

FASPEC  
A PROGRAM TO DETERMINE GROUP CONSTANTS  
FOR UP TO 47 GROUPS IN A FAST NEUTRON SPECTRUM

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## I. INTRODUCTION

### 1.1 General View

Reactor core design is an iterative process in which core "constants," such as rod diameter and pitch, are first chosen. Once these choices are made, the designer has a choice of two methods. He may hand calculate group constants using a small number of energy groups or he may use a large, expensive-to-run computer program with many energy groups. The first method usually uses two groups, fast and thermal. A number of simplifying assumptions must be made to allow hand calculation. The necessity of the assumptions and the small number of groups combine to produce inherent inaccuracies, but the process is still quite time consuming. It also does not give the student or inexperienced designer an "intuitive feel" of the relative effects of small changes in design. Effects such as inelastic scattering are often ignored with this method because they are more time consuming than they are worth.

In either case, group constants, system reactivity and burnup are calculated. If the results are not satisfactory, one or more of the design parameters must be changed, the entire set of calculations repeated and the results evaluated. This process must continue until an acceptable core design is reached. Since this is a time consuming and tedious process, a method which is simpler, less tedious, and less costly is needed.

One such method would bring together several program modules to determine multi-group constants, criticality and burnup calculations to provide core design criteria, core life results and design optimization. As a result of this approach, changes can be made to the design and the results of those changes seen quickly. The time and expense of the design process should thus be drastically reduced and the large, expensive programs used only to confirm and refine the design.

In this study, the infinite-medium Boltzmann, or transport, equation is solved numerically using a linear approximation to determine fast group constants for up to 47 energy groups. Cross sections used in the solution were provided from the "Very Improved Monte Carlo" Code (VIM) for an infinitely repeating hexagonal, mid-range lattice. Though the FASPEC program incorporates a homogeneous medium only, the VIM Code does calculate microscopic cross sections which are varied to include the effects of self shielding. The FASPEC program does, therefore, incorporate self shielding indirectly.

Because the core design used in cross section determination is based on a regionalized, as opposed to a homogeneous medium, and because the cross sections and other constants used are necessarily averaged, deviations from this average core introduce further inaccuracies. These inaccuracies should be small because the individual effects of regions and self-shielding changes are relatively small.

The transport equation is an energy dependent balance equation which describes neutron slowing down by scattering, while taking into account the addition of fast neutrons by the fission process. The equation and its various terms are discussed individually in Chapter

2. The appendix contain both the program listing and a short users guide for the program.

## 1.2 Purpose

The primary objective of the work described in this thesis is to provide fast-spectrum multi-group constants quickly and inexpensively while retaining reasonable accuracy. Further, when combined with thermal group constants, this program should provide input for a criticality program, such as ODMUG [1], as well as to a burnup program such as the RFD program series [2]. When so combined, the user need only calculate the atomic number densities of the various isotopes present in the system to determine group constants for any number of energy groups from one to 47. The energy of the groups varies from that of the fastest expected fission-produced neutrons,  $1.0 \times 10^7$  eV, down to that of the upper limit of thermal neutrons, 0.625 eV. System criticality and burnup estimates may then be calculated from the calculated group constants.

As an additional benefit, students may use the program to determine, quickly and easily, the result of any change in lattice design. While this will not take the place of design experience, it will help the student develop an intuitive understanding of core lattice design and constraints.



## II. DESCRIPTION

### 2.1 General Description

In a reactor, neutrons are produced at high energies (with the average around 2 MeV) and interact with materials present in the reactor by nuclear collisions. These collisions slow the neutrons toward the thermal energy range ( $< 0.625$  eV) by transfer of energy through both elastic and inelastic scattering. This slowing of neutrons is the purpose of moderators in thermal reactors, so-called because most fission events in thermal reactors occur through absorption of thermal neutrons by fissile fuel material.

Because of the large number of neutrons involved and, consequently, the large number of collisions, the energy distribution of neutrons in the steady state system is a continuous function [3] and solutions to the transport equation are energy-dependent. The energy dependent equations may, however, be solved approximately by dividing the energy spectrum into many micro-groups, each having an average set of group constants within the respective micro-groups. Further, the micro-groups may be collapsed to one or more macro-groups for use in the appropriate few-group calculations.

This thesis will briefly discuss neutron slowing down processes, present the neutron transport equation, discuss what each of the terms describes and present one solution to the transport equation as well as the calculation of group constants in the form of the computer program, FASPEC. A listing of the FASPEC code and its attendant data and control files together with sample output and a user's guide are provided in the appendix.

## 2.2 Neutron Slowing Down in an Infinite Medium

Most fission-produced neutrons have energies in the 1 to 3 MeV range and slow down by collisions with materials in the reactor system. This slowing down is through two distinct scattering mechanisms: elastic scatter and inelastic scatter.

In the elastic scatter mechanism, both neutrons and target nuclei behave as though they were hard elastic spheres. The analogy most often drawn for visualization by students is that of two billiard balls in collision. Visualization of the inelastic collision event involves, instead, two plastic spheres. In this collision, part of the system's kinetic energy is used to deform the target sphere. Thus kinetic energy is not conserved in the inelastic collision. More detailed treatment of these collisions as they pertain to the problem at hand will be given in the following sections.

In order to treat quantitatively the slowing down mechanisms, some assumptions must be made. First, we assume that, since we are dealing with an infinite homogeneous medium, neutron escape from that medium is either impossible or sufficiently small to be irrelevant. We also assume that the nuclei are not tightly bound and therefore that every collision between a neutron and a target nucleus results in an energy loss by the neutron through either elastic or inelastic scatter. These assumptions are reasonable for this treatment [4]. Also, for the purposes of this study, upscattering, the gain of energy by the neutron in collision, is ignored, since we are dealing with only those energy levels above the thermal range. Though these assumptions do necessarily introduce some slight inaccuracies, they are common assumptions in the

solution of the transport equation which greatly simplify later mathematical treatment.

### 2.3 Elastic Scatter

There are actually two types of elastic scattering [4]. These are potential scattering, resulting from short range nuclear forces acting on the neutron, and resonance scattering, in which a compound nucleus is formed when the neutron is first absorbed then re-emitted by the target nucleus. In either case, elastic scatter may be visualized as a collision of billiard balls because of the rapid re-emission of the neutron in the resonance scatter case. Since both kinetic energy and momentum of the neutron-target system are conserved, elastic scattering may be treated by means of classical mechanics.

In a scattering event (in the laboratory system), when a neutron of unit rest mass, traveling at a velocity  $v_0$ , strikes a stationary target nucleus of rest mass =  $A$  units, it may be shown [5] that, when scattered through an angle,  $\theta$ , the resulting neutron velocity,  $v$ , may be described by

$$v^2 = \frac{A^2 + 2 A \cos \theta + 1}{(A + 1)^2} ,$$

which is also the ratio of the new to the original kinetic energy,  $KE/KE_0$  [6]. It is obvious that the resulting neutron energy is a minimum when  $\cos \theta = -1$ , or  $\theta = \pi$ . In this case of direct backscatter

$$\frac{KE}{KE_0} = \frac{A^2 - 2 A + 1}{(A + 1)^2} = \frac{(A - 1)^2}{(A + 1)^2} \equiv \alpha .$$

For convenience, we will also define here the quantity  $\xi$ , the logarithmic energy decrement, which is the average change in the logarithm of neutron energy per collision. This quantity may be shown [7] to be

$$\xi = 1 + \frac{\alpha}{1 - \alpha} \ln \alpha . \quad (2.3.1)$$

It should be noted that both  $\alpha$  and  $\xi$  are functions of the rest mass of the target nucleus and are independent of neutron energy.

One other quantity which may be defined for convenience is the logarithmic energy, or lethargy,  $u$  [8], where

$$u \equiv \ln \left( \frac{E_0}{E} \right) ,$$

which indicates that

$$E = E_0 e^{-u} .$$

For the purposes of this study,  $E_0$  is taken to be  $1.0 \times 10^7$  eV or 10 MeV, a reasonable energy above which it is assumed no fission neutrons are emitted [7].

The Boltzmann (or Neutron Transport) Equation for an infinite medium may now be written as [8]

$$\Sigma_T(E) \phi(E) = S(E) + \int_E^\infty \Sigma_S(E') \phi(E') F(E' \rightarrow E) dE' + \Gamma(E)$$

or, in the lethargy domain,

$$\Sigma_T(u) \phi(u) = S(u) + \int_0^u \Sigma_S(u') \phi(u') F(u' \rightarrow u) du' + \Gamma(u), \quad (2.3.2)$$

where

$\Sigma_T(u)$  = the total macroscopic cross section at the lethargy (energy) of interest,

$\phi(u)$  = the neutron flux at the given lethargy,

$S(u)$  = the source term of fission neutrons which are produced at the given lethargy

$\Sigma_S(u)$  = the macroscopic elastic scatter cross section,

$F(u' \rightarrow u)$  = the function describing the scatter of neutrons from lethargy  $u'$  to  $u$ , by elastic scattering, and

$\Gamma(u)$  = the scatter of neutrons into  $u$  by inelastic scatter.

The function  $F$  is generally written [8] in terms of lethargy as

$$F(u' \rightarrow u) = \frac{e^{(u'-u)}}{1 - \alpha}, \quad ,$$

which is the probability of neutrons scattering into lethargy interval  $du$  about  $u$ .

### 2.3.1 Elastic Scatter by Hydrogen

Since for hydrogen,

$$\alpha_H = \frac{(1 - 1)^2}{(1 + 1)^2} = 0 \text{ and } \xi_H = 1 ,$$

one may see that, dependent upon scattering angle, the incident neutron may lose up to 100 percent of its original energy. This is the case only for collision with hydrogen. A neutron striking a hydrogen atom may thus emerge with any energy from slightly less than the incident energy,  $E_0$  for example, down to thermal energies. For this reason, hydrogen is treated separately from all other isotopes present in the system. In writing the term for scattering in hydrogen, we note that  $\alpha_H = 0$ , so [8]

$$\int_0^u \Sigma_S^H(u') \phi(u') F(u' \rightarrow u) du' = \int_0^u \Sigma_S^H(u') \phi(u') e^{(u'-u)} du' , \quad (2.3.3)$$

indicating that scatter from hydrogen into  $du$  about  $u$  may occur from any lower lethargy (higher energy) group and is a function of the macroscopic scattering cross section and the flux in the lethargy group from which the scatter occurs.

Let us here define the slowing down density,  $q$ , such that

$$q(u) = q_H(u) + q_e(u) , \quad (2.3.4)$$

where

$q(u)$  = the total slowing down density at the given lethargy,  
 $q_H$  = the contribution from interactions with hydrogen, and  
 $q_e$  = the contributions from interactions with all other isotopes in the system combined.

The slowing down by hydrogen alone then is [8]

$$q_H(u) = \int_0^u \Sigma_S^H(u') \phi(u') e^{(u'-u)} du' \quad . \quad (2.3.5)$$

This shows that slowing down by hydrogen collision is accomplished only by elastic scattering and that the conditions stated earlier apply also to the slowing down density. As will be shown in the next section, such turns out not to be the case with other isotopes.

### 2.3.2 Elastic Scatter in Isotopes Other than Hydrogen

For purposes of developing the term for slowing down in isotopes other than hydrogen, we will develop the term first for a single isotope, then extend this term to incorporate all the isotopes in the system other than hydrogen.

If we assume that neutrons are produced only at lethargy  $u$  then the scattering term for any isotope,  $i$ , other than hydrogen is [3]

$$\Sigma_S^i(u) \phi(u) = \int_{u-\epsilon_i}^u \Sigma_S^i(u') \phi(u') \frac{e^{(u'-u)}}{1-\alpha_i} du' \quad . \quad (2.3.6)$$

This equation states that scatter into  $du$  about  $u$  may occur only within the lethargy region from  $u-\epsilon$  to  $u$  where

$$\varepsilon_1 \equiv \ln\left(\frac{1}{\alpha_1}\right) , \quad (2.3.6a)$$

and that the probability of this occurring is  $F(u' \rightarrow u)$  where

$$F(u' \rightarrow u) = \frac{e^{(u'-u)}}{1 - \alpha_1} .$$

One may see, then, that scattering is a function not only of flux and cross section, but also of the mass of the target nucleus. This mass dependence is a result of classical mechanics as applied to the neutron-target collision.

