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**INCORPORATION OF EPITHERMAL PROTON
CHEMICAL BINDING EFFECTS IN HAMMER**

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INCORPORATION OF EPITHERMAL PROTON CHEMICAL BINDING EFFECTS IN HAMMER*

Arthur Buslik and John Herczeg

I. Introduction

This reports those changes to the hydrogen epithermal library in HAMMER, and those changes to the HAMMER program^(1,2) itself, which are required to incorporate the effects of the chemical binding and thermal motion of the protons in water on the epithermal neutron flux and reaction rates. The changes to the hydrogen epithermal library required are changes to the slowing-down power $\xi\sigma_s$, the Greuling-Goertzel parameter γ , and the P-1 component of the scattering cross-section τ_{s1} . These changes are based on the kernel developed by Cady, Kirouac and McInerney.⁽³⁾

The changes to the HAMMER program which are required consist of changes to the program to ensure that the slowing-down power $\xi\sigma_s$ and the Greuling-Goertzel parameter γ for hydrogen are used in all of the subroutines (HAMMER at present assumes in certain of its subroutines that the hydrogen slowing-down power $\xi\tau_s$ is equal to the P-0 component of the scattering cross-section σ_{s0} , and that the parameter γ for hydrogen is equal to unity). In addition, changes are required to modify the Dancoff factor used in the Pu-240 1 eV resonance treatment and the cosine current calculation of the lattice escape probabilities used in the resonance absorption calculation. These changes are along the lines discussed in references 7 and 8.

Another approach to obtaining cross-sections for hydrogen which account for epithermal chemical binding effects is to obtain values of $\xi\sigma_s$ by multigroup so as to reproduce the Corngold asymptotic expansion fluxes exactly for plain water, and to leave the value of the Greuling-Goertzel parameter γ equal to unity. This is the approach used by J. Hardy, Jr.⁽⁶⁾ as suggested by E. M. Colbard. However, by also varying γ (as is done in the method presented here), one would hope to get better accuracy in cases of heavy absorption. Moreover, this is more consistent with the changes made in the resonance absorption treatment for the Pu-240 1 eV resonance.

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The changes to the HAMMER hydrogen epithermal library will first be presented, and a comparison of fluxes as calculated with these hydrogen cross-sections and parameters to fluxes as calculated by the Corngold asymptotic expansion^(4,5) will be presented. This comparison acts as a check on the correctness of the hydrogen cross-sections and parameters obtained. (The comparisons do not check σ_{g1} .)

II. The Changes to the HAMMER Epithermal Library

The formulae used for the values of ξ_{gs} and γ for hydrogen are derived in reference 8. These formulae are:

$$\xi_{gs}(E) = \left(1 - \frac{1}{2} \frac{kT^*}{E}\right)^2, \quad (1)$$

and

$$\gamma(E) = 1 - \frac{1}{2} \frac{kT^*}{E} \quad (2)$$

Here σ is the asymptotic value of the hydrogen scattering cross-section, and was taken as 20.4 barns in the computations; E is the neutron energy and T^* is the effective temperature associated with the short collision time approximation⁽⁹⁾. The value of T^* used in the computations corresponds to a moderator temperature of 500°F (= 533°K) in a Melkin kernel model.⁽¹⁰⁾ The value of T^* obtained is 1453°K. One should note that the values of the hydrogen epithermal library parameters are therefore dependent on the water temperature, and that the calculated parameters correspond to a water temperature of 500°F. The temperature dependence of the parameters is rather weak, however, since T^* depends rather weakly on T . (At room temperature T^* is 1360°K, while at 533°K, T^* is 1453°K.)

The value of $\sigma_{g1}(E)$ is the same as in an effective temperature kernel model, and is given by

$$\sigma_{g1}(E) = \frac{2}{3} \sigma \left[1 - \frac{1}{2} \frac{kT^*}{E} + \frac{5}{16} \left(\frac{kT^*}{E}\right)^2 - \frac{1}{4} \left(\frac{kT^*}{E}\right)^3 \right] \quad (3)$$

This formula was taken from the Cady, Kirouac and McInerney article.⁽³⁾

The value of $\sigma_{80}(E)$ is also the same as that for an effective temperature kernel and the formula for $\tau_{80}(E)$,

$$\sigma_{80}(E) = \sigma \left(1 + \frac{1}{2} \frac{kT^*}{E} \right), \quad (4)$$

is also taken from reference 3.

Group averages of the various parameters were obtained by taking the arithmetic average of the quantity at the upper and lower energies bounding the multigroup. For example,

$$\bar{\sigma}_{s,j} = \frac{1}{2} [\sigma_{s0}(E_{j+1}) + \sigma_{s0}(E_j)]$$

where E_j and E_{j+1} are the energies bounding the j th multigroup.

The chemical binding effects were included for energies up to and including group 36; for energies greater than the upper cutpoint of this group, chemical binding effects were neglected and the values of the parameters used in the previous library for hydrogen were used.

The hydrogen cross-sections obtained are given in Table I. The isotope identity number is 2001001, and the cross-sections are on tape N35838. Note that the cross-sections in Table I are not in the same format as a printout of the HAMMER epithermal library -- some columns have been omitted and others have been rearranged. The column labelled "age number" is what we have denoted by γ . The omitted parameters (inelastic scattering, fission cross-section, neutrons per fission) are all zero for hydrogen.

III. Verification of the Hydrogen Cross-Section Changes

In order to verify the cross-section changes made, the neutron fluxes in a medium composed of plain water (with oxygen scattering effects neglected) were computed by means of the Corngold asymptotic expansion and compared to the fluxes obtained by running a HAMMER problem using the new hydrogen library. In addition, water poisoned with a $\frac{1}{v}$ absorber was considered. Five terms in the Corngold asymptotic expansion were used. It turns out that to this order the expansion is identical to an expansion derived in a much simpler fashion by Parks⁽¹¹⁾ (see also pages 103 ff of reference 5). The

TABLE I. Hydrogen cross-sections including binding effects.

IDENT=2001UG1, MASS= 1.0091 H1 CADDY MODEL (BUSL: 5/74
 PARTIAL CROSS SECTIONS (BARNS)

