04	0.375000E-01
0.638000E+01	0.450000E-01	0.280000E-03	0.150000E-01
0.709000E+01	0.330000E-01	0.109000E-03	0.220000E-01
0.879000E+01	0.410000E-01	1.000000E-03	0.520000E-01
0.928000E+01	0.330000E-01	0.122000E-03	0.440000E-02
0.970000E+01	0.330000E-01	0.400000E-04	0.375000E-01
0.101600E+02	0.330000E-01	0.640000E-04	0.375000E-01
0.106400E+02	0.330000E-01	0.330000E-04	0.375000E-01
0.111100E+02	0.330000E-01	0.470000E-04	0.375000E-01
0.116400E+02	0.330000E-01	0.680000E-03	0.260000E-02
0.123800E+02	0.420000E-01	0.137000E-02	0.180000E-01
0.132600E+02	0.330000E-01	0.990000E-03	0.375000E-01
0.138000E+02	0.330000E-01	0.150000E-03	0.375000E-01
0.141000E+02	0.330000E-01	0.200000E-03	0.375000E-01
0.145300E+02	0.330000E-01	0.15 E-03	0.4 E-01
<u>U²³⁸</u>			
0.668 E+02	0.25 E-01	0.148 E-02	
0.102 E+02	0.246 E-01	0.140 E-05	
0.21 E+02	0.25 E-01	0.900 E-02	
<u>Au¹⁹⁷</u>			
0.4906 E+01	0.125 E-00	0.156 E-01	

V. OUTPUT

Since the program is compiled to run on the Argonne Monitor system, all output is on tape 6. (Tape 2 is used as a scratch tape.)

The first page of output includes the problem identification (cards 1 and 2) and the input data on card 3. The rest of the input data, for each isotope in turn, are printed on the next pages. Each isotope starts a new page.

Following this are sheets labeled alternately: "Resonance Integral, Fission" with columns labeled ENERGY, COLLISION DENSITY, FLUX, RESINT ISOTOPE 1, etc. (Recall that the term "FLUX" is a misnomer since the quantity in question is just the energy times the collision density.) The entries on each page correspond to the quantities calculated during one major cycle of the code, 10N lethargy steps.

A typical code listing is given in Appendix A. Since the code is experimental, this listing is not necessarily the one in current use, but all the vital features of the code are present. Possible changes in the code are discussed in the next section.

VI. EARLY RESULTS AND PROGRAM OF FUTURE WORK

Results

An interesting case to study is a low-enrichment, high-conversion lattice. We took as an example a mixture of water and uranium in equal volumes. (The effects of rod size were neglected at this point.) The temperature was taken as 0°K and the heavy atom scattering mass was 238. Three U^{235} enrichments were studied: 1, 2, and 3 per cent. In addition, gold at 10^{-6} atom/(b-cm) was included to study the response of a typical monitor foil.

Resonance parameters are given in Table I; the U^{235} data were taken from Harvey⁽³⁾ and WCAP-1434⁽⁴⁾, whereas the data for U^{238} and gold come from BNL-325⁽⁵⁾.

We used a version of the code which calculated the real fluxes, and these are plotted, for 1% enrichment, in Fig. I. Also shown on Fig. I by means of dashed lines are the changes in the flux when calculated for 3% enrichment. The flux perturbations from the various resonances are clearly seen. Also to be noted are the effects of the 6.68-ev U^{238} resonance and the 4.84-ev U^{235} resonance on the gold resonance at 4.91 ev. The gold resonance integral over the energy range indicated is given in Table II for the various enrichments. The shielding mostly comes from U^{238} , but there is a small U^{235} effect.

Fig. I. Flux Per Unit Lethargy
in an H/U Mixture

Table II

RESONANCE INTEGRAL OF DILUTE GOLD
IN H:U = 1 MIXTURE.
ENERGY RANGE 3 - 10 ev.

Enrichment, %	Integral (b)
1	1357
2	1337
3	1333

(Resonance integral over this energy range,
1/E spectrum: 1445.)

Figure II shows graphs of the U^{235} resonance integrals as a function of enrichment. Based on moderator scattering per U^{235} atom, a larger variation in the cross section as well as a larger cross section would be expected. The U^{238} dominates the spectrum and suppresses the scattering effect. The shielding by the U^{238} amounts to about 20% of the cross section [see, e.g., the tabulation in Resonance Integral Newsletter No. 8⁽⁶⁾]. The ratio of capture to fission in U^{235} , α , also shown in Fig. II, is practically independent of enrichment.