Since  $\Sigma_S(u)\phi(u)$  may be called the scattering collision density, the slowing down density may be written as

$$q_e^1(u) = \int_{u-\varepsilon_1}^u \Sigma_S^1(u')\phi(u') \frac{e^{(u'-u)} - \alpha_1}{1 - \alpha_1} du' ,$$

where the quantity  $(e^{(u'-u)} - \alpha_1)/(1 - \alpha_1)$  is the probability that neutrons scattering from lethargy  $u'$  will scatter to a lethargy greater than  $u$ .

Generalizing the above term to multiple-isotope media, and reserving the isotope number 1 for hydrogen, we have [3]

$$\sum_{i=2}^N \Sigma_S^i(\theta)\phi(u) = \sum_{i=2}^N \int_{u-\varepsilon}^u \Sigma_S^i(u')\phi(u') \frac{e^{(u'-u)} - \alpha_i}{1 - \alpha_i} du' , \quad (2.3.7)$$

and

$$q_e(u) = \sum_{i=2}^N \int_{u-\varepsilon_i}^u \Sigma_S^i(u')\phi(u') \frac{e^{(u'-u)} - \alpha_i}{1 - \alpha_i} du' . \quad (2.3.8)$$



For a more rigorous and detailed treatment of this development see Ferziger and Zweifel [7] and Bowden and Edlund [3].

Since only 13 isotopes are included in the data files for the program,  $N = 13$  in the above equation.

## 2.4 Inelastic Scatter

When a neutron and a target nucleus are involved in an inelastic scattering event, a compound nucleus is formed in which the kinetic energy of the incident neutron is transferred to the compound nucleus [6]. While often part of this transfer results in motion of the compound nucleus, with the attendant resulting kinetic energy, the remainder of the transferred energy results in an excited compound nucleus. This excited nucleus then re-emits a neutron at a lower energy than that of the incident neutron. The remaining excitation energy is then emitted in the form of one or more gamma-ray photons.

Though a detailed description of the physics of the event is beyond the scope of this work, a simplified visualization is somewhat analogous to the situation in which an orbital electron is struck by an incident photon. In this analogy, if the incident photon has energy equal to or greater than a certain threshold energy, dependent upon the isotope and electron struck, the electron can become excited to the next higher orbital and will subsequently decay by emitting a photon of energy equal to its excitation energy as it drops back to the ground state orbital. Similarly, a distinct threshold exists for each isotopic nucleus. the incident neutron must have energy at least equal to that threshold energy to excite the nucleus and thus undergo inelastic scattering. So,

if  $E_\gamma$  is the excitation energy of a given isotope,  $E_1$  the energy of the incident neutron and  $E_2$  the energy of the emitted neutron [4],

$$E_1 = E_2 + E_\gamma$$

and the energy of the gamma(s) emitted during the decay to the ground state is also  $E_\gamma$ .

Although there are exceptions, generally the lower the atomic mass of the target nucleus, the higher the threshold energy. For purposes of this study, only the heavy isotopes need be considered.

In developing the inelastic term for the transport equation, we may begin as we have for each of the preceding terms by stating the inelastic term,  $\Gamma_i(u)$ , as

$$\Gamma_i(u) = \int_0^u \Sigma_{in}^i(u') \phi(u') f(u' \rightarrow u) du' \quad (2.4.1)$$

In this case, however, the probability of inelastic scatter into  $du$  about  $u$  is different from those similar functions in preceding terms.

By beginning at low lethargies (high energies), we start with fast neutrons, above the required energy threshold. To simplify the development of the inelastic term, we assume that a neutron at a given incident energy,  $E_j$ , will scatter with only one energy,  $E_k$ , when inelastically scattered by an isotope of mass  $A_j$ . The energy of the scattered neutron,  $E_k$ , is found from

$$E_k = \frac{6.4}{\sqrt{A_j}} \sqrt{E_j} \quad (2.4.1a)$$

where energies are in MeV and

The general term for all isotopes present is then

$$\Gamma(u) = \sum_{i=0}^N \int_0^u \Sigma_{in}^i(u') \phi(u') f_{j \rightarrow k}^i du' \quad , \quad (2.4.2)$$

where  $f_{j \rightarrow k}^i$  must satisfy equation (2.4.1a). Note that the total inelastic term is simply the sum of the contributions of the separate isotopes.

Inelastic collisions in low mass isotopes are negligible and are non-existent in the case of hydrogen. Therefore, for the purposes of this study, Eq. 2.4.2 will take into account only the heavy isotopes, those of uranium and plutonium, numbered 2 through 7 in the data files.

## 2.5 A Solution of the Neutron Transport Equation

The infinite-medium Boltzmann equation (2.3.2), as stated earlier is

$$\Sigma_T(u) \phi(u) = S(u) + \int_0^u \Sigma_S(u') \phi(u') F(u' \rightarrow u) du' + \Gamma(u) \quad (2.5.1)$$

By introducing Eqs. 2.3.3, 2.3.7 and 2.4.2 into 2.5.1 and taking absorption into account [3], the equation may be rewritten as

$$\begin{aligned} \Sigma_T(u) \phi(u) = & \int_0^u \Sigma_S^H(u') \phi(u') e^{(u'-u)} du' + \\ & \sum_{i=2}^{13} \int_{u=\epsilon_i}^u \Sigma_S^i(u') \phi(u') \frac{e^{(u'-u)}}{1 - a_i} du' + \end{aligned}$$

$$\sum_{i=2}^7 \int_0^u \Sigma_{in}^i(u') \phi(u') f_{j \rightarrow k} du' + S(u) \quad . \quad (2.5.2)$$

Since the point of the solution of (2.5.2) is to determine the average group flux in each lethargy group, the equation must have a form which expresses the flux in the  $j^{\text{th}}$  group in terms of fluxes and cross sections of previously evaluated groups,  $k = 1$  to  $j - 1$ . We therefore wish to integrate across the micro-group to determine a micro-group average flux rather than integrating across the entire spectrum. The source term in Eq. 2.5.2,  $S(u)$ , was provided by VIM as a group average across each of the 47 groups. The inelastic term is handled within the program using the simplification noted in the previous section. Renaming the group-average inelastic flux contribution and the VIM provided group-average source term as  $I(u)$  and  $X(u)$  respectively, we may begin the solution by considering first the term for isotopes other than hydrogen, the total cross section term on the left of the equality, and finally the hydrogen term. For convenience, we will use an abbreviated notation in which a subscript  $j$  will indicate that the particular cross section, flux, etc. is evaluated in the  $j^{\text{th}}$  lethargy group, such as  $\Sigma_S^i(u_j) = \Sigma_{Sj}^i$ , the elastic scattering cross section of the  $i^{\text{th}}$  isotope evaluated in the  $j^{\text{th}}$  lethargy group.

We shall now consider separately the first two terms to the right of the equality in Eq. 2.5.2.

### 2.5.1 Isotopes Other than Hydrogen

We may state this term from Eq. 2.5.2 as

$$A(u) = \sum_{i=2}^{13} \int_{u-\epsilon_i}^u \Sigma_S^i(u') \phi(u') \frac{e^{(u'-u)}}{1-\alpha_i} du' , \quad (2.5.3)$$

and, for a single isotope, which is less cumbersome,

$$A_i(u) = \int_{u-\epsilon_i}^u \Sigma_S^i(u') \phi(u') \frac{e^{(u'-u)}}{1-\alpha_i} du' . \quad (2.5.4)$$

We must also note that, from age theory [9],

$$q_e(u) \approx \sum_{i=2}^{13} \xi_i \Sigma_S^i(u) \phi(u) \quad (2.5.5)$$

or

$$q_e^i(u) \approx \xi_i \Sigma_S^i(u) \phi(u) \quad (2.5.6)$$

in terms of the single,  $i^{\text{th}}$  isotope. The slowing down density,  $q$ , for isotopes other than hydrogen was earlier stated as Eq. 2.3.8 as

$$q_e(u) = \sum_{i=2}^{13} \int_{u-\epsilon_i}^u (u') \phi(u') \frac{e^{(u'-u)} - \alpha_i}{1-\alpha_i} du' ,$$

which may be separated as

$$\begin{aligned} q_e^i(u) = & \int_{u-\epsilon_i}^u \Sigma_S^i(u') \phi(u') \frac{e^{(u'-u)}}{1-\alpha_i} du' \\ & - \frac{\alpha_i}{1-\alpha_i} \int_{u-\epsilon_i}^u \Sigma_S^i(u') \phi(u') du' , \end{aligned} \quad (2.5.7)$$

considering only the single isotope. Substituting Eq. 2.5.4 and 2.5.6 into 2.5.7 gives

$$\xi_1 \Sigma_S^1(u) \phi(u) = A_1(u) - \frac{\alpha_1}{1 - \alpha_1} \int_{u-\epsilon_1}^u \Sigma_S^1(u') \phi(u') du' . \quad (2.5.8)$$

Noting that  $\Delta u$  in isotopes other than hydrogen is

$$\Delta u = u - (u - \epsilon) = \epsilon ,$$

and is thus very small in most instances, we may assume that  $\Delta \phi(u)$  is sufficiently small to be almost negligible, which will be shown in the discussion of the program itself. Therefore,

$$\int_{u-\epsilon_1}^u \Sigma_S^1(u) \phi(u') du' \simeq \Sigma_{Sj}^1 \phi_j \int_{u-\epsilon_1}^u du' = \Sigma_{Sj}^1 \phi_j \epsilon_1 , \quad (2.5.9)$$

and Eq. 2.5.8 becomes

$$\xi_1 \Sigma_{Sj}^1 \phi_j = A_{1j} - \frac{\alpha_1}{1 - \alpha_1} \Sigma_{Sj}^1 \phi_j \epsilon_1 ,$$

which is rearranged as

$$A_{1j} = \Sigma_{Sj}^1 \phi_j \xi_1 + \Sigma_{Sj}^1 \phi_j \frac{\alpha_1}{1 - \alpha_1} \epsilon_1 . \quad (2.5.10)$$

When terms are combined and Eqs. 2.3.1 and 2.3.6a are substituted for  $\xi$  and  $\epsilon$  respectively, we have

$$A_{1j} = \Sigma_{Sj}^1 \phi_j \left( 1 + \frac{\alpha_1}{1 - \alpha_1} \ln \alpha + \frac{\alpha_1}{1 - \alpha_1} \ln \frac{1}{\alpha_1} \right)$$

or

$$A_{ij} = \sum_{Sj}^i \phi_j \left( 1 + \frac{\alpha_i}{1-\alpha_i} \ln \alpha - \frac{\alpha_i}{1-\alpha_i} \ln \alpha \right) = \sum_{Sj}^i \phi_j \quad (2.5.11)$$

The term for isotopes other than hydrogen is then, returning to Eq. 2.5.3 and summing the contributions of each of the isotopes considered here,

$$\sum_{i=2}^{13} \int_{u-\epsilon_i}^u \sum_{Sj}^i (u') \phi(u') \frac{e^{(u'-u)}}{1-\alpha_i} du' = \sum_{i=2}^{13} \sum_S^i (u) \phi(u) \quad (2.5.12)$$

Equation 2.5.12 may be combined with the expression to the left of the equality in Eq. 2.5.2 as

$$\sum_T(u) \phi(u) - \sum_{i=2}^{13} \sum_S^i (u) \phi(u) = \phi(u) \left( \sum_T(u) - \sum_{i=2}^{13} \sum_S^i (u) \right) = \Sigma(u) \phi(u) \quad (2.5.13)$$

where  $\Sigma(u)$  is now a composite term on the left of the equality, reducing the transport equation to

$$\Sigma(u) \phi(u) = \int_0^u \sum_S^H(u') \phi(u') e^{(u'-u)} du' + \Gamma(u) + S(u) \quad (2.5.14)$$

### 2.5.2 The Hydrogen Term

The hydrogen term of equation 2.5.2 is the first term to the right of the equality,

$$\int_0^u \sum_S^H(u') \phi(u') e^{(u'-u)} du' = e^{-u} \int_0^u \sum_S^H(u') \phi(u') e^{u'} du' \quad (2.5.15)$$

where we have taken the liberty of separating the exponential component and moving the constant multiplier outside the integral.