GRP	SIGMA-S0	SIGMA-C	AGE NUMBER	SIGMA-S1	X1.SIGMA-S0
1	1.050000E+00	0.	1.000000E+00	7.000000E-01	1.050000E+00
2	1.300000E+00	0.	1.000000E+00	8.670000E-01	1.300000E+00
3	1.550000E+00	0.	1.000000E+00	1.033000E+00	1.550000E+00
4	1.850000E+00	0.	1.000000E+00	1.233000E+00	1.850000E+00
5	2.150000E+00	0.	1.000000E+00	1.433000E+00	2.150000E+00
6	2.500000E+00	0.	1.000000E+00	1.667000E+00	2.500000E+00
7	2.900000E+00	0.	1.000000E+00	1.933000E+00	2.900000E+00
8	3.350000E+00	0.	1.000000E+00	2.233000E+00	3.350000E+00
9	3.850000E+00	0.	1.000000E+00	2.567000E+00	3.850000E+00
10	4.400000E+00	1.000000E+04	1.000000E+00	2.933000E+00	4.400000E+00
11	5.050000E+00	1.000000E+04	1.000000E+00	3.367000E+00	5.050000E+00
12	5.750000E+00	1.000000E+04	1.000000E+00	3.834000E+00	5.750000E+00
13	6.500000E+00	1.000000E+04	1.000000E+00	4.334000E+00	6.500000E+00
14	7.350000E+00	1.000000E+04	1.000000E+00	4.900000E+00	7.350000E+00
15	8.250000E+00	1.000000E+04	1.000000E+00	5.500000E+00	8.250000E+00
16	9.300000E+00	1.000000E+04	1.000000E+00	6.200000E+00	9.300000E+00
17	1.045000E+01	1.000000E+04	1.000000E+00	6.967000E+00	1.045000E+01
18	1.160000E+01	1.000000E+04	1.000000E+00	7.734000E+00	1.160000E+01
19	1.270000E+01	2.000000E+04	1.000000E+00	8.467000E+00	1.270000E+01
20	1.375000E+01	2.000000E+04	1.000000E+00	9.167000E+00	1.375000E+01
21	1.520000E+01	2.000000E+04	1.000000E+00	1.013000E+01	1.520000E+01
22	1.680000E+01	3.000000E+04	1.000000E+00	1.120000E+01	1.680000E+01
23	1.810000E+01	4.000000E+04	1.000000E+00	1.207000E+01	1.810000E+01
24	1.880000E+01	5.000000E+04	1.000000E+00	1.253000E+01	1.880000E+01
25	1.930000E+01	6.000000E+04	1.000000E+00	1.287000E+01	1.930000E+01
26	1.960000E+01	8.000000E+04	1.000000E+00	1.307000E+01	1.960000E+01
27	1.980000E+01	1.000000E+03	1.000000E+00	1.320000E+01	1.980000E+01
28	1.990000E+01	1.300000E+03	1.000000E+00	1.327000E+01	1.990000E+01
29	2.000000E+01	1.700000E+03	1.000000E+00	1.333000E+01	2.000000E+01
30	2.010000E+01	2.200000E+03	1.000000E+00	1.340000E+01	2.010000E+01
31	2.020000E+01	2.800000E+03	1.000000E+00	1.347000E+01	2.020000E+01
32	2.030000E+01	3.600000E+03	1.000000E+00	1.353000E+01	2.030000E+01
33	2.030000E+01	4.400000E+03	1.000000E+00	1.353000E+01	2.030000E+01
34	2.040000E+01	4.900000E+03	1.000000E+00	1.360000E+01	2.040000E+01
35	2.040000E+01	5.600000E+03	1.000000E+00	1.360000E+01	2.040000E+01
36	2.041900E+01	6.300000E+03	9.990900E-01	1.355600E+01	2.036300E+01
37	2.042400E+01	7.200000E+03	9.988400E-01	1.355700E+01	2.035200E+01
38	2.043100E+01	8.100000E+03	9.985100E-01	1.354500E+01	2.033900E+01
39	2.043900E+01	9.200000E+03	9.980800E-01	1.353000E+01	2.032200E+01
40	2.045000E+01	1.040000E+02	9.975300E-01	1.351200E+01	2.030000E+01
41	2.046500E+01	1.180000E+02	9.968400E-01	1.349000E+01	2.027100E+01
42	2.048300E+01	1.340000E+02	9.959400E-01	1.346100E+01	2.023500E+01
43	2.050600E+01	1.520000E+02	9.947800E-01	1.342500E+01	2.018800E+01
44	2.053700E+01	1.720000E+02	9.933000E-01	1.338100E+01	2.012800E+01
45	2.057500E+01	1.950000E+02	9.914000E-01	1.332700E+01	2.005100E+01
46	2.062500E+01	2.210000E+02	9.889600E-01	1.325100E+01	1.995200E+01
47	2.068900E+01	2.500000E+02	9.858200E-01	1.318100E+01	1.982600E+01
48	2.077100E+01	2.840000E+02	9.817900E-01	1.309400E+01	1.966400E+01
49	2.087700E+01	3.220000E+02	9.766200E-01	1.298000E+01	1.945700E+01
50	2.101300E+01	3.640000E+02	9.699800E-01	1.283200E+01	1.919400E+01
51	2.118800E+01	4.130000E+02	9.613600E-01	1.265800E+01	1.885500E+01
52	2.141200E+01	4.680000E+02	9.504100E-01	1.247900E+01	1.842800E+01
53	2.173400E+01	5.370000E+02	9.345300E-01	1.222700E+01	1.782200E+01
54	2.218800E+01	6.229000E+02	9.123600E-01	1.190500E+01	1.698400E+01

CAPTURE INTEGRAL = 1.33403E+01

FISSION INTEGRAL = 0.

expansion, to the order given, may be written in the form

$$E\phi(E) = 1 - \frac{3R}{\rho} + \frac{6R^2+1}{\rho^2} - \frac{10R^3 + \frac{4}{3}R}{\rho^3} + \left[\frac{15}{4} + \frac{43}{4}R^2 + 15R^4 - \frac{1}{2} \frac{B_{av}}{T^2} \right] \frac{1}{\rho^4} \quad (5)$$

where

$$R = \frac{\Sigma_a(RT^*)}{\Sigma}, \quad \rho = \sqrt{\frac{E}{R.T^*}}, \quad B_{av}^2 = \int_0^\infty (\hbar\omega)^2 f(\omega) d\omega \quad (6)$$

and the effective temperature is given by

$$RT^* = \frac{1}{2} \int_0^\infty \hbar\omega f(\omega) d\omega \coth \frac{\hbar\omega}{2kT}$$

Here $f(\omega)$ is the phonon frequency spectrum; for the Nelkin model it is given by

$$f(\omega) = \sum_{i=1}^4 \frac{A_i}{\hbar\omega} \delta(\omega - \omega_i) \quad (7)$$

where

$A_1 = 18$	$\hbar\omega_1 = 0$
$A_2 = 2.32$	$\hbar\omega_2 = .06 \text{ eV}$
$A_3 = 5.84$	$\hbar\omega_3 = .205 \text{ eV}$
$A_4 = 2.92$	$\hbar\omega_4 = .481 \text{ eV}$

(8)

It is assumed that the absorption cross-section has a $\frac{1}{v}$ energy dependence; the quantity Σ is the asymptotic macroscopic scattering cross-section of hydrogen ($= 20.4 N^H$, where N^H is the atom density of hydrogen). The quantity B_{av}^2 is computed to be

$$B_{av}^2 = .087981,$$

in a Nelkin model.

Computations of $E\phi(E)$ from Eq. (5) were first performed corresponding to room temperature water; these were compared to computations done by J. Hardy and reported in reference 6 (a larger version of Figure 1 of

reference 6 was obtained directly from J. Hardy.) The purpose of this comparison was to verify our use of the Corngold asymptotic expansion. J. Hardy, Jr. used seven terms in the expansion, while we used five terms. Agreement within .2% was obtained. Calculations for both a plain water case and water poisoned such that the absorption cross-section (including the hydrogen absorption) was 6 barns per hydrogen atom at .0253 eV were performed.

Calculations of epithermal fluxes by the Corngold asymptotic expansion were then performed at reactor operating temperature (more precisely, 500°F = 533°K). The calculations were for plain water and for water poisoned with a $\frac{1}{v}$ absorber such that the poison absorption cross-section per hydrogen atom was 6 barns at .0253 eV. The results are compared to similar cases at room temperature in Figure 1. The effects of moderator temperature on the epithermal flux is seen to be fairly small.