For check purposes, infinite dilution integrals were calculated through use of small abundances, and these were checked against results obtained by use of the code RE-266,⁽⁷⁾ a code designed especially for computing infinite dilution integrals. For U^{235} , agreement was better than 0.1%.

Fig. II. Effective Resonance Integrals of U^{235} in $H/U = 1$ Mixture; and α of U^{235}

Future Program

The code is too slow. Future work has the main task of speeding the code. At temperatures other than $0^\circ K$, the W subroutine requires about 8 ms per entry and roughly triples the running time. It is not clear that a faster W subroutine exists; instead, it may prove useful to change the form of access to the W routine. In particular, with a larger machine with disc files, it will probably save time to enter the ψ and χ functions as a table for a given problem and refer to that. Some small gain can be made by changing the order of computing σ_0 , etc.; the main difficulty however, comes from the attempt to compute a sum over all levels.

It is not clear how to eliminate levels in a systematic way. The -1.4-ev level in U^{235} contributes about 2 b to the resonance

integral from 3 to 10 ev. Since some levels in the range 0-3 ev contribute much less than 2 b, mere displacement along the energy scale is not a good test. A test of $\sigma_0/(1+x^2)$ is not a time saver.

For the present, we make a survey of a problem by taking an actual decimal dump of a typical problem and examining the cross-section contributions PP SIGA, PP SIGH from each level. Levels whose contribution is small may then be removed from the data deck and the full problem run.

The use of a uniform mesh is clearly wasteful; a variable mesh spacing would help. In this case, small resonances or the resonance capture in elements of low abundance would have to be calculated analytically in regions of large mesh spacing.

The investigation of these points together with such obvious topics as inclusion of unresolved resonances, effects of lumping, differences in scattering mass, and exact moderator effect forms an ambitious program of work.

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ACKNOWLEDGEMENT

I wish to acknowledge the patient and helpful assistance given me by Mrs. D. Bingaman and other members of the Applied Mathematics Division. Messrs. Paul J. Persiani and A. E. McCarthy were helpful in the selection of the U²³⁵ negative energy parameters and the calculation of resonance integrals at infinite dilution.

APPENDIX A

Typical Fortran Listing for 1559/RE

* 004 3/7/63 MEYER, L. 1559/RE 3627 *** 6296
 0307631503 C KELBER 44111-051111559RE 70420
 \$COMPILE 3 03 RM 3/7/63 1559

C 1559/RE.GEAR FOUR. A PROGRAM TO COMPUTE THE RESONANCE INTEGRALS
 C FOR UP TO FOUR ISOTOPES WITH AS MANY AS 75 LEVELS EACH.
 C PLEASE RETURN ALL RESULTS TO C.N.KELBER,D-208.
 DIMENSIONE(1000),TPSIGA(4),TPSIGH(4),TPSIGS(4),
 XJ(4),GAMT(75,4),GG(75,4),GN(75,4),GF(75,4),ZETA(75,4),AMAS(4),
 XEX(75,4),ER(75,4),PSY(75,4),CHY(75,4),SIGO(75,4),SW(4),ABUN(4),
 XPPSIGA(75,4),PPSIGH(75,4),PPSIGS(75,4),SIGPT(4),
 X PRAT(1000,4),PRFT(1000,4),A(1000),G(101),H(101),
 XAJ(1000),F(1000),PHY(1000),RESINT(1000,4),P(20),Z(5)
 DIMENSIONASTART(4),FSTART(4)

SAN ALF N
 SAIP ALF IP
 SAEU ALF EU
 SAEL ALF EL
 SAAO ALF AO
 SAATE ALF TEMP
 SASMO ALF SMOD

1 FORMAT(12A6)
 2 FORMAT(4I3,5E12.6)
 3 FORMAT(4I12)
 4 FORMAT(4E12.6)

410 READINPUTTAPE7,1,(P(IA),IA=1,20)
 READINPUTTAPE7,2,N,IP,IFP,ICOUNT,EU,EL,AO,TEMP,SMOD
 READINPUTTAPE7,3,(J(L),L=1,IP)
 READINPUTTAPE7,4,(AMAS(L),SW(L),SIGPT(L),ABUN(L),L=1,IP)
 DO5L=1,IP
 JL=J(L)
 5 READINPUTTAPE7,4,(ER(K,L),GG(K,L),GN(K,L),GF(K,L),K=1,JL)
 6 FORMAT(1H1/1H0/1H0/1H0/1H0/

X94H 1559 RE A PROGRAM TO COMPUTE THE EFFECTS OF
 XINTERFERENCE BETWEEN RESONANCES///
 X61H PROBLEM IDENTIFICATION//
 X)