Recalling that the macroscopic cross sections are group averaged and applying the definition of an integral, and evaluating the entire term across the micro-group for an average flux, we have

$$\begin{aligned} \int_{u_{j-1}}^{u_j} e^{-u} du \int_0^u \Sigma_S^H(u') \phi(u') e^{u'} du' \\ = \int_{u_{j-1}}^{u_j} e^{-u} du \left[ \sum_{k=1}^J \Sigma_{S_k}^H \frac{\phi_k + \phi_{k-1}}{2} (e^{u_k} - e^{u_{k-1}}) \right] . \end{aligned}$$

Finally, the integral of the multiplier is evaluated as

$$\int_{u_{j-1}}^{u_j} e^{-u} du = e^{-u_{j-1}} - e^{-u_j} .$$

The hydrogen term now becomes

$$\int_0^u \Sigma_S^H(u') \phi(u') e^{(u'-u)} du' = (e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^J \Sigma_{S_k}^H \frac{\phi_k + \phi_{k-1}}{2} (e^{u_k} - e^{u_{k-1}}) .$$

(2.5.16)

As previously stated, what is needed is an expression for flux in the  $j^{\text{th}}$  group in terms of the constants of previous groups. The hydrogen term must therefore be separated into two terms, one for the  $j^{\text{th}}$  group and one for all previous groups, becoming



$$\begin{aligned}
& (e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^J \frac{\phi_k + \phi_{k-1}}{2} (e^{u_k} - e^{u_{k-1}}) \\
&= (e^{-u_{j-1}} - e^{-u_j}) \sum_{S_j}^H \frac{\phi_j + \phi_{j-1}}{2} (e^{u_j} - e^{u_{j-1}}) \\
&+ (e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^{J-1} \sum_{S_k}^H \frac{\phi_k + \phi_{k-1}}{2} (e^{u_k} - e^{u_{k-1}}) \quad . \quad (2.5.17)
\end{aligned}$$

For convenience, we note that

$$\Phi_j \equiv \int_{u_{j-1}}^{u_j} \phi(u) du = \frac{\phi_j + \phi_{j-1}}{2} \Delta u_j \quad (2.5.18)$$

and therefore

$$\frac{\phi_j + \phi_{j-1}}{2} = \frac{\Phi_j}{\Delta u_j} \quad . \quad (2.5.19)$$

With the substitution of Eq. 2.5.19 into 2.5.17, the hydrogen term now becomes

$$\begin{aligned}
& (e^{-u_{j-1}} - e^{-u_j}) \frac{\sum_{S_j}^H \Phi_j}{\Delta u_j} (e^{u_j} - e^{u_{j-1}}) \\
&+ (e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^{J-1} \frac{\sum_{S_k}^H \Phi_k}{\Delta u_k} (e^{u_k} - e^{u_{k-1}}),
\end{aligned}$$

or, combining the exponential expression in the left portion,

$$\int_0^u \sum_S^H(u') \phi(u') e^{(u'-u)} du' = (e^{\Delta u_j} + e^{-\Delta u_j} - 2) \frac{\sum_{S_j}^H \Phi_j}{\Delta u_j}$$

$$+ (e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^{J-1} \frac{\Sigma_{S_k}^H \Phi_k}{\Delta u_k} (e^{u_k} - e^{u_{k-1}}) . \quad (2.5.20)$$

### 2.5.3 Total Flux and the Group Averaged Solution

The term to the left of the equality in Eq. 2.5.14 must still be integrated over the individual lethargy group. This is done as in sections 2.5.1 and 2.5.2 and becomes

$$\int_{u_{j-1}}^{u_j} \Sigma(u) \phi(u) du = \Sigma_j \frac{\phi_j + \phi_{j-1}}{2} \Delta u_j = \Sigma_j \Phi_j . \quad (2.5.21)$$

The transport equation becomes, by substituting 2.5.20 and 2.5.21 into Eq. 2.5.14, and remembering the group averaged source and inelastic terms,

$$\begin{aligned} \Sigma_j \Phi_j &= (e^{\Delta u_j} + e^{-\Delta u_j} - 2) \frac{\Sigma_{S_j}^H \Phi_j}{\Delta u_j} \\ &+ (e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^{J-1} \frac{\Sigma_{S_k}^H \Phi_k}{\Delta u_k} (e^{u_k} - e^{u_{k-1}}) \\ &+ I_j + X_j . \end{aligned}$$

Combining terms on  $\Phi_j$ , we obtain

$$\begin{aligned} &\Phi_j \left[ \Sigma_j - (e^{\Delta u_j} + e^{-\Delta u_j} - 2) \frac{\Sigma_{S_j}^H}{\Delta u_j} \right] \\ &= (e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^{J-1} \frac{\Sigma_{S_k}^H \Phi_k}{\Delta u_k} (e^{u_k} - e^{u_{k-1}}) + I_j + X_j . \end{aligned}$$

The expression for flux in the  $j^{\text{th}}$  group is then

$$\Phi_j = \frac{[(e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^{J-1} \frac{\Sigma_{S_k}^H \Phi_k}{\Delta u_k} (e^{u_k} - e^{u_{k-1}}) + I_j + X_j]}{[\Sigma_j - (e^{\Delta u_j} + e^{-\Delta u_j} - 2) \frac{\Sigma_{S_j}^H}{\Delta u}]}, \quad (2.5.22)$$

which is the expression to be evaluated for averaged group fluxes in the FASPEC program, and is used to determine the macrogroup constants.

## 2.6 Other Group Constants

The group constants required for determination of such design criteria as criticality and burnup are the macroscopic absorption cross section,  $\Sigma_a$ , the removal cross section,  $\Sigma_R$ , the product of the average number of fission neutrons per fission event and the fission cross section,  $\nu\Sigma_f$ , and the diffusion coefficient,  $D$ , which may be expressed as a function of the transport cross section,  $\Sigma_{tr}$ . In addition, to determine flux in any group we must calculate the total cross section,  $\Sigma_T$ . We remember that

$$\Sigma = N \sigma$$

where

$\Sigma$  = is any given macroscopic cross section, such as elastic scatter,  $\Sigma_s$

$\sigma$  = is the same microscopic cross section (e.g.,  $\sigma_s$ )

$N$  = is the atomic number density of the isotope whose cross section corresponds with  $\Sigma$  and  $\sigma$ .

Similarly, we note that

$$\Sigma_a = \Sigma_c \text{ (capture)} + \Sigma_f \text{ (fission) and}$$

$$\Sigma_T = \Sigma_s + \Sigma_a + \Sigma_{in} \text{ (inelastic scatter).}$$

Using the above relationships, together with user-supplied number densities and VIM-supplied cross sections, values for the group constants except  $\Sigma_R$ ,  $D$  and flux  $\phi$ , may be determined.

To find  $D$ , the diffusion coefficient, we must first calculate  $\Sigma_{tr}$  from [10]

$$\frac{1}{\Sigma_{tr_j}} = \frac{1}{\Sigma_{s_j} \left(1 - \frac{2}{3A}\right)} .$$

Then  $D$  is found as

$$D_j = [2 \Sigma_{tr_j}]^{-1} . \quad (2.6.1)$$

The removal cross section, like the flux, must be calculated from a defining equation.

## 2.7 The Removal Cross Section

The removal cross section multiplied by the flux is equal to the total slowing down density [11], or

$$\Sigma_R(u) \phi(u) = q(u) = q_H(u) + q_e(u) \quad (2.7.1)$$

recalling Eq. 2.3.4. Substituting Eq. 2.3.5 for  $q_H(u)$  and Eq. 2.5.5 for  $q_e(u)$ , we have, after integrating  $q_e$  over the lethargy group,

$$\begin{aligned} \Sigma_R(u) \phi(u) &= \int_0^u \Sigma_S^H(u') \phi(u') e^{(u'-u)} du' \\ &+ \sum_{i=2}^{13} \xi_i \Sigma_S^i(u) \Phi(u) \end{aligned} \quad (2.7.2)$$

where the hydrogen term is identical to that found in section 2.5.2 as Eq. 2.5.16,

$$\begin{aligned} &\int_0^u \Sigma_S^H(u') \phi(u') e^{(u'-u)} du' \\ &= (e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^{J-1} \frac{\Sigma_{S_k}^H \Phi_k}{\Delta u_k} (e^{u_k} - e^{u_{k-1}}) . \end{aligned} \quad (2.7.3)$$

Integrating the left side of Eq. 2.7.1 over the lethargy group  $u_j \rightarrow u_{j-1}$  in a manner similar to Eq. 2.5.21 yields

$$\int_{u_{j-1}}^{u_j} \Sigma_R(u) \phi(u) du = \Sigma_{R_j} \Phi_j \quad (2.7.4)$$

Substituting Eqs. 2.7.3 and 2.7.4 into Eq. 2.7.2 produces

$$\begin{aligned} \Sigma_{R_j} \Phi_j &= (e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^J \frac{\Sigma_{S_k}^H \Phi_k}{\Delta u_k} (e^{u_k} - e^{u_{k-1}}) \\ &+ \sum_{i=2}^{13} \xi_i \Sigma_{S_j}^i \Phi_j . \end{aligned} \quad (2.7.5)$$

With the flux for the  $j^{\text{th}}$  group already calculated, we may rearrange Eq. 2.7.5 to produce an expression for the macroscopic removal cross section.

$$\Sigma_{R_j} = \frac{(e^{-u_{j-1}} - e^{-u_j}) \sum_{k=1}^J \frac{\Sigma_k^H \Phi_k}{\Delta u_k} (e^{u_k} - e^{u_{k-1}}) + \sum_{i=2}^{13} \xi_i \Sigma_j^i \Phi_j}{\Phi_j} .$$

These calculations and the corresponding output provide the required data for entry into the ODMUG program [1] and should provide sufficient group constant data for the user to enter most criticality and burnup programs.

### III. FASPEC

#### 3.1 General Description

The FASPEC program determines neutron flux and group constants for up to 47 macrogroups. This is done by first dividing the original 47 groups into 20 sub-groups each for a total of 940 microgroups. Calculations of group constants are then carried out as noted in Chapter 2.

After all group constants have been calculated, the 940 microgroups are then collapsed to 47 macrogroups as flux weighted macrogroup constants, which are available for use as is or may be further collapsed into the desired number of macrogroups.

The program was written to be as user-friendly as possible. The only input values required are the atomic number densities for fuel, moderator and clad, and the desired number of final macrogroups and their upper and lower group numbers. A set of default number densities is provided (see user's guide) which may be substituted at the choice of the user. Number densities, number of macrogroups and the macrogroup delimiters are requested via prompting from the program together with examples in each case.

Output is in file form, which may be printed at the discretion of the user, in both "microgroup" (47) and "macrogroup" (user specified) files. See the appendix for sample output.

In the following sections the method of input, microgroup expansion, macrogroup collapse, some calculations within the program and output format will be discussed.

### 3.2 Input and Output

There are two types of input used in the FASPEC program. Data files are used to supply data such as cross section ( $\sigma_c, \sigma_x, \sigma_f, \sigma_{in}$ ),  $v, \xi, \alpha, A, u$  and  $X$  which are isotope and/or energy dependent. A number density file is also provided for the default case. This file may also be used in lieu of the prompting if more than one run with the same number density set is anticipated. Any data in these files may be modified by the user (see user's guide) but care should be taken as changes here can be very time consuming unless the changes can be read directly into the files in the correct order and format.

Double precision format was used for the input files to improve accuracy. E, or simple exponential, format has been used successfully in number density input with nominal results. The first step in the program is a read in of all the data files into the appropriate arrays.

After the file supplied data are read and stored, the program asks the user, "DO YOU WISH TO USE DEFAULT NUMBER DENSITIES? (YES/NO)." If the user reply is yes, the statement "DEFAULT NUMBER DENSITIES WILL BE USED. SEE USER'S GUIDE FOR DEFAULT VALUES" will appear and the program will begin running. If the user replies "NO" to the question, the program begins prompting for number densities of each of the 13 isotopes provided in the data files (see user's guide). The prompting is of the form "NUMBER DENSITY OF HYDROGEN?(EG. .46800D-01)" and continues through all 13 isotopes. When the last of the 13 number densities has been entered, the program begins to run.