Comparison of epithermal fluxes as calculated by the Corngold asymptotic expansion, and by the HAMMER program with the new hydrogen library representing hydrogen bound in water, are presented in Figure 2. The same figure shows the fluxes as calculated with the old hydrogen library which corresponds to a free proton at rest model. These comparisons are for the case of plain water; Figure 3 gives a similar comparison for the case of water poisoned with a $\frac{1}{v}$ absorber, with the poison absorption being 6 barns per hydrogen atom at .0253 eV. The fluxes calculated using the new HAMMER hydrogen cross-section set agree rather well with the Corngold expansion fluxes, and represent a considerable improvement over those calculated with the old HAMMER hydrogen cross-section set.

IV. The Changes to the HAMMER Program

In addition to the changes to the HAMMER epithermal library, it is necessary to make changes to the HAMMER program in order that chemical binding effects be taken into account properly.

The first of these changes is in the subroutine SØRE to ensure that the library values of ξ_0 and v for hydrogen are used in the heterogeneous part

of the slowing-down calculation. Originally, HAMMER treated the slowing-down density due to hydrogen everywhere by the equation

$$\frac{dq_H}{du} + q_H = \Sigma_{sH}\phi,$$

where q_H is the slowing-down density due to hydrogen, Σ_{sH} is the scattering cross-section due to hydrogen, and ϕ is the flux per unit lethargy. (See reference 2 for a good description of the HAMMER code from the viewpoint of the physical approximations and numerical techniques used.)

HAMMER was later modified so that in that part of the above-thermal calculation where the homogeneous slowing-down calculation is done the slowing-down density due to hydrogen is treated by

$$Y_H \frac{dq_H}{du} + q_H = \xi_H \Sigma_{sH} \phi$$

The homogeneous slowing-down calculation is done in subroutine SLODON. However, the SØRE subroutine was left unmodified.

The primary reason that the changes in the subroutine SØRE are important is that the regionwise multigroup fluxes and slowing-down densities calculated in the heterogeneous part of the calculation are used in the calculation of the resonance absorption probability. In particular (see Eq. (73) of reference 2), the resonance absorption probability for a resonance with resonance integral I is given by

$$A = 1 - \exp \left\{ - (N_0 I \bar{\phi}_0 V_0) / \sum_n q_{ni} V_n \right\}$$

where q_{ni} is the slowing-down density in the nth region at the lower energy limit of the ith multigroup (before the ith multigroup resonance absorption depletes the slowing-down density), and is due to all isotopes, both hydrogen and heavy elements. The quantity $\bar{\phi}_0 V_0$ is the integral of the ith multigroup flux over the regions containing the resonance isotope, and N_0 is the number density of the resonance absorber averaged over these regions. Consequently, the resonance absorption probability is affected directly by the slowing-down densities and fluxes entering into the heterogeneous part of the above-thermal HAMMER calculation.

In addition to the changes in the SØRE subroutine, changes must be made to the Dancoff factor calculation and the calculation of the collision probability calculations used in the resonance integral calculation for the Pu-240 1 eV resonance. In point of fact, the changes are made for all resonances which occur in multigroups 53 and 54. They are made only on option in the program. The option is used whenever the 30th element on the batch control card is a 1. (This sets a flag ICADY equal to unity in the program.)

Before discussing these changes in detail, it should be pointed out that the older version of HAMMER did not recalculate the Dancoff factor in each multigroup, but rather used the Dancoff factor calculated in a given multigroup in all succeeding multigroups. Thus the Dancoff factor, if it was calculated at all, was calculated only once per problem. Whether or not the collision probabilities used in the resonance integral calculation are obtained from a formula using a Dancoff factor or whether they are calculated by the method of cosine currents depends on whether the flux across the lattice cell is sufficiently flat (see reference 2 here). If the flux is sufficiently flat, then a parameter KEY is set equal to unity, and the Dancoff factor method is used when the resonance absorber is in the fuel pellet. However, once the parameter KEY is set equal to unity it is not reset in any succeeding multigroup, and moreover the collision probability table is not recalculated in the succeeding multigroup. This had to be changed in order to modify the resonance integral calculation for the Pu-240 1 eV resonance so that proton chemical binding effects could be taken into account. Changes were therefore made to the subroutine FLUX so that the Dancoff factor would be recalculated in each multigroup.

In accordance with the method described in references 7 and 8, the modifications to the Dancoff factor are made by computing the "optical thickness" $\Sigma \Delta r$ of each region external to the fuel pellet stack with

$$\Sigma = \frac{E_H \Sigma_{sH}}{v_H} + \Sigma_a$$

where the value of Σ_{sH} and v_H are the values appropriate to hydrogen for that group; here Δr is the difference between the outer and inner radii for the particular region, and Σ_a is the absorption cross-section

for the given region. The change is made only if there is a 1 in column 30 of the batch control card in the input to HAMMER. Under these circumstances, it affects all resonances in multigroups 53 and 54. This change occurs in the subroutine DANC. The change implicitly assumes that the resonances in question are wide with respect to scattering from all isotopes except hydrogen.

As mentioned earlier, if the flux is not sufficiently flat across the lattice cell the Dancoff factor is not used to calculate the table of collision probabilities used in the resonance integral calculation. Instead a method of cosine currents is used. Here the collision probability calculation was modified by using $\bar{\Sigma}_{SH}/\gamma_H$ as the cross-section in each region (except in the region containing the resonance absorber) where previously the quantity Σ_s , the scattering cross-section of all materials, appeared. This change occurs in the subroutine PTBL.

The appendix gives, along with some comments, a Fortran listing of the subroutines which have been changed. This is a preliminary version of the program.

In an early version of the program there were certain indications of errors in the resonance integral calculation performed for the Pu-240 1 eV resonance. These errors could have been associated with the coarseness of the energy mesh used in the numerical calculation of the resonance integral, or possibly some sort of numerical instability (see reference 12). Later work indicated that the numerical instability problem is not serious, and that the use of a finer mesh in the resonance integral calculation was sufficient. The changes to the subroutine GRID which are required to permit a finer mesh in the resonance integral calculation are included in the appendix.

Concerning limitations on the use of the new program and the new hydrogen library, one should probably use the new library at all times; the use of the ICADY = 1 option (activated by putting a 1 in column 30 of the batch control card) should be used only if the principal moderator is hydrogen.

APPENDIX I

This appendix gives a Fortran listing of those subroutines which have been changed, with some explanatory comments. The new cards added to the source are readily identifiable since they are labelled with the identification "HAMMER". The deleted cards are not shown, however.

The changes to the subroutine RTBLIB consist in:

- (1) Setting the flag ICADY by equating it to ICNTRL (158), which (see LINK 1 of the HAMMER program) is equal to the item in column 30 of the batch control card.
- (2) Computing the parameter $\frac{\xi_H \bar{s}_H}{Y_H}$ for each mixture. For the Mth mixture this variable is called CDYC(M). If, in any mixture M, the hydrogen concentration is so low that the value of $N^H Y_H \xi_H \bar{s}_H$ is less than .0001, CDYC(M) is set equal to zero.
- (3) A labelled common block CADY is used to transmit CDYC(M) and ICADY to other subroutines where they are required.