7 FORMAT(20A6)
 WRITEOUTPUTTAPE6,6
 WRITEOUTPUTTAPE6,7,(P(IA),IA=1,20)
 8 FORMAT(1H1/1H0/1H0/

X64H INPUT DAT
 XA//)

9 FORMAT(65H FOR THIS
 X PROBLEM,//43H THE LOGARITHMIC DECREMENT IS DIVIDED INTO 13,21H IN
 XTERVALS.THERE ARE 13,14H ISOTOPES,AND 13,17H OF THEM FISSION.//)
 10 FORMAT(20H THE UPPER ENERGY ISE12.5,17H EV.,THE LOWER ISE12.5,35H
 XEV. HEAVY ATOM SCATTERING ALPHA ISE12.5//26H THE TEMPERATURE IN EV
 X. ISE12.5,28H THE MODERATOR SCATTERING ISE12.5,8H PER CM.//))

11 FORMAT(71H RESULTS ARE PRINTED A
 XT INTERVALS OF 13,16H LETHARGY STEPS.//)
 WRITEOUTPUTTAPE6,9,N,IP,IFP
 WRITEOUTPUTTAPE6,10,EU,EL,AC,TEMP,SMOD
 WRITEOUTPUTTAPE6,11,ICOUNT

C IN CASE OF INPUT ERROR

12 FORMAT(32H INPUT ERROR. SEE ON LINE PRINT.)

C TEST INPUT

13 FORMAT(7H ERROR.A6,31H OUT OF RANGE.RETURN TO SENDER.//)
 ATEMP=TEMP+1.E-9

II=I

14 IF(N)15,15,17

```

15 WRITEOUTPUTTAPE6,12
16 PRINT13,AN
   II=1
17 IF(IP)18,18,20
18 WRITEOUTPUTTAPE6,12
19 PRINT13,AIP
   II=1
20 IF(100-N)21,24,24
21 WRITEOUTPUTTAPE6,12
22 PRINT13,AN
   II=1
23 EQUIVALENCE(Z(1),EU),(Z(2),EL),(Z(3),AO),(Z(4),ATEMP),
   X(Z(5),SMOD)
24 DO34J=1,5
25 IF(Z(J))26,26,34
26 WRITEOUTPUTTAPE6,12
28 GO TO(29,30,31,32,33),J
29 PRINT13,AEU
   II=1
   GO TO 34
30 PRINT13,AEL
   II=1
   GO TO 34
31 PRINT13,AAO
   II=1
   GO TO 34
32 PRINT13,AATE
   II=1
   GO TO 34
33 PRINT13,ASMOD
   II=1
   GO TO 34
34 CONTINUE
35 IF(II-1)37,36,36
36 GOTO410
37 GOTO40
C   READ OUT ISOTOPE DATA
50 FORMAT(1H1//67H                                     IN
   XPUT DATA,ISOTOPEI3//)
51 FORMAT(25H      THIS ISOTOPE HAS14,8H LEVELS.//)
52 FORMAT(21H      ATOMIC MASS=E12.6,12H  STAT.WT.=E12.6,
   X13H  POT.SCAT.=E12.6,13H  ABUNDANCE=E12.6//)
53 FORMAT(80H      LEVEL ENERGY          GAMMA GAMMA          GAM
   XMA N          GAMMA F//)
54 FORMAT(4E20.6)
40 DO46L=1,IP
41 WRITEOUTPUTTAPE6,50,L
42 WRITEOUTPUTTAPE6,51,J(L)
43 WRITEOUTPUTTAPE6,52,AMAS(L),SW(L),SIGPT(L),ABUN(L)
44 WRITEOUTPUTTAPE6,53
45 JL=J(L)
46 WRITEOUTPUTTAPE6,54,{ER(K,L),GG(K,L),GN(K,L),
   XGF(K,L),K=1,JL)
   GOTO70
70 TSIGPT=0.
71 DO72L=1,IP
72 TSIGPT=TSIGPT+SIGPT(L)*ABUN(L)
73 D=LOGF(1./(1.-AO))/FLOATF(N)
74 IMAX=10*N
75 GOTO80
C   AFTER THE INPUT HAS BEEN READ IN WE GET SET.
80 IB=0

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81 E1=EU
82 D083J=1,IP
83 ASTART(J)=0.
84 D085J=1,IFP
85 FSTART(J)=0.
   GOT09C
90 CONTINUE
91 REWIND2
92 REWIND3
93 REWIND4
95 D0110I=1,IMAX
   PSIGA=0.
   PSIGS=0.
96 U=FLOATF(I)*D
97 E(I)=E1/EXPF(U)
   D0105L=1,IP
   TPSIGA(L)=0.
   TPSIGH(L)=0.
   TPSIGS(L)=0.