When calculations are complete, including the collapse from 940



microgroups to 47 macrogroups, the program stops and tells the user to "ENTER NUMBER OF MACRO GROUPS DESIRED.(EG. 05)" and waits for a two-digit number to be entered. After the number of macrogroups is entered, the programs prompts with "ENTER LOWER GROUP NO. AND UPPER GROUP NO. FOR MACRO GROUP 01 (EG. 05 16)". After the entry of the group number delimiters for group 01, the prompting continues through the group number initially entered by the user. Following entry of the last set of macrogroup delimiters, the program performs the collapse to the required number of macrogroups and sets the results into the output files.

There are four output files: AMICRO, BMICRO, AMACRO and BMACRO. The MICRO files contain the output for 47 groups; the MACRO files contain the user selected number of groups. The two A files (MICRO & MACRO) each contain data for the same parameters, as do the two B files. Column headings are provided to indicate the contents of each column. All output is truncated to exponential (single precision) form.

In addition to the normal output files, two diagnostic files, TEST DATA and TESTOUT DAT, are inactive within the program. Either or both may be activated by the user and used to display any given parameter(s) in any position(s) within the program by simply placing the activated statements in the correct location(s) and supplying the variable names of the desired parameters (see user's guide for details). The appendices contain samples of input and output files.

### 3.3 Microgroup Expansion and Macrogroup Collapse

To determine more accurately the various group constants from the VIM-supplied cross section data, each of the original 47 groups is divided into 20 microgroups for a total 940 microgroup calculation. The resulting 940 sets of group constants are then collapsed back to 47 macrogroups for initial output, then collapsed again to the number of macrogroups required by the user. By adjusting certain loop and variable parameters, the user may select a wide range of output groups (see user's guide for details).

The expansion to 940 microgroups is accomplished as follows:

1. The original cross sections (and other energy-dependent parameters) are subtracted and divided to form an appropriate  $\Delta$  function, such as

$$(\sigma_j - \sigma_{j-1})/20 = \Delta\sigma_j$$

2. This  $\Delta$  function is then successively added to the cross section of the low (u) end of the macrogroup, such as

$$\sigma_{j1} = \sigma_{j-1} + \Delta\sigma_j ,$$

$$\sigma_{j2} = \sigma_{j-1} + 2\Delta\sigma_j ,$$

and so on to  $\sigma_{j20}$ .

3. Each of the VIM-provided energy-dependent parameters is subdivided in this manner prior to the initiation of calculations of group constants.

Calculations are then made in the 940 microgroup structure before being collapsed back to 47 groups.

Collapsing back to 47 groups and the further collapse to a user-specified number of macrogroups are handled in the same manner, though with necessarily different routines within the program. The collapse is accomplished using the accepted method of group collapse,

$$\overline{\Sigma}_j = \frac{\sum_{M=1}^{20} \Sigma_M \phi_M \Delta u_M}{\sum_{M=1}^{20} \phi_M \Delta u_M} . \quad (3.3.1)$$

Average flux was found as

$$\overline{\Phi}_j = \frac{\sum_{M=1}^{20} \phi_M \Delta u_M}{\sum_{M=1}^{20} \Delta u_M} . \quad (3.3.2)$$

The macrogroup diffusion coefficient,  $\overline{D}_j$ , was determined by first collapsing the transport cross section as in Eq. 3.3.1, then applying Eq. 2.6.1 to obtain

$$\overline{D}_j = [3 \Sigma_{tr_j}]^{-1} . \quad (3.3.3)$$

#### 3.4 Some Calculations Within FASPEC

All calculations of group constants are carried out in as straightforward a manner as possible using the relationships and equations presented and derived in Chapter 2. The determination of the inelastic scattering contribution to flux does, however, deserve a more detailed treatment.

The inelastic scatter flux contribution from a particular originating group (incident neutron energy) by a particular isotopic target nucleus (of mass  $A$  - see Section 2.4) is determined using an array which is set by two nested do loops: the outer loop for isotopes, the inner loop for the lethargy group into which the energy of the scattered neutron falls. Since there is no contribution by inelastic scattering within the originating group and there is, therefore, no inelastic scatter contribution in the first group, the calculation is performed as the last step before returning to the start of the calculation loop at the next higher lethargy.

The calculation simply converts the energy of the incident neutron, found from the lethargy, to MeV instead of eV, then searches the lethargy groups to find the group into which the energy of the scattered neutron falls. If there is no match, the program returns to the next isotope, and so on until all heavy isotopes have been considered. If a match is found, the macroscopic inelastic cross section is multiplied by the flux, both evaluated at the lethargy of the incident neutron, and the product is added to the number already residing in the inelastic array in the lethargy group corresponding to the energy of the scattered neutron. The array thus not only holds the values of inelastic flux contribution for the down-scatter neutrons but also acts as an adder for the contributions from any isotope at any appropriate incident energy. This method is more economical of storage space than the somewhat more easily understood 2D array system which could be used.

## IV. RESULTS AND CONCLUSIONS

### 4.1 Results

The case from which VIM supplied cross section data is that of a hexagonal infinitely repeating lattice which is also infinite in the axial direction. Rod pitch and diameter are near the middle of the accepted design range. Table IV.1 contains the lattice parameters for this core as well as those for two other cases. The initial core design was run on both VIM and FASPEC for comparison and evaluation of FASPEC in both beginning of life and end of life isotopic concentrations. Beginning of life calculations were also run on both programs for the two other lattices to verify the operation of FASPEC in cases other than the one from which the initial data were taken.

Figure 4.1 shows a comparison of fluxes calculated by both VIM and FASPEC for the beginning of life case. FASPEC fluxes in the higher energy ranges (lower lethargies) are somewhat higher than those calculated by VIM. The peak flux differs by 3.68 percent, while at higher lethargies, the difference between the two calculated values varies in the 4 to 8 percent range. The calculated fluxes maintain about the same difference throughout the remainder of the spectrum, including the obvious resonances, except at the end point ( $E = 0.6253$  eV) where the difference is 15 percent. This divergence is most likely due to upscatter, the gain of energy by the neutron from the moderator. VIM takes upscatter into account while FASPEC does not, which produces the higher VIM flux.

Table 4.I Test Case Lattice Parameters

	Initial (A)	B	C
Pitch	1.27 cm	1.60	1.50 cm
Fuel diameter	0.8000 cm	1.0287 cm	0.8000 cm
Rod O.D.	0.8888 cm	1.143 cm	0.8888 cm
Clad thickness	0.0444 cm	0.0572 cm	0.0444 cm
Fuel to water ratio	0.6474	0.6979	0.37846
Fuel (BOL)	3% enriched $\text{UO}_2$		
Clad	Zircalloy		
Moderator	$\text{H}_2\text{O}$		

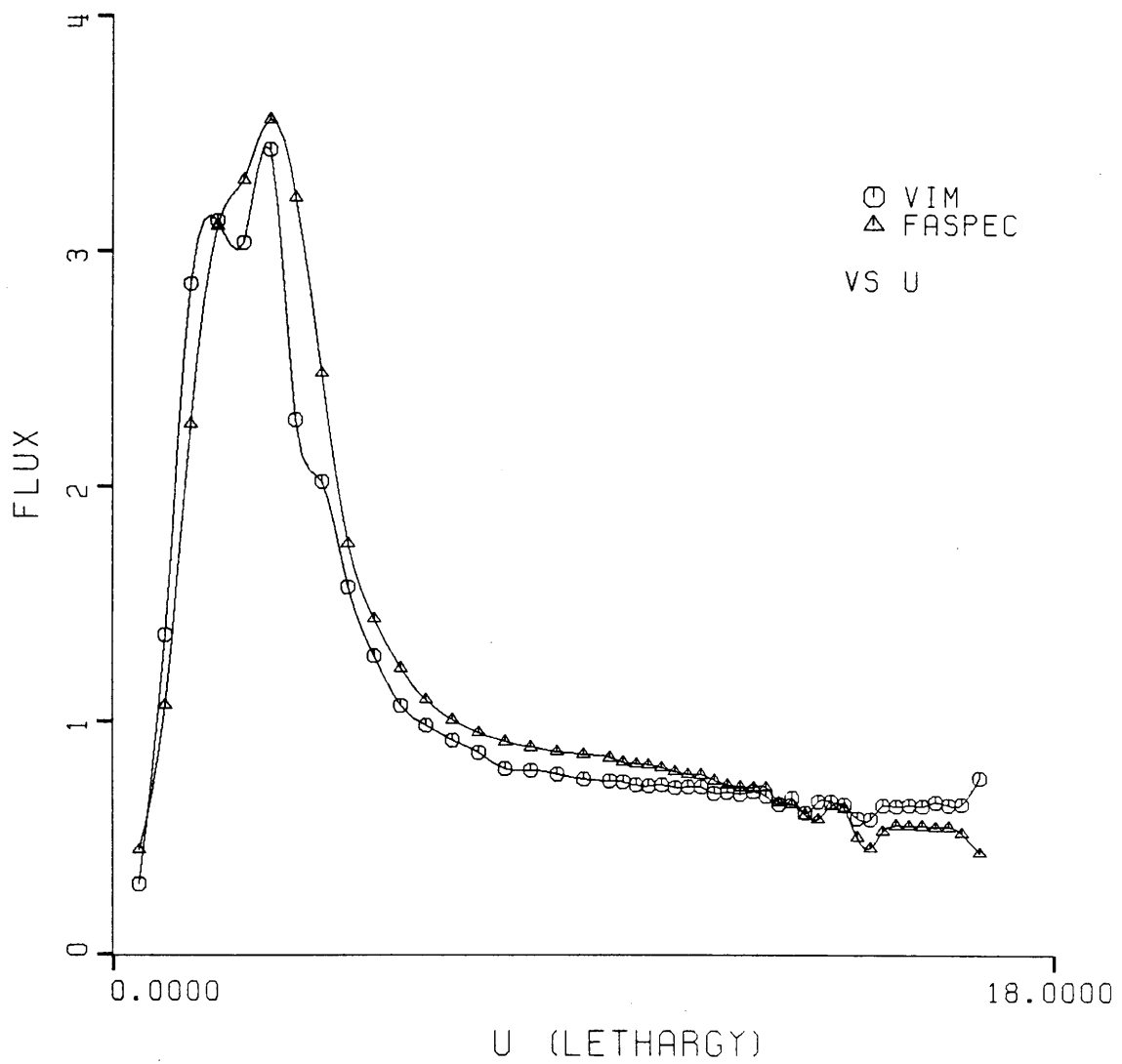


Figure 4.1 Flux Comparison for Initial Case (BOL)

Figure 4.2 is a similar comparison of calculated fluxes for the end of life case for the same core. In this case, peak flux differs by 5.75 percent, higher lethargies differ by 4 to 8 percent while the endpoints differ by 9.65 percent.

Figures 4.3 and 4.4 show flux comparisons for the other two cores noted in Table IV.1. One may see from these figures that the differences in the VIM and FASPEC results are very similar to those of Figs. 4.1 and 4.2, indicating that FASPEC performs the flux calculations reasonably well over the range of lattice parameters tested.

Figures 4.5 through 4.7 show comparisons of  $\Sigma_f$ ,  $v\Sigma_f$  and  $v$  respectively for the end of life case of the initial core. FASPEC calculated values for  $\Sigma_f$  differ from VIM-generated values by less than one percent in the lower lethargies (less than 13.0). Higher lethargy values show differences ranging from less than 0.5 percent to about 40 percent at the maximum in group 36 ( $u = 13.75$ ). Similar results were obtained for both the beginning of life case and the case labeled "C" in Table IV.1, as shown in Figs. 4.8 and 4.9 respectively.