The changes to the subroutine SØRE consist in:

- (1) The computation of ν for hydrogen from the ratio of $(N\nu\xi\sigma_s)_H$ to $(N\xi\sigma_s)_H$.
- (2) The kernel $P_{n,i}$ (see eq. (44) of reference 2) is modified to use the library value of ν and $\xi\Sigma_s$ for hydrogen. This kernel expresses the effect of in-group scattering in the equation determining the fluxes in the various regions of the cell. It is denoted by GRP(N) in the program.
- (3) The slowing-down density due to hydrogen (called ETA(N) in the program) is computed with ν and $\xi\Sigma_s$ for hydrogen used where unity and Σ_s were used previously. The equation is now completely analogous to the equation for Q(N), the nonhydrogenous slowing-down density.

- (4) The source term ($S_{n,i}$ of eq. (48) of reference 2) is modified also to use the γ and \sum_s for hydrogen. This term is denoted by $SOR(N)$ in the program.

The source $S_{n,i}$ and the kernel $P_{n,i}$ discussed above occur in eq. (40) of reference 2,

$$\phi_{ni} = \sum_{n'} T_{nn',i} (P_{n',i} \phi_{n',i} + S_{n',i})$$

where n and n' are region indices and i is a group index. This equation determines the regionwise fluxes.

A change to the subroutine FLUX is made so that the flat flux flag KEY is initialized to zero in each group and is reset to 1 only if the flat flux criterion is met. Certain indices MDONE(I) are reset to zero in each group. This ensures that the collision probability tables will be recalculated in each group.

Changes to PTBL are made. They consist of

- (1) Defining IGGDY as IG, the group index. This index is transmitted to DANC through the labelled common block CADY.
- (2) The cross-section XT(N) used in regions not containing the resonance absorber for the collision probability calculation when the method of cosine currents is used is set equal to CDYC(M) instead of the scattering cross-section for groups 53 and 54 if ICADY = 1.

Changes to DANC are made, to the calculation of the moderator optical thickness SL, for groups 53 and 54, if ICADY = 1. In such cases the optical thickness SL is computed with CDYC(M) instead of the scattering cross-section SSC(M).

Changes to subroutine GRID have been made so that more than 501 mesh points (in lethargy) can be used per resonance. The mesh for all resonances in multigroup 53 is changed to half that used in other multigroups. These changes reduce the mesh error in the treatment of the 1 eV resonance of Pu-240 to an acceptable level (about 1%).

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SUBROUTINE FLUX(IG)
CFLOW =====HAMMER=====BNL-SRL LATTICE ANALYSIS PROGRAM=====HAMLET
CFLOW ITERATE ON SPATIAL DISTRIBUTION OF FLUX
DIMENSION CNTRL(200),BTTL(9),LNK(10)
COMMON CNTRL
EQUIVALENCE
X(CNTRL( 1),IDBCH),(CNTRL( 2),ACASE),(CNTRL( 3),NFLOG),
1(CNTRL( 4),BTTL(1)),(CNTRL(13),NTIN),(CNTRL(14),NTOUT),
2(CNTRL(15),NTPUN),(CNTRL(16),NCHAIN),(CNTRL(17),LIB1),
3(CNTRL(18),LIB2),(CNTRL(19),LIB3),(CNTRL(20),INT1),
4(CNTRL(21),INT2),(CNTRL(22),NSC1),(CNTRL(23),LNK(1)),
5(CNTRL(33),NTHCS),(CNTRL(34),NEPCS),(CNTRL(35),KLIB1),
6(CNTRL(36),KLIB2),(CNTRL(37),KLIB3),(CNTRL(126),NCPRN),
7(CNTRL(130),NCPPT),(CNTRL(141),NTHRN),(CNTRL(142),NTHPT),
8(CNTRL(143),NTHPN),(CNTRL(153),NEPRA),(CNTRL(154),NEPPT),
9(CNTRL(155),NEPPN),(CNTRL(156),NEPSG),(CNTRL(157),NEPAG),
A(CNTRL(165),NFGPN),(CNTRL(166),NFGPT),(CNTRL(167),NFGPN),
B(CNTRL(168),NFGPB),(CNTRL(169),NFGJB),(CNTRL(177),NEDRN),
C(CNTRL(178),NEDPT),(CNTRL(179),NEDPA),(CNTRL(180),NEDNB),
D(CNTRL(181),NEDFW),(CNTRL(182),NEDHB),(CNTRL(183),NEDAX),
E(CNTRL(184),NEDNU)
DIMENSION LIMP(600),HOL(9),NPT(20),THT(20),MXAS(20),
1ILHI(20),NRBP(20),DEGC(20),WSTBA(18),WSTBB(18),
2CONCTA(18,10),LIMT(10),RIN(20),RAD(20),ROUT(20),VOL(20),
3MTBL(20),REGV(20),FISD(20),HOLIC(3,18)
COMMON LIMP
EQUIVALENCE
1(LIMP( 1), IDENT),(LIMP( 2), NX),(LIMP( 3), MX),
2(LIMP( 4), NRX),(LIMP( 5), ISOX),(LIMP( 6), ISCXE),
3(LIMP( 7), NGEOM),(LIMP( 8), NP1B1),(LIMP( 9), NECT),
4(LIMP(10), NXP),(LIMP(11), BSOD),(LIMP(12), HOL(1)),
5(LIMP(21), NPT(1)),(LIMP(41), THT(1)),(LIMP(61), MXAS(1)),
6(LIMP(81), ILHI(1)),(LIMP(101), NRBP(1)),(LIMP(121), DEGC(1)),
7(LIMP(141),WSTBA(1)),(LIMP(159),WSTBB(1)),(LIMP(177),CONCTA(1,1)),
8(LIMP(357),LIMT(1)),(LIMP(367),RIN(1)),(LIMP(377),RAD(1)),
9(LIMP(407),ROUT(1)),(LIMP(427),VOL(1)),(LIMP(447),MTBL(1)),
A(LIMP(467),REGV(1)),(LIMP(487),FISD(1)),(LIMP(507),HOLIC(1,1))
DIMENSION LOUT(1100),HOLA(9),BALT(18,4,5),FOIL(20,4,5),
1FOGX(4,6),FOX(20,4),DUMH(20),CTGC(5),CTGA(30,6)
COMMON LOLT
EQUIVALENCE ( LOUT(1),ID),(LOUT(2),HOLA(1)),
1(LOUT(11),BALT(1,1,1)),(LOUT(371),FOIL(1,1,1)),
2(LOUT(771),FOGX(1,1)),(LOUT(795),FOX(1,1)),(LOUT(875),DUMH(1)),
3(LOUT(895),OTGC(1)),(LOUT(900),CTGA(1))
DIMENSION ERASE(3500)
COMMON ERASE
DIMENSION SSC(10),S1(10),SIGABS(10),SIGIN(10),SIGX(10),C(10),
1AN(10),SD(10),PROB(25,10),SIGY(18,54),GNU(18,54),SIGA(18,54),
2NRIG(18),ER(200),GMN(200),GMGM(200),GMF(200),SPIN(200),
3AMASS(18),SIGP(18),JONE(18),JTWC(18),DZERO(18),DONE(18),DTWC(18),
4ETA(20),Q(20),FS(54),FX(20),DEL(54),F(20,54),HDONE(18),P(18,54),
5PF(18,54),PZ(1001),PZ1(1001),A1(18),EEK(55),TEMP(18),SIGEFY(18),
6CT(18,10)
COMMON IX,SIGY,GNU,SIGA,P,PF,F,DEL,FS,SSC,S1,SIGABS,SIGIN,SIGX,
1C,AN,SD,PROB,NRIG,ER,GMN,GMGM,GMF,SPIN,AMASS,SIGP,JONE,JTWC,