   JL=J(L)
   D0100K=1,JL
   GAMT(K,L)=GG(K,L)+GN(K,L)+GF(K,L)
597 IF(TEMP)598,598,98                                XGAMT
598 EX(K,L)=2.*(E(I)-ER(K,L))/GAMT(K,L)
599 PSY(K,L)=1./(1.+EX(K,L)**2)
600 CHY(K,L)=2.*EX(K,L)/(1.+EX(K,L)**2)
   GOT099
98 ZETA(K,L)=SQRTF((AMAS(L)*GAMT(K,L)**2)/(4.*E(I)*TEMP))
   EX(K,L)=2.*(E(I)-ER(K,L))/GAMT(K,L)
   CALLW(ZETA(K,L)*EX(K,L)/2.,ZETA(K,L)/2.,REW,AIMW)
   PSY(K,L)=ZETA(K,L)*.8862265*REW
   CHY(K,L)=ZETA(K,L)*1.772453*AIMW
99 SIGO(K,L)=(2.62E+6)*SW(L)*GN(K,L)/(ABSF(ER(K,L))*GAMT(K,L))
   PPSIGA(K,L)=(GG(K,L)+GF(K,L))*SIGO(K,L)*PSY(K,L)
   X*SQRTF(ABSF(ER(K,L))/E(I))/GAMT(K,L)
   PPSIGH(K,L)=GF(K,L)*PPSIGA(K,L)/(GG(K,L)+GF(K,L))
   TPSIGA(L)=TPSIGA(L)+ABUN(L)*PPSIGA(K,L)
   TPSIGH(L)=TPSIGH(L)+ABUN(L)*PPSIGH(K,L)
   PPSIGS(K,L)=(GN(K,L)*SIGO(K,L)*PSY(K,L)/GAMT(K,L))+
   X*SQRTF(SIGPT(L)*SIGO(K,L)*SW(L)*GN(K,L)/GAMT(K,L))*CHY(K,L)
100 TPSIGS(L)=TPSIGS(L)+ABUN(L)*PPSIGS(K,L)                END K
   PSIGA=PSIGA+TPSIGA(L)
105 PSIGS=PSIGS+TPSIGS(L)
106 D0109L=1,IP
   PRAT(I,L)=TPSIGA(L)/(PSIGS+PSIGA+TSIGPT+SMOD)
109 PRFT(I,L)=TPSIGH(L)/(PSIGS+PSIGA+TSIGPT+SMOD)
110 A(I)=(PSIGS+TSIGPT)/((PSIGS+TSIGPT+PSIGA+SMOD)*A0)
   GOT012C
C   PREPARE TO GENERATE FLUXES
120 IF(IB)200,125,200
C   IF IB IS ZERO WE GENERATE SOME STARTING FLUXES
C   THE ASYMPTOTIC VALUES ARE USED
125 MN=N+1
   D0130J=1,MN
   AD=FLOATF(N+1)*D
   EUU=EU*EXPF(AD)
   UU=FLOATF(J)*D
   AE=EUU/EXPF(UU)
   G(J)=(TSIGPT+SMOD)/AE
130 H(J)=TSIGPT/(A0*(TSIGPT+SMOD))
131 WRITETAPE2,(G(J),J=1,MN)
   WRITETAPE2,(H(J),J=1,MN)

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      ENDFILE2
      REWIND2
132  FF=G(N+1)
      AA=H(N+1)
      AAJ=(TSIGPT/(EU*D))-0.5*FF*AA
      GOT02C)
C     NOW WE GO INTO THE ITERATION ROUTING
C     CALCULATE F(I) AND PHY(I)
200  WRITEOUTPUTTAPE6,202
202  FORMAT(1H1/85H
      X   RESONANCE INTEGRALS,ABSORPTION//119H      ENERGY COLLISION
      XDENSITY          FLUX RESINT ISOTOPE 1 RESINT ISOTOPE 2 RESINT
      XISOTOPE 3 RESINT ISOTOPE 4//)
201  MN=N+1
      READTAPE2,(G(I),I=1,MN)
      READTAPE2,(H(I),I=1,MN)
      AJ(1)=AAJ-0.5*(G(1)*H(1)+G(2)*H(2))+FF*AA
      F(1)=(D*AJ(1)+(SMOD/E(1)))/(1.-0.5*D*A(1))
      REWIND2
205  DO220I=2,IMAX
      NN=N+2
      IF(I-NN)210,215,215
210  AJ(I)=AJ(I-1)-0.5*(G(I)*H(I)+G(I+1)*H(I+1))
      X+F(I-1)*A(I-1)
      F(I)=(D*AJ(I)+(SMOD/E(I)))/(1.-0.5*D*A(I))
      PHY(I)=F(I)*E(I)
      GOT022)
215  NI=I-N
216  AJ(I)=AJ(I-1)-0.5*(F(NI-1)*A(NI-1)+F(NI)*A(NI))
      X+F(I-1)*A(I-1)
217  F(I)=(D*AJ(I)+(SMOD/E(I)))/(1.-0.5*D*A(I))