The comparison of  $v\Sigma_f$  values (Fig. 4.6) for the end of life case shows results which are very similar to those for  $\Sigma_f$ . Differences between VIM and FASPEC generated values of  $v\Sigma_f$  range from less than 1 percent in the low lethargies to the 10 to 40 percent range in groups 31 through 39. Similar results were also obtained in the other cases shown in Figs. 4.10 and 4.11.

As a further check on FASPEC performance, values for  $v$  were hand calculated from VIM results and compared with values calculated by



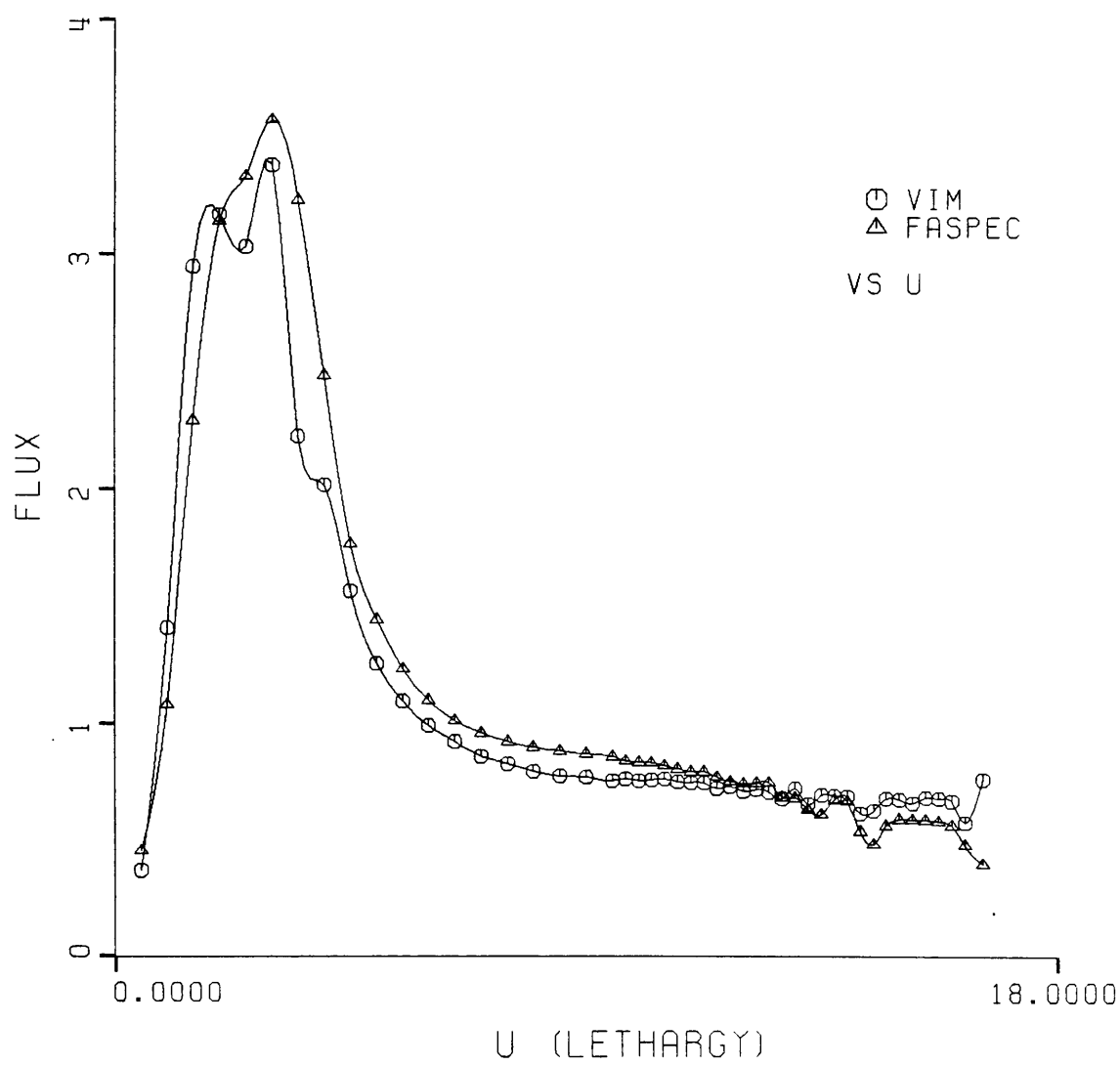


Figure 4.2 Initial Case (EOL)