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```

2DZERC,DCNE,DTWO,ETA,0,ESC,HCONE,KEY,MCURR,PZ,PZ1,DELSIG,A1,ESK, FLUX
STEMP,SIGEFY,NDONE FLUX
DIMENSION DATA(165),DZ(18),GRP(20),SOR(20),T(20,20),XT(20),V1(20); FLUX
1V2(20),V3(20),V4(20),V5(20),CP(20),CN(20),CP2(20),CN2(20),Y(21), FLUX
2F1(20),F2(20),S2(20),Q1(20),QC(20),TO(20),T1(20) FLUX
EQUIVALENCE (ERASE(1),DATA(1),DZ(1),GRP(1)), FLUX
1(ERASE(21),SOR(1)),(ERASE(41),T(1)),(ERASE(441),XT(1)), FLUX
2(ERASE(461),V1(1)),(ERASE(481),V2(1)),(ERASE(501),V3(1)), FLUX
3(ERASE(521),V4(1)),(ERASE(541),V5(1)),(ERASE(561),CP(1)), FLUX
4(ERASE(581),CN(1)),(ERASE(601),CP2(1)),(ERASE(621),CN2(1)), FLUX
5(ERASE(641),Y(1)),(ERASE(441),F1(1)),(ERASE(461),F2(1)), FLUX
6(ERASE(481),S2(1)),(ERASE(501),C1(1)),(ERASE(481),QC(1)), FLUX
7(ERASE(461),TO(1)),(ERASE(441),T1(1)) FLUX
EQUIVALENCE (FX(1),FISD(1)),(CT(1),CONCTA(1)),(LIB2,NLIB2) FLUX
COMMON ALIB FLUX
ITCNT=0 FLUX
XNORM=0, FLUX
DO 9999 N=1,NX FLUX
XNORM=XNORM+SOR(N)+VOL(N) FLUX
M=MT=L(N) FLUX
Q1(N)=(SSC(M)-S1(M)+SIGIN(M)+SIGABS(M)-GRP(N))+VOL(N) FLUX
9999 CONTINUE FLUX
IF(IG=1) 5,1,5 FLUX
1 ITMX=0 FLUX
RNX=1, FLUX
IGI=1 FLUX
IGR=1 FLUX
EPSF=0,1 FLUX
ITMAX=100 FLUX
EPS=1,E-3 FLUX
DO 3 N=1,NX FLUX
3 F1(N)=SCF(N) FLUX
GO TO 20 FLUX
5 DO 6 N=1,NX FLUX
6 F1(N)=F(N,IG=1) FLUX
20 RNORM=0,0 FLUX
DO 30 N=1,NX FLUX
30 RNORM=RNORM+Q1(N)*F1(N) FLUX
RNORM=XNORM/RNORM FLUX
DO 40 N=1,NX FLUX
F1(N)=F1(N)*RNORM FLUX
S2(N)=SCR(N)+F1(N)*GRP(N) FLUX
40 CONTINUE FLUX
45 RNORM=0,0 FLUX
DO 53 N=1,NX FLUX
F2(N)=0,0 FLUX
DO 50 M=1,NX FLUX
DUMMY=DUMMY FLUX
50 F2(N)=F2(N)+T(N,M)*S2(M) FLUX
53 RNORM=RNORM+Q1(N)*F2(N) FLUX
RNORM=XNORM/RNORM FLUX
DO 55 N=1,NX FLUX
55 F2(N)=F2(N)*RNORM FLUX
DO 60 N=1,NX FLUX
DUMMY=DUMMY FLUX

```

3/

```

60 IF (ABS((F1(N)-F2(N))/F2(N))-EPS) 60,60,70      FLUX
    CONTINUE                                       FLUX
    GO TO 90                                       FLUX
70 DO 80 N=1,NX                                   FLUX
    S2(N)=SCR(N)*F2(N)+GRP(N)                     FLUX
    F1(N)=F2(N)                                    FLUX
80 CONTINUE                                       FLUX
    ITCNT=ITCAT+1                                  FLUX
    IF (ITCNT-ITMAX) 45,90,90                     FLUX
90 IF (ITCNT-ITMX) 92,92,91                       FLUX
91 ITMX=ITCNT?                                     FLUX
    IGI=IG                                          FLUX
92 IF (ABS(RNCRM-1.)-ABS(RMX-1.)) 94,94,93        FLUX
93 RMX=RNCRM                                       FLUX
    IGR=IG                                          FLUX
94 CONTINUE                                       FLUX
    DO 100 I=1,NX                                  FLUX
100 F(N,IG)=F2(N)                                  FLUX
    KEY=0                                           FLUX
105 IF (NX=1) 125,125,110                          FLUX
110 DO 120 N=2,NX                                  FLUX
    IF (ABS(F2(N)/F2(1)-1.)-EPS) 120,120,130      FLUX
120 CONTINUE                                       FLUX
125 KEY=1                                           FLUX
130 DO 140 I=1,ISGX                                 FLUX
    SIGEFY(I)=0.                                    FLUX
140 MDONE(J)=0                                      FLUX
    MCURR=0                                          FLUX
    MDONE=0                                          FLUX
    REWINDASC1                                       FLUX
150 IF (54-IG) 152,151,152                         FLUX
151 WRITE(NTOLT,160) ITMX,IGI,RMX,IGR             FLUX
160 FORMAT(59H-MAXIMUM ITERATIONS ON THE FLUX SHAPE IN ANY MACRO GROU FLUX
    1P = 15,6H GROUP 12/39H MAXIMUM RENORMALIZATION IN ANY GROUP = FLUX
    1F9,5,6H GROUP 12)                             FLUX
152 RETURN                                         FLUX
    END                                             FLUX

```

ION
SIGNED OVER THE LCOPI BEGINNING AT LINE 92
SIGNED OVER THE LCOPI BEGINNING AT LINE 95
SIGNED OVER THE LCOPI BEGINNING AT LINE 102
SIGNED OVER THE LCOPI BEGINNING AT LINE 107

7

ROUTINE RTBL14

CDC 6600 FTN V3.0-P261 DPT=2 11/20/

```
1WRITE(NTOUT,1112) (CDYC(M),M=1,MX)
1112 FORMAT(5E20.8)
1114 FORMAT(* IG=110)
1113 FORMAT(* CDYC(M),M=1,MX*)
RETURN
END
```

HAMM
HAMM
HAMM
HAMM
RTHL
RTHL

E SORE

```

SDH1(M)=SDH(M)
50 SD1(M)=SD(M)
IF(IG-25)60,60,80
60 IG1=IG-1
DO70N=1,N*
M=MTBL(N)
GRP(N)=CRF(N)+PROB(IG,M)
DO70I=1,IG1
70 SOR(N)=SOR(N)+PROB(I,M)*F(N,I)/DEL(IG)*DEL(I)
80 RETURN
END

```

HAMMER
SORE
SORE
SORE
SORE
SORE
SORE
SORE
SORE
SORE
SORE

ES MADE BY THE OPTIMIZER
VARIANT RLST REMOVED FROM THE LOOP STARTING AT LINE 83

ION
SIGNED OVER THE LOOP BEGINNING AT LINE 77
SIGNED OVER THE LOOP BEGINNING AT LINE 81
SIGNED OVER THE LOOP BEGINNING AT LINE 86

ROUTINE PTEL

CDC 6600 FTN V3.0-P261 UPT=2 11/20/