218  PHY(I)=E(I)*F(I)
      GOT022)
220  CONTINUE
      J=IMAX-N-1
      WRITETAPE2,(F(I),I=J,IMAX)
      WRITETAPE2,(A(I),I=J,IMAX)
      ENDFILE2
      REWIND2
C     TAPE 2 IS NOW READY FOR THE NEXT TIME THRU.
C     SET THE AUXILLARY CONSTANTS
      AAJ=AJ(IMAX)
      FF=F(IMAX)
      AA=A(IMAX)
      GOT023)
C     NOW START THE EDIT ROUTINE
230  DO240L=1,IP
      RESINT(1,L)=ASTART(L)
232  DO240I=2,IMAX
235  RESINT(I,L)=RESINT(I-1,L)+0.5*D*(PHY(I)*PRAT(I,L)
      X+PHY(I-1)*PRAT(I-1,L))
240  CONTINUE
      GOT0242
242  IF(IP-1)243,243,247
243  DO245I=1,IMAX
      RESINT(I,2)=0.
      RESINT(I,3)=0.
245  RESINT(I,4)=0.
      GOT0255
247  IF(IP-2)255,248,250
248  DO249I=1,IMAX

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SEE 230

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      RESINT(I,3)=0.
249 RESINT(I,4)=0.
      GOTO255
250 IF(IP-3)255,251,255
251 D0252I=1,IMAX
252 RESINT(I,4)=0.
      GOTO255
255 ICON=1
256 D0260I=1,IMAX
      ICON=ICON+1
      IF(ICON-ICOUNT)260,257,260
257 WRITEOUTPUTTAPE6,265,(E(I),F(I),PHY(I),
      XRESINT(I,1),RESINT(I,2),RESINT(I,3),RESINT(I,4))
      ICON=1
260 CONTINUE
265 FORMAT(7E17.5)
      GOTO465
465 D0466J=1,IP
466 ASTART(J)=RESINT(IMAX,J)
      GOTO266
266 IF(IFP)270,350,270
270 WRITEOUTPUTTAPE6,272
272 FORMAT(1H1/82H
      X   RESONANCE INTEGRALS,FISSION//119H           ENERGY COLLISION DEN
      XSITY           FLUX RESINT ISOTOPE 1 RESINT ISOTOPE 2 RESINT ISO
      XTOPE 3 RESINT ISOTOPE 4//)
      GOTO280
280 D0290L=1,IFP

      RESINT(1,L)=FSTART(L)
282 D0291I=2,IMAX
285 RESINT(I,L)=RESINT(I-1,L)+.5*D*(PHY(I)*PRFT(I,L)
      X+PHY(I-1)*PRFT(I-1,L))
290 CONTINUE
292 IF(IFP-1)293,293,297
293 D0295I=1,IMAX
      RESINT(I,2)=0.
      RESINT(I,3)=0.
295 RESINT(I,4)=0.
      GOTO303
297 IF(IFP-2)303,298,300
298 D0299I=1,IMAX
      RESINT(I,3)=0.
299 RESINT(I,4)=0.
300 IF(IFP-3)303,303,303
301 D0302I=1,IMAX
302 RESINT(I,4)=0.
      GOTO303
303 ICON=1
304 D0310I=1,IMAX
      ICON=ICON+1
      IF(ICON-ICOUNT)310,305,310
305 WRITEOUTPUTTAPE6,265,(E(I),F(I),PHY(I),
      XRESINT(I,1),RESINT(I,2),RESINT(I,3),RESINT(I,4))
      ICON=0
310 CONTINUE
311 D0312J=1,IFP
312 FSTART(J)=RESINT(IMAX,J)
      GOTO350
350 FE=E(IMAX)
351 IF(FE-EL)400,400,380
380 IB=IB+1
      GOTO385
385 E1=FE
      GOTO90
C   START OVER AGAIN
400 WRITEOUTPUTTAPE6,405
      GOTO410
405 FORMAT(1H1/34H           THIS PROBLEM IS COMPLETE.)
      END ( 1 , 1 , 0 , 1 , 0 )

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SEE 265

SEE 310