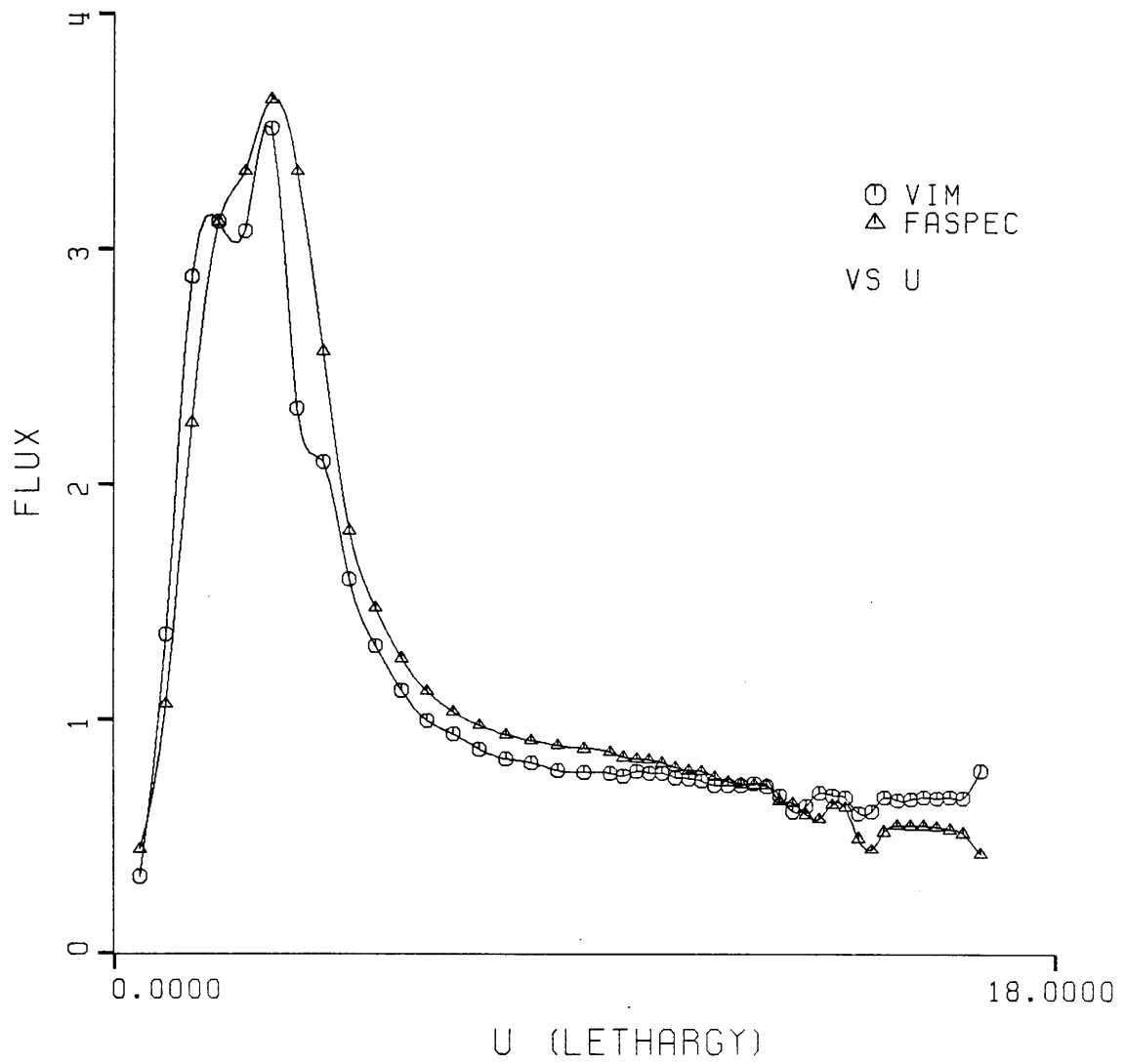


Figure 4.3 Case B, BOL Core

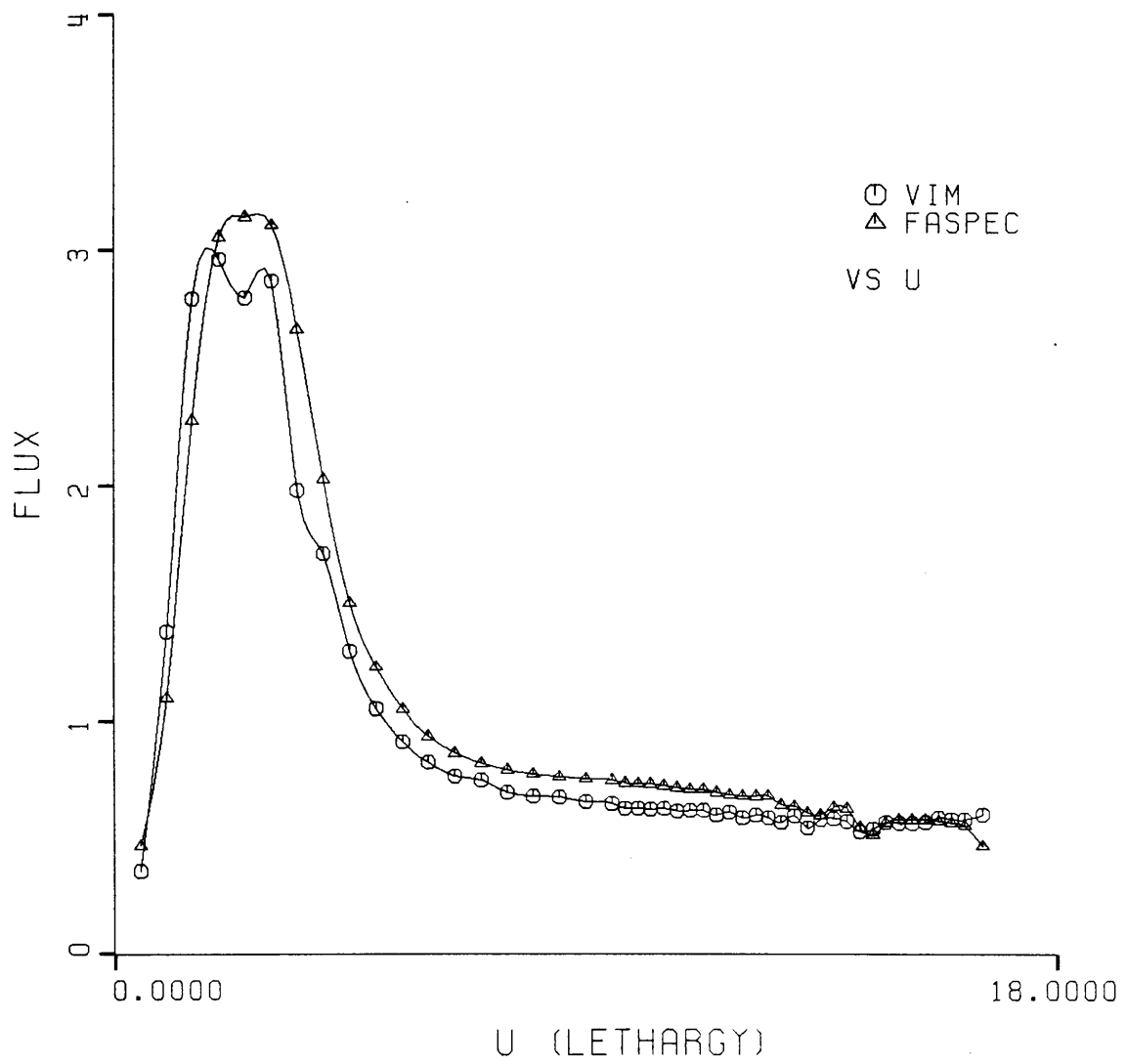


Figure 4.4 Case C, BOL Core

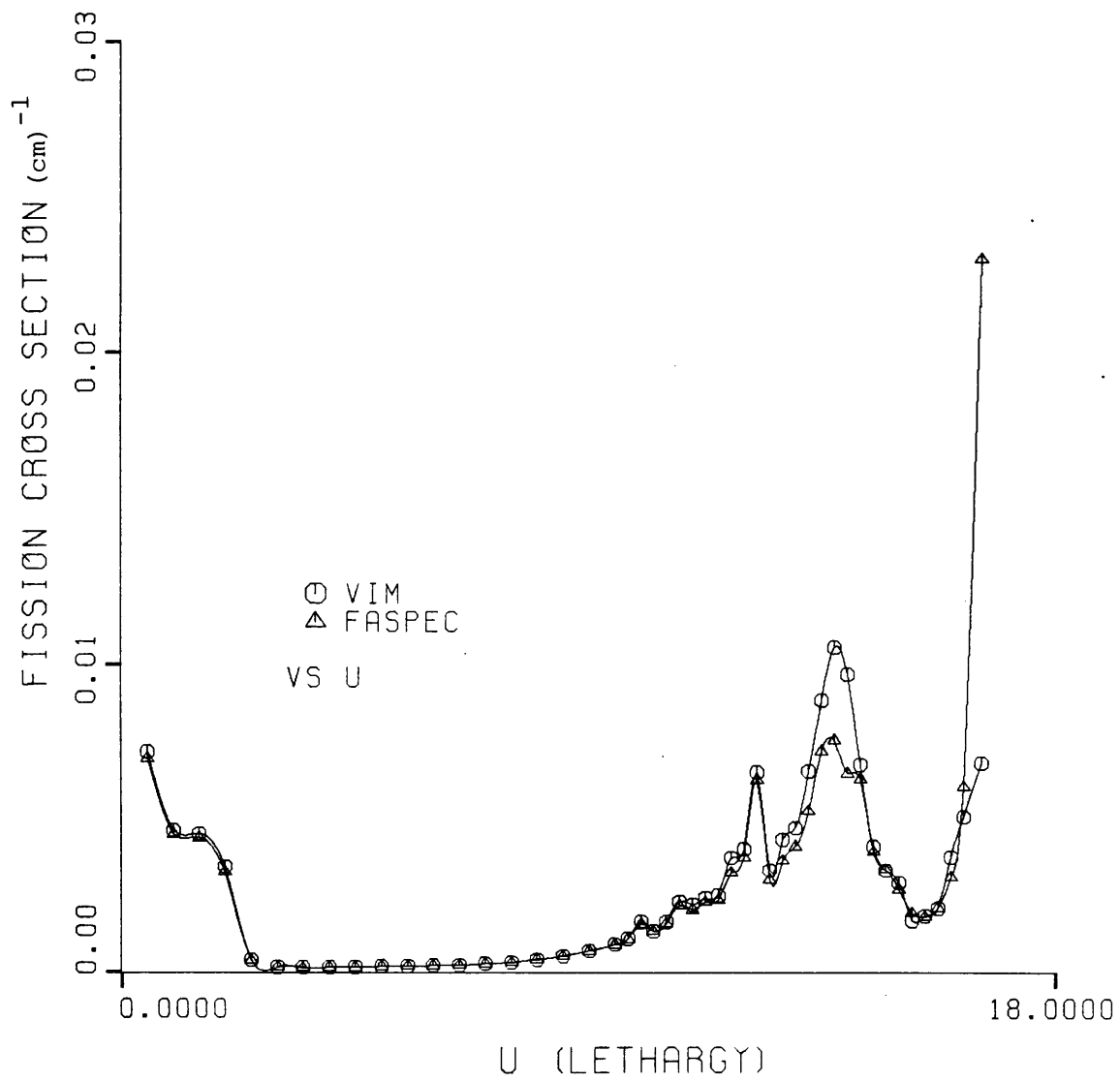


Figure 4.5 Comparison of  $\Sigma_f$  for Case A, EOL

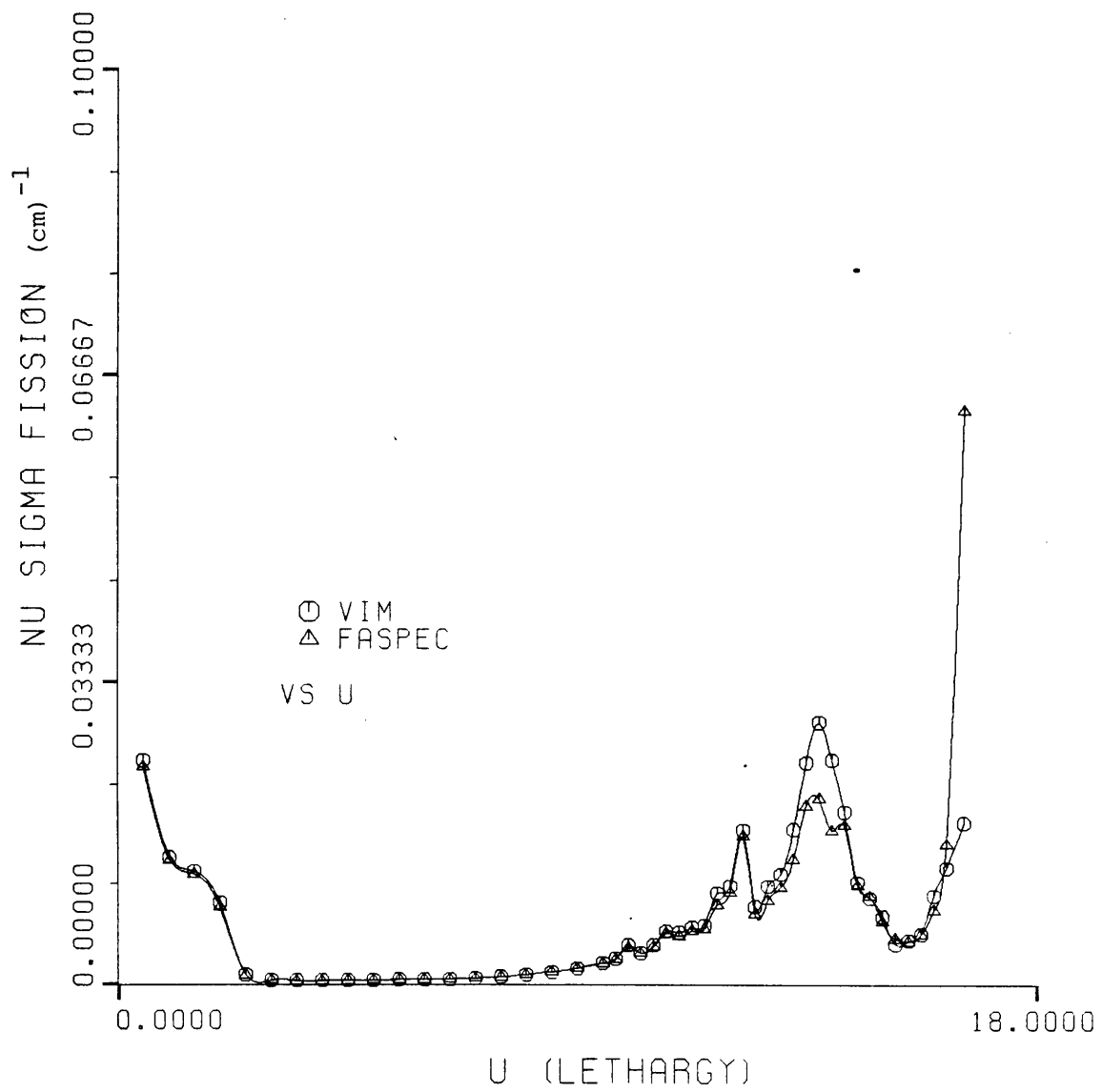


Figure 4.6  $\nu\Sigma_f$  Comparison for Case A, EOL

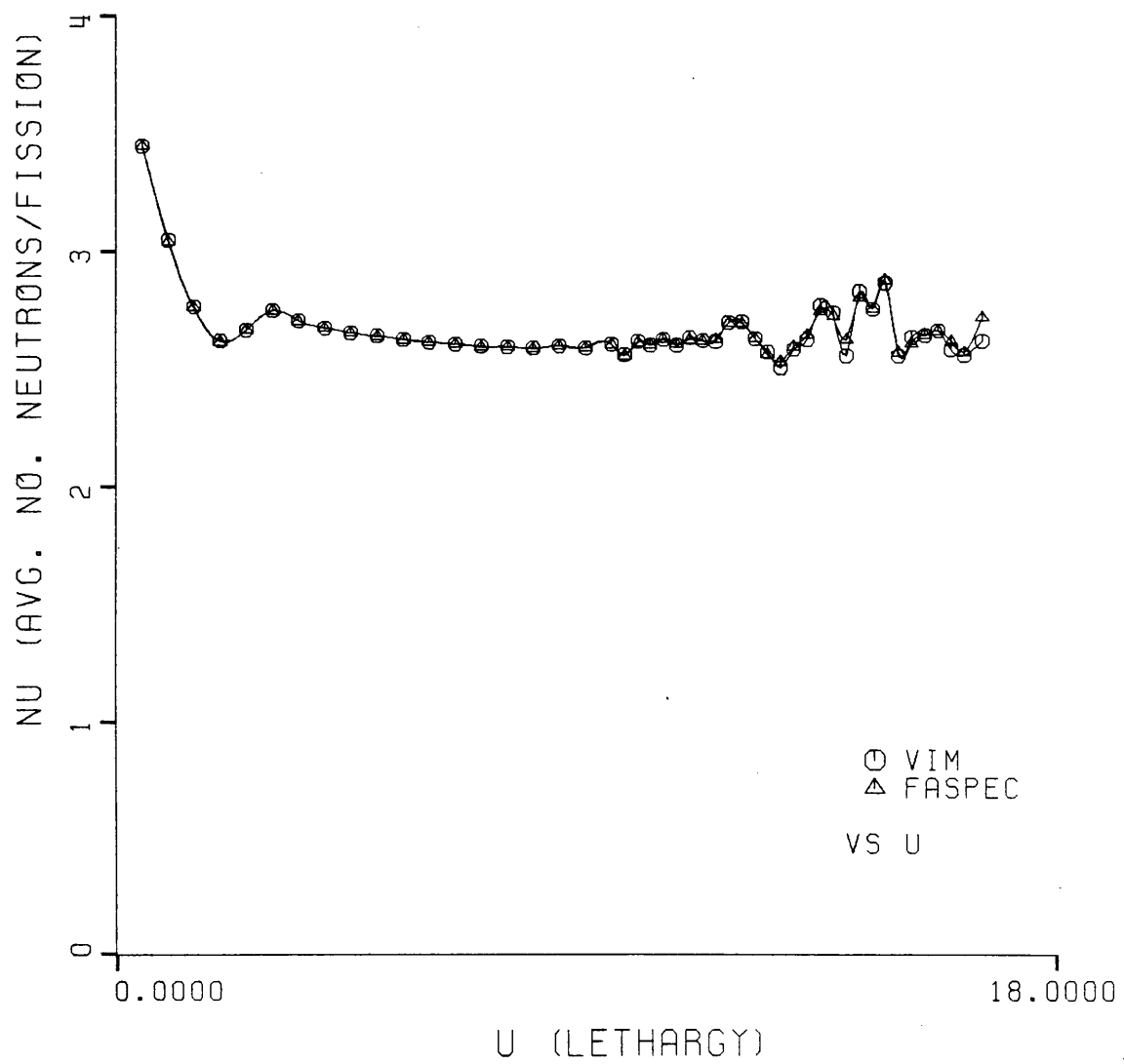


Figure 4.7 v Comparison for Case A, EOL

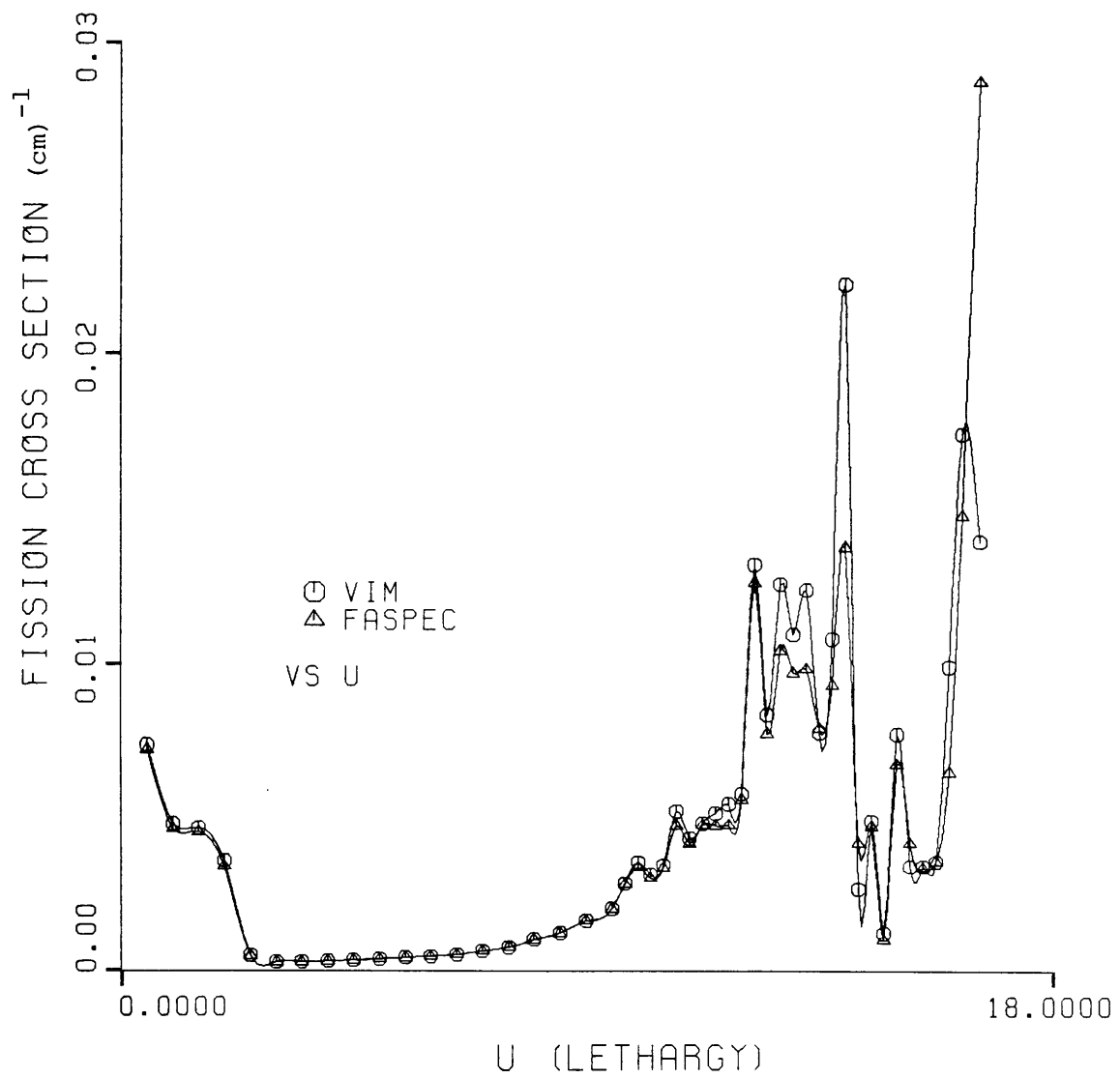


Figure 4.8  $\Sigma_f$  Comparison for Case A, BOL

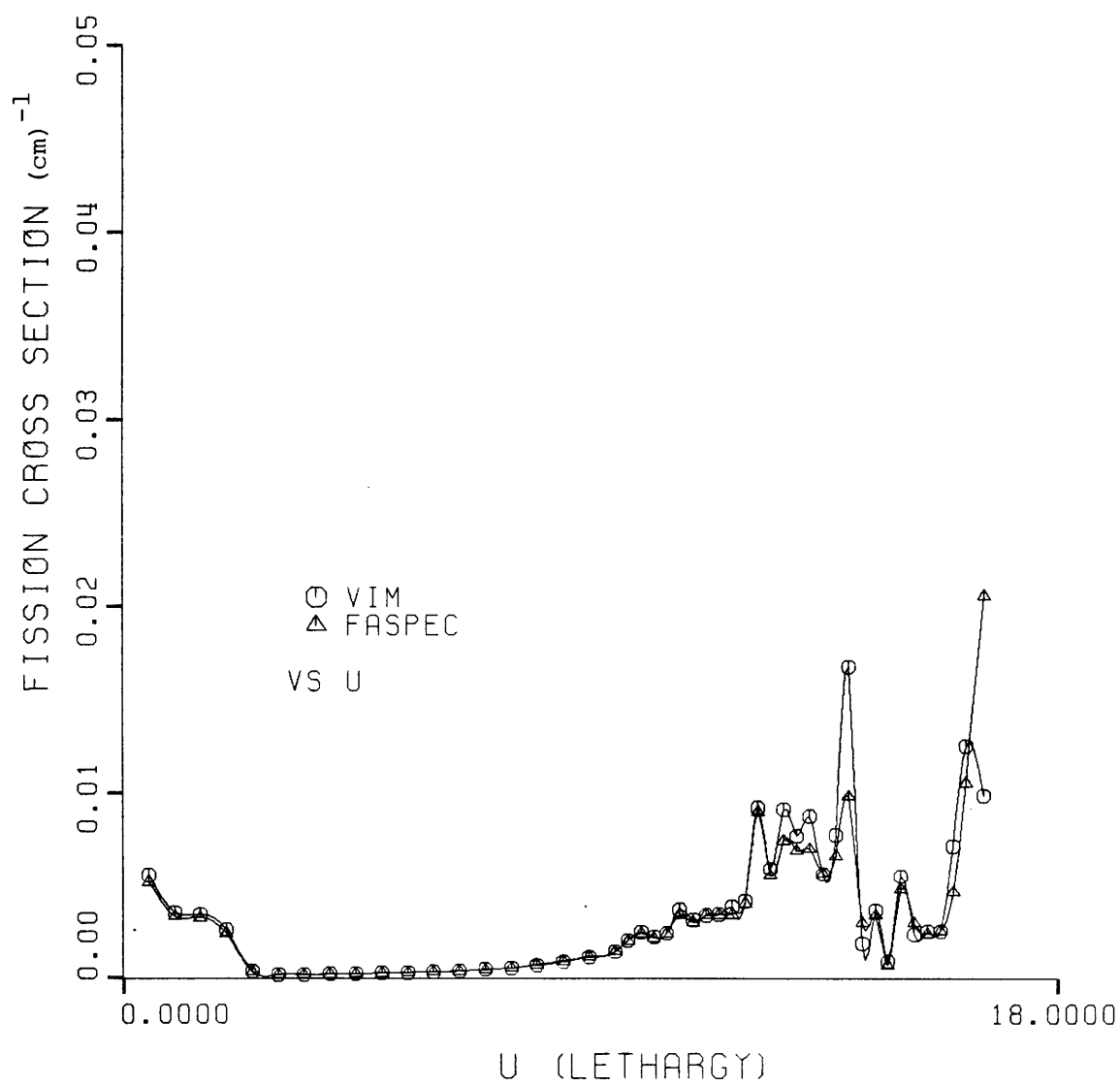


Figure 4.9  $\Sigma_f$  Comparison for Case C, BOL



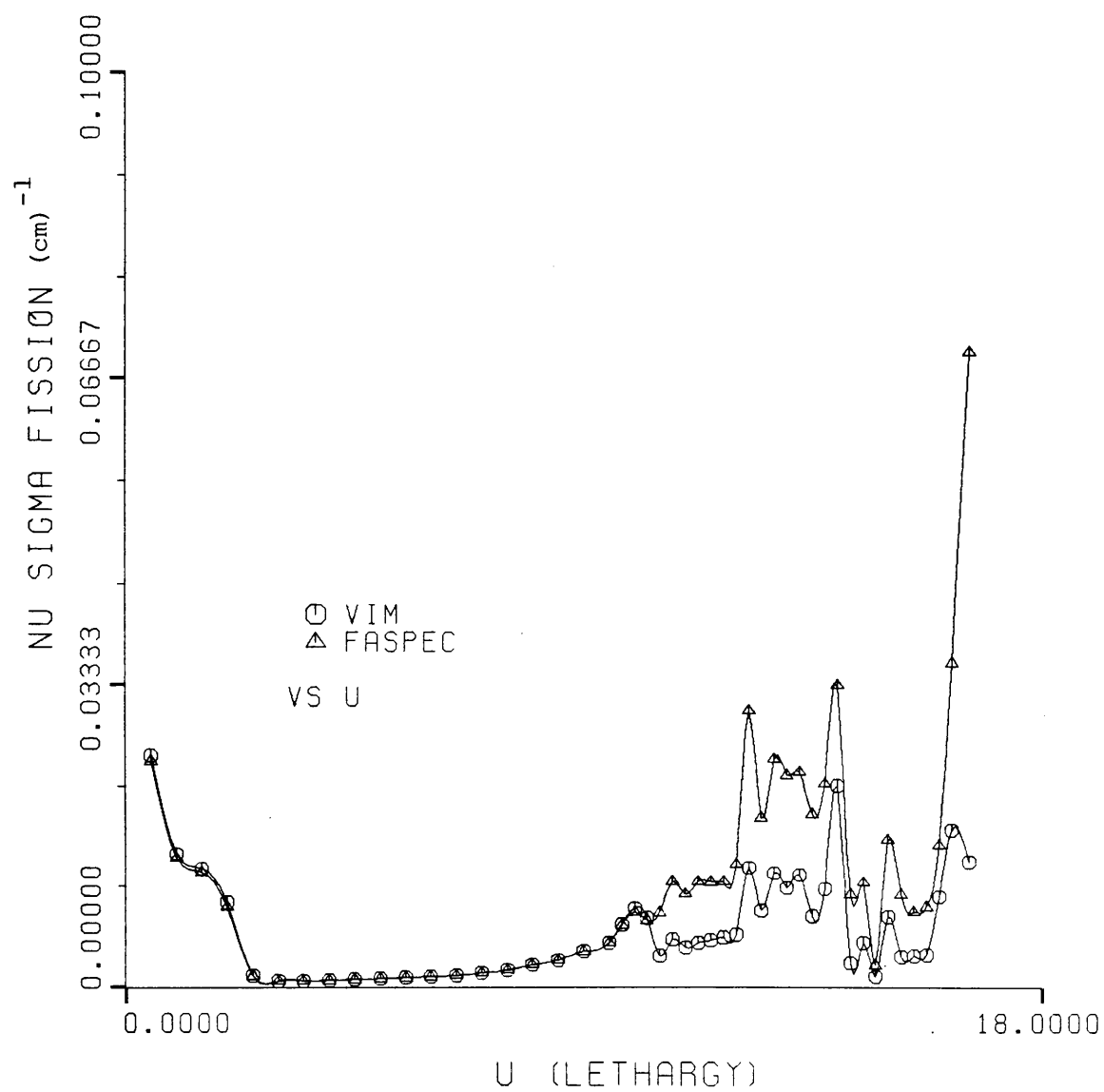


Figure 4.10  $\nu\Sigma_f$  Comparison for Case A, BOL

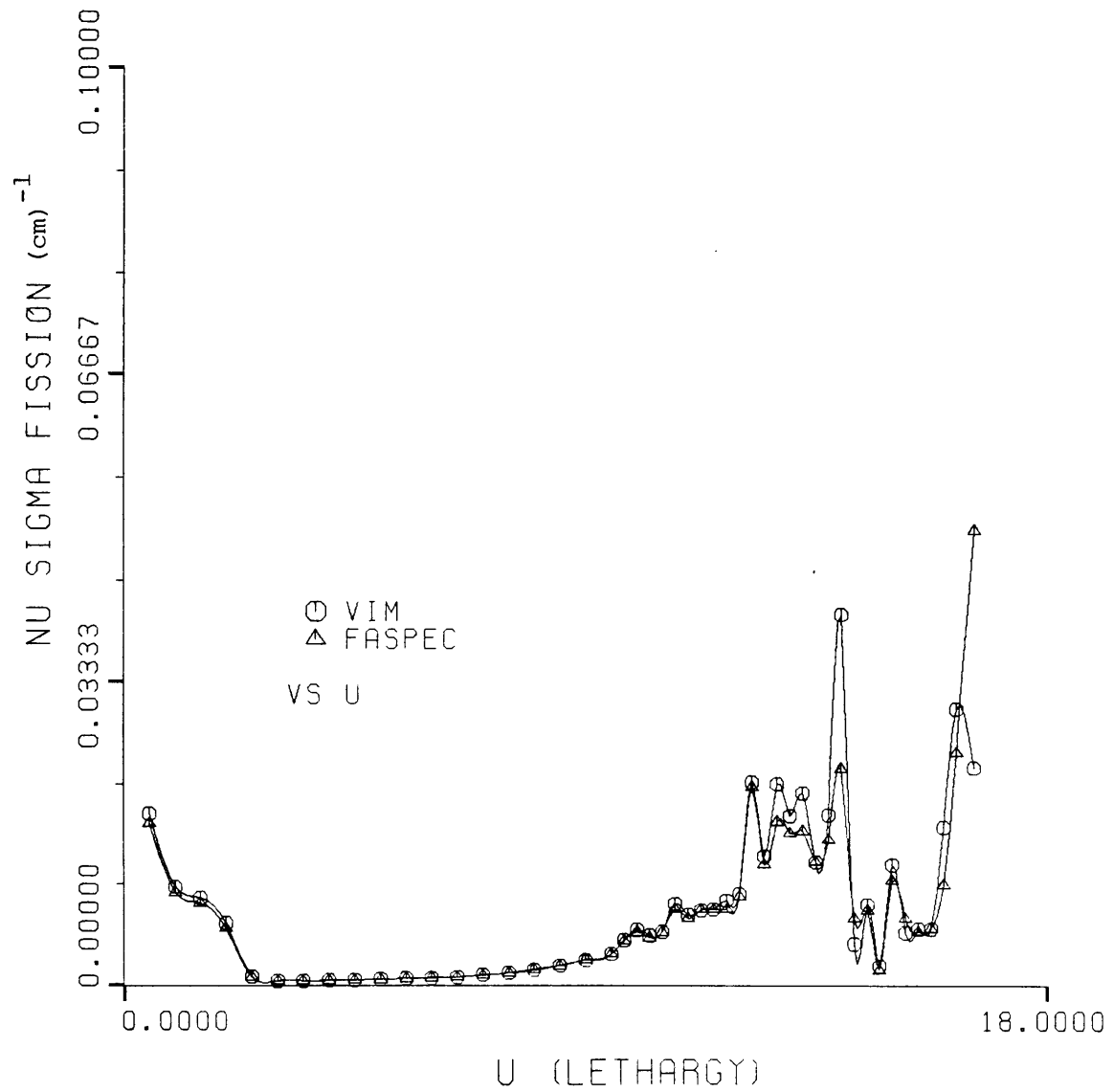


Figure 4.11  $\nu\Sigma_f$  Comparison for Case C, BOL