```

2DZERO,DONE,DTWO,ETA,Q,ESC,MDONE,KEY,MCURR,PZ,PZ1,DELSIG,A1,EBK; PTHL
3TEMP,SIGEFY,NDONE PTHL
DIMENSION DATA(165),DZ(18),GRP(20),SOR(20),T(20,20),XT(20),V1(20), PTHL
1V2(20),V3(20),V4(20),V5(20),CP(20),CN(20),CP2(20),CN2(20),V(21), PTHL
2F1(20),F2(20),S2(20),Q1(20),QO(20),TO(20),T1(20) PTHL
EQUIVALENCE (ERASE(1),DATA(1),DZ(1),GRP(1)), PTHL
1(ERASE(21),SOR(1)),(ERASE(41),T(1)),(ERASE(441),XT(1)), PTHL
2(ERASE(461),V1(1)),(ERASE(481),V2(1)),(ERASE(501),V3(1)), PTHL
3(ERASE(521),V4(1)),(ERASE(541),V5(1)),(ERASE(561),CP(1)), PTHL
4(ERASE(581),CN(1)),(ERASE(601),CP2(1)),(ERASE(621),CN2(1)), PTHL
5(ERASE(641),Y(1)),(ERASE(441),F1(1)),(ERASE(461),F2(1)), PTHL
6(ERASE(481),S2(1)),(ERASE(501),Q1(1)),(ERASE(481),QO(1)), PTHL
7(ERASE(461),TO(1)),(ERASE(441),T1(1)) PTHL
EQUIVALENCE (FX(1),FISD(1)),(CF(1),CONCTA(1)),(LIB2,NLIB2) PTHL
COMMON NLIB PTHL
COMMON/CADY/CDYC(10),IGCDY,ICADY HAMM
IGCDY=IG HAMM
SIGPZ=SIGP(J) PTHL
J1=JUNE(J) PTHL
IF(J1)20,10,20 PTHL
10 SIGM1=0. PTHL
GOTO31 PTHL
20 SIGM1=SIGP(J1)+DONE(J)/DZERO(J) PTHL
30 J2=JTWO(J) PTHL
IF(J2)20,40,50 PTHL
40 SIGM2=0. PTHL
GOTO61 PTHL
50 SIGM2=SIGP(J2)+DTWO(J)/DZERO(J) PTHL
60 SIGT=(SIGPZ+SIGM1+SIGM2)+DZERO(J) PTHL
FLX=0. PTHL
V0=0. PTHL
DO110N=1,NX PTHL
Q0(N)=0. PTHL
M=MTBL(N) PTHL
IF(CI(J,M))80,70,90 PTHL
70 XT(N)=SSC(M) PTHL
IF(IG,55,53,AND,ICADY,EQ,1) XT(N)=CDYC(M) HAMM
GOTO110 PTHL
80 XT(N)=SIGT PTHL
DO90NR=1,NRX PTHL
IF(N-NRBP(NR))100,100,90 PTHL
90 CONTINUE PTHL
NR=NRX PTHL
100 RMAX=THT(NR) PTHL
Q0(N)=VOL(N) PTHL
V0=V0+VOL(N) PTHL
130 FLX=FLX+VOL(N)*F(N,IG) PTHL
110 CONTINUE PTHL
IF(NRIG(J))160,160,<0 PTHL
160 CALLPZCALC PTHL
P0=0. PTHL
P1=0. PTHL
DO120N=1,NX PTHL
IF(Q0(N))170,160,170 PTHL
170 P0=P0+I0(N) PTHL

```

GOTO120	PTB
180 P1=P1+T0(N)*F(N,IG)	PTB
120 CONTINUE	PTB
PD=PO/VC	PTB
IF(KEY)121,122,121	PTB
121 P1=P1-PD	PTB
GOTO125	PTB
122 P1=P1/FLX	PTB
123 A1(J)=P1+PD	PTB
SIGEV(J)=SIG*(P1/PD)	PTB
GOTO415	PTB
200 DELSIG=0,02/RMAX	PTB
TEST=RMAX-THT(1)	PTB
CALLUANG(C1)	PTB
IF(IG,EQ,53) WRITE(6,500) IG,C1,KEY	HAM
500 FORMAT(1HG='IG=',13,'C1= ',E20.8,'KEY= ',13)	HAM
SIG=C1	PTB
PZ1(1)=1.	PTB
PZ(1)=0.	PTB
DO310=2,1001	PTB
SIG=SIG+DELSIG	PTB
IF(KEY)210,230,210	PTB
210 IF(TEST)230,220,230	PTB
220 ARG=SIG+RMAX	PTB
IF(VGEUM=1)221,221,222	PTB
221 ARG=ARG+ARG	PTB
CALLESCAPE(1., ARG,P1,PD)	PTB
PZ1(N)=P1+P1	PTB
GOTO225	PTB
222 CALLESCAPE(0,ARG,P1,PD)	PTB
PZ1(N)=P1	PTB
223 PZ1(N)=PZ1(N)*(1.-C1)/(1.+(1.-2.*ARG+PZ1(N))*C1)	PTB
GOTO310	PTB
230 DO250K=1,NA	PTB
IF(QO(K))240,250,240	PTB
240 XT(K)=SIG	PTB
250 CONTINUE	PTB
260 CALLPZCALC	PTB
PZ(N)=0.	PTB
270 PZ1(N)=0.	PTB
IF(KEY)305,275,305	PTB
275 DO300K=1,NA	PTB
IF(QO(K))290,260,290	PTB
280 PZ1(N)=PZ1(N)+T0(K)*F(K,IG)	PTB
GOTO301	PTB
290 PZ(N)=PZ(N)+T0(K)	PTB
300 CONTINUE	PTB
PZ1(N)=PZ1(N)/FLX	PTB
PZ(N)=PZ(N)/VC	PTB
GOTO310	PTB
305 DO307K=1,NA	PTB
IF(QO(K))306,307,306	PTB
306 PZ1(N)=PZ1(N)+T0(K)	PTB
307 CONTINUE	PTB
PZ(N)=PZ(N)/VC	PTB


```

SUBROUTINE DANC(C1)
CDANC *****HAMMER*****BNL-SRL LATTICE ANALYSIS PROGRAM*****HAMLET
CDANC DANC OFF CORRECTION FOR SINGLE RODS
DIMENSION CNTRL(200),BTTL(9),LNK(10)
COMMON CNTRL
EQUIVALENCE
X(CNTRL( 1),IDBCH),(CNTRL( 2);NCASE),(CNTRL( 3),NFLOG),
1(CNTRL(4),BTTL(1)),(CNTRL(13);NTIN),(CNTRL(14),NTOUT),
2(CNTRL( 15),NTPUN),(CNTRL(16);NCHAIN),(CNTRL( 17),LIB1),
3(CNTRL( 18), LIB2),(CNTRL( 19); LIB3),(CNTRL( 20),INT1),
4(CNTRL( 21), INT2),(CNTRL( 22); NSC1),(CNTRL( 23),LNK(1)),
5(CNTRL( 33),NTHCS),(CNTRL( 34);NEPCS),(CNTRL( 35),KL1B1),
6(CNTRL( 36),KL1B2),(CNTRL( 37);KL1B3),(CNTRL(129),NCPRN),
7(CNTRL(130),NCPPT),(CNTRL(141);NTMRN),(CNTRL(142),NTHPT),
8(CNTRL(143),NTHPN),(CNTRL(153);NEPRN),(CNTRL(154),NEPPT),
9(CNTRL(155),NEPPN),(CNTRL(156);NEPSG),(CNTRL(157),NEPAG),
A(CNTRL(165),NFGRN),(CNTRL(166);NFGPT),(CNTRL(167),NFGPN),
J(CNTRL(168),NFGPB),(CNTRL(169);NFGJO),(CNTRL(177),NEDRN),
C(CNTRL(178),NEDPT),(CNTRL(179);NEUPN),(CNTRL(180),NEDNB),
H(CNTRL(181),NEDFW),(CNTRL(182);NEURB),(CNTRL(183),NEDAX),
E(CNTRL(184),NEUNU)
DIMENSION LIMP(600),HOL(9),NPT(20),THT(20),MXAS(20),
1(LHI(20),NRHP(20),DEGC(20),WSTBA(18),WSTBB(16),
2(CONCTA(16,10),LIMT(10),RIN(20);RAD(20),ROUT(20),VOL(20),
3(MTBL(20),REGV(20),FISD(20),HOLID(3,18)
COMMON LIMP
EQUIVALENCE
1(LIMP( 1), IDENT),(LIMP( 2), NX),(LIMP( 3), MX),
2(LIMP( 4), NRX),(LIMP( 5), ISOX),(LIMP( 6), ISUXE),
3(LIMP( 7), NGEOM),(LIMP( 8), NP1B1),(LIMP( 9), NACT),
4(LIMP(10), NKP),(LIMP(11), BSQD),(LIMP(12), HOL(1)),
5(LIMP(21), NPT(1)),(LIMP(41), THT(1)),(LIMP(61), MXAS(1)),
6(LIMP( 91), LHI(1)),(LIMP(101), NRBP(1)),(LIMP(121), DEGC(1)),
7(LIMP(141),WSTBA(1)),(LIMP(159),WSTBB(1)),(LIMP(177),CONCTA(1,1)),
8(LIMP(357), LIMT(1)),(LIMP(367), RIN(1)),(LIMP(397), RAD(1)),
9(LIMP(407), ROUT(1)),(LIMP(427), VOL(1)),(LIMP(447), MTBL(1)),
A(LIMP(467), REGV(1)),(LIMP(487), FISD(1)),(LIMP(507),HOLID(1,1))
DIMENSION LOU(1100),HOLA(9),BALT(16,4,5),FOIL(20,4,5),
1FOGX(4,6),FOX(20,4),DUMB(20),OTGC(5),OTGA(30,6)
COMMON LOU
EQUIVALENCE ( LOU(1),ID),(LOU(2),HOLA(1)),
1(LOU(11),BALT(1,1,1)),(LOU(371),FOIL(1,1,1)),
2(LOU(771),FOGX(1,1)),(LOU(795),FOX(1,1)),(LOU(875),DUMB(1)),
3(LOU(895),OTGC(1)),(LOU(900),OTGA(1))
DIMENSION ERASE(3500)
COMMON ERASE
DIMENSION SSC(10),S1(10),SIGABS(10),SIGIN(10),SIGX(10);C(10),
1A(10),SD(10),PROB(25,10),SIGY(18,54),GNU(18,54),SIGA(18,54),
2NR(3(18),ER(200 ),GMV(200 ),GMGM(200 ),GMF(200 ),SPIN(200 ),
3AMASS(18),SIGP(18),JONE(18),JTWO(18),DZERO(18),DONE(18),DTWO(18),
4ETA(20),Q(20),FS(54),FX(20),DEL(54),F(20,54),MONE(18),P(18,54),
5PF(18,54),PZ(1001),FZ1(1001),A1(18),EBK(55),TEMP(18),SIGEV(18),
ACT(18,10)
COMMON IX,SIGY,GNU,SIGA,P,PF,F,DEL,FS,SSC,S1,SIGABS,SIGIN,SIGX,
1C,AN,SD,PROB,NRIG,EF,GMV,GMGM,GMF,SPIN,AMASS,SIGP,JONE,JTWO,

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20ZEHO,DUNE,DTWO,ETA,U,ESC,MDONE,KEY,MCURR,PZ,PZ),DELSIG,A1,EBK; DANC
JTEMP,SIGEFY,NDONE DANC
DIMENSION DATA(165),DZ(18),GRP(20),SOR(20),T(20,20),XT(20),V1(20), DANC
1V2(20),V3(20),V4(20),V5(20),CP(20),CN(20),CP2(20),CN2(20),Y(21), DANC
2F1(20),F2(20),S2(20),Q1(20),Q0(20),TD(20),T1(20) DANC
EQUIVALENCE (ERASE(1),DATA(1),DZ(1),GRP(1)), DANC
1(ERASE(21),SOR(1)),(ERASE(41),T(1)),(ERASE(441),XT(1)); DANC
2(ERASE(461),V1(1)),(ERASE(481),V2(1)),(ERASE(501),V3(1)), DANC
3(ERASE(521),V4(1)),(ERASE(541),V5(1)),(ERASE(561),CP(1)), DANC
4(ERASE(581),CN(1)),(ERASE(601),CP2(1)),(ERASE(621),CN2(1)); DANC
5(ERASE(641),Y(1)),(ERASE(441),F1(1)),(ERASE(461),F2(1)), DANC
6(ERASE(481),S2(1)),(ERASE(501),Q1(1)),(ERASE(481),Q0(1)), DANC
7(ERASE(461),TD(1)),(ERASE(441),T1(1)) DANC
EQUIVALENCE (FX(1),ISD(1)),(CT(1),CONCTA(1)),(LIR2,NLIB2) DANC
COMMON NLIB DANC
COMMON/CADY/CDYC(10),IGCDY,ICADY DANC
IG=IGCDY HAMMER
IF(MRX=1)200,200,1 HAMMER
1 NX=IX DANC
IF(NGEUM=2)10,10,20 DANC
10 C2=0.95231261 DANC
C3=0.12 DANC
GOTO3 DANC
20 C2=0.8862269 DANC
C3=0.11 DANC
35 L04=NOI(1)+1 DANC
SL=0.1 DANC
IF(L04+NX)35,35,45 DANC
35 U740N=L04,NX DANC
M=MTBL(N) DANC
IF(IG,LT,53,OR,ICADY,VE,1) DANC
1SL=SL+(ROUT(N)-ROJT(N-1))*(SSC(M)+SIGIN(M)+SIGABS(M)) HAMMER
IF(IG,GE,53,AND,ICADY,ED,1) HAMMER
1SL=SL+(ROUT(N)-ROJT(N-1))*(CDYC(M)+ HAMMER
2SIGIN(M)+SIGABS(M)) HAMMER
40 CONTINUE HAMMER
45 IF(NGEUM=1)70,70,73 DANC
70 SL=SL*2. DANC
IF(SL=1.)71,71,72 DANC
71 C1=1.-SL+(2.*SL*(ALOG(SL)-.9228-SL*(.332-.6354*SL))) DANC
GOTO111 DANC
72 C1=EXP(-SL)*(2.+6.16/(SL+3.))**2)/(SL+3.) DANC
GOTO111 DANC
73 CONTINUE DANC
VMOF=(ROUT(NX)/ROJT(L04-1)) DANC
SL=SL*2.*(VMOF+1.) DANC
VMOF=VMOF**2-1. DANC
VMOF=(C2*SQRT(VMOF+.1)-1.)/VMOF-C3 DANC
IF(VMOF)51,51,52 DANC
52 C2=VMOF*SL DANC
IF(C2=20.)50,60,60 DANC
51 C2=. DANC
53 C1=EXP(-C2)/(1.+SL-C2) DANC
GOTO111 DANC
60 C1=. DANC

```

18

ROUTINE DANC

```

111 IF(NEPT)110,113,110
110 WRITE(NTOUT,112)C1
112 FORMAT(1H 75X2MC=1PE10.6)
113 RETURN
200 C1=1.0
    GOTD111
    END

```

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DAI
DAI
DAI
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DAI

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      EPSIL(IG) = )
      ENE(IG)=EZERO(IG)*EXP(EPSIL(IG)+FLOAT(MESH(IG)-1))*CUT
300 IF (MESH-MESH(IG)) 220,320,320
      MESH EXCEEDS STORAGE LIMITS
220 CONTINUE
      ITEMP=1
      IF (ITEMP, EQ, 1) GO TO 316
      GO TO (221, 222), NYX
316 IF (MESH(IG).GT. MMSH) WRITE(NOUT,317) MESH(IG), MMSH
317 FORMAT(10 NUMBER OF MESH PTS FOR THIS RESONANCE **,120 ,* THIS
      * MAX NUMBER*,120 )
      WRITE(NOUT,325) EZERO, GAMN, GMGM, GFG, SPIN, H, S
325 FORMAT(10 THIS RESONANCE IS AT *E20.8/* IT HAS *WIDTHS*3E20.8/
      * SPIN, H, S ARE *3E20.8)
      GO TO 320
221 MESH=MP
      WRITE(NOUT,223)EZERO, GAMN, GMGM, GFG, SPIN, H, S
223 FORMAT(14M RESONANCE AT E20.8, 14M, WITH WIDTHS 3E20.8/6M SPIN =20
      1.8, 4M, R E20.8, 4M, S E20.8/30M CANNOT BE PROCESSED PROPERLY./)
      NYX=2
222 IF (N(JG)-2, 1300, 330, 500
500 N(JG)=N(JG)-1.
      GO TO 6
307 MESH(IG)=MMSH
      IF (ZUNE=0.57142857) 301, 301, 302
301 EPSIL(IG)=ALOG(ENE(IG))/(2.*EZENO(IG)-EDNE(IG))/(FLOAT(MMSH-3))
      GO TO 320
302 EPSIL(IG)=ALOG(2.3333333*ENE(IG)/EZENO(IG))/(FLOAT(MMSH-3))
320 CONTINUE
      MESH=
      END
      END

```

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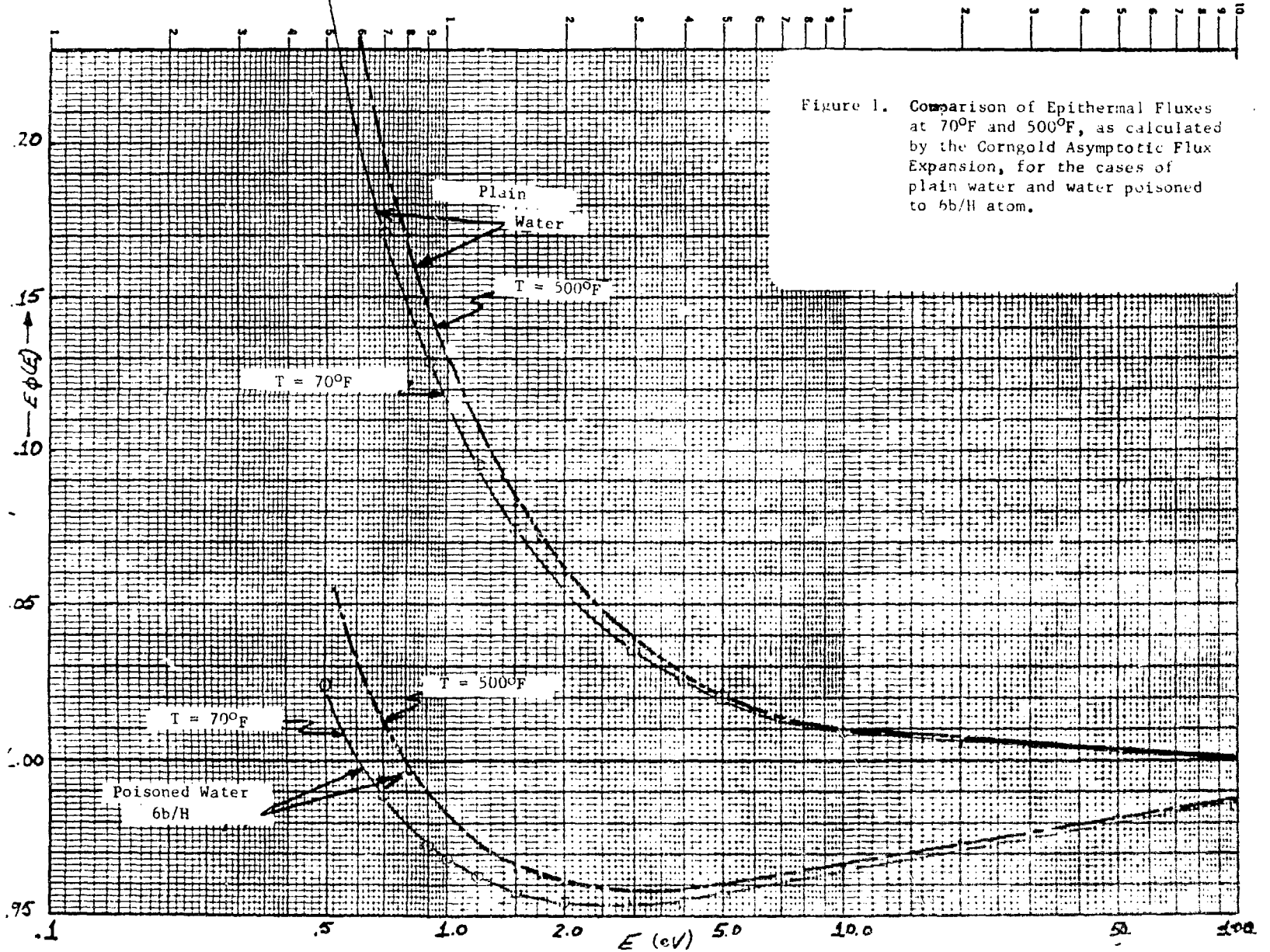


Figure 1. Comparison of Epithermal Fluxes at 70°F and 500°F, as calculated by the Corngold Asymptotic Flux Expansion, for the cases of plain water and water poisoned to 6b/H atom.