FASPEC. The greatest point of difference was found to be group 47, as would be expected from the previously mentioned figures. Here the difference between VIM values and FASPEC values of  $\nu$  was 3.8 percent, with many values across the spectrum either agreeing exactly or differing by less than one percent, as may be seen in Fig. 4.7.

Comparisons of values for  $\Sigma_a$  (Figs. 4.12 through 4.15) show agreement similar to those for  $\Sigma_f$ . At lethargies above the resonance range, agreement is generally within one percent. Within the resonance region of the spectrum, results differ by as much as 40 percent, as was the case with  $\Sigma_f$  and  $\nu\Sigma_f$ . The fact that this discrepancy is in the resonance region indicates that, while working well generally, FASPEC is not as accurate as VIM in the resonance region of the spectrum.

#### 4.2 Conclusions

As noted in the previous section, the FASPEC program does produce reasonably accurate group constant values within the limited design parameters it is intended to serve. FASPEC is not intended to replace the large Monte Carlo or statistically based programs, but to complement them. As such, it is much more restricted in terms of the core design parameters which can be expected to yield accurate results. It does not agree exceptionally well with VIM generated results of some group constants within the resonance region. This would be expected because of the nature of the equations used and the physical occurrences within that region of the spectrum. It should also be noted that the differences between the VIM and FASPEC values in the resonance region are differences in magnitude, rather than location of the resonances.

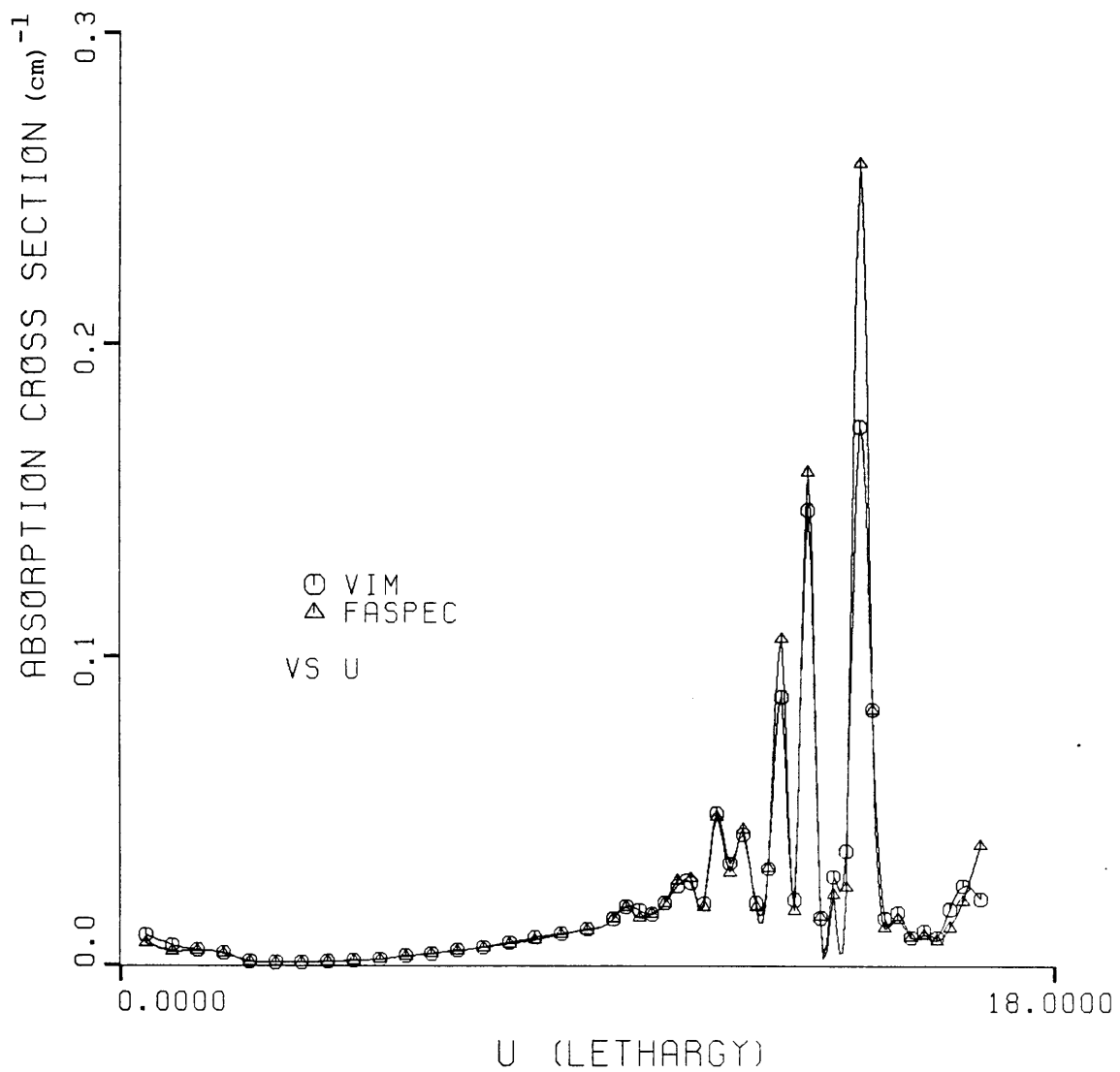


Figure 4.12  $\Sigma_a$  Comparison for Case A, BOL

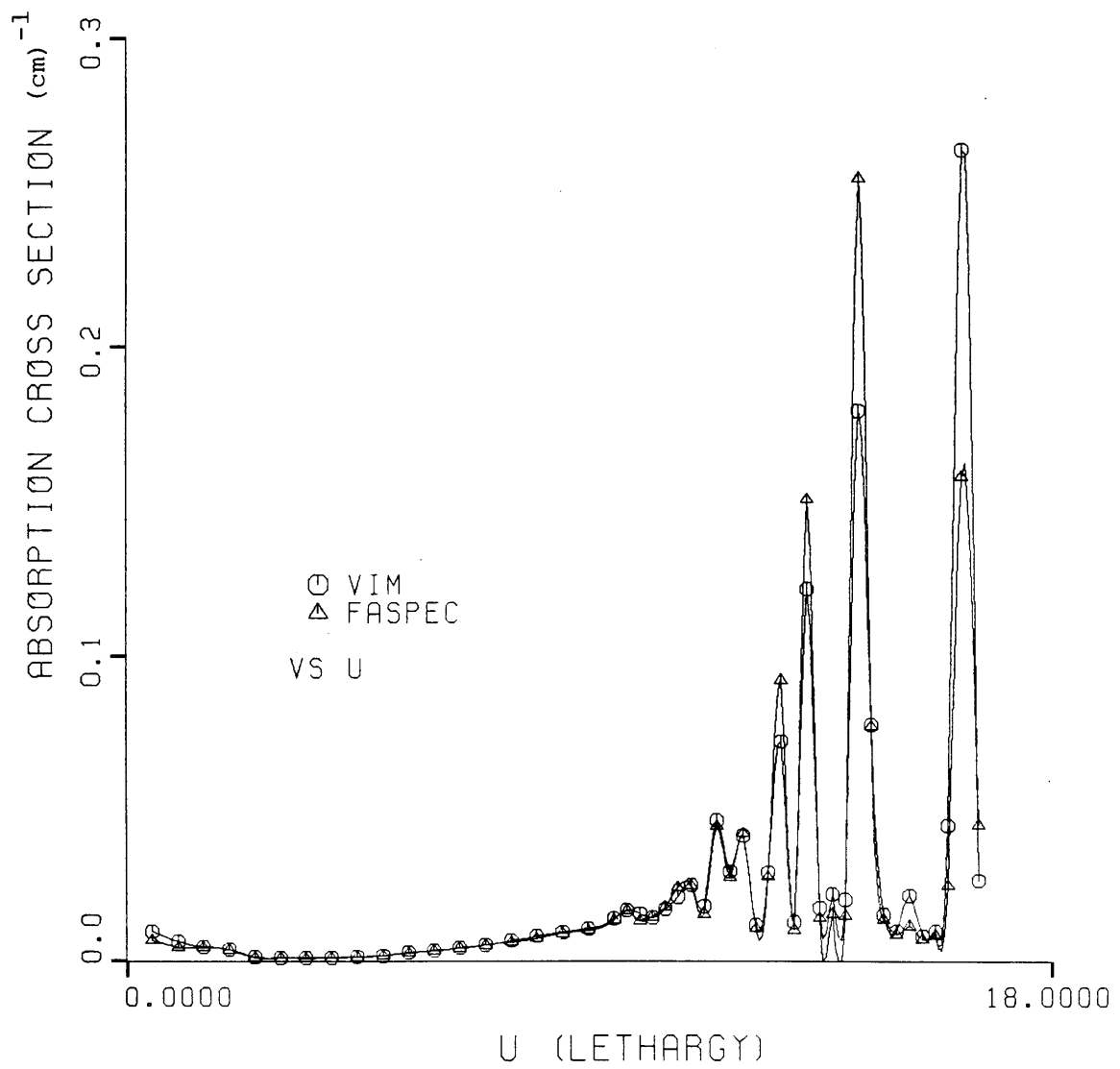


Figure 4.13  $\Sigma_a$  Comparison for Case A, EOL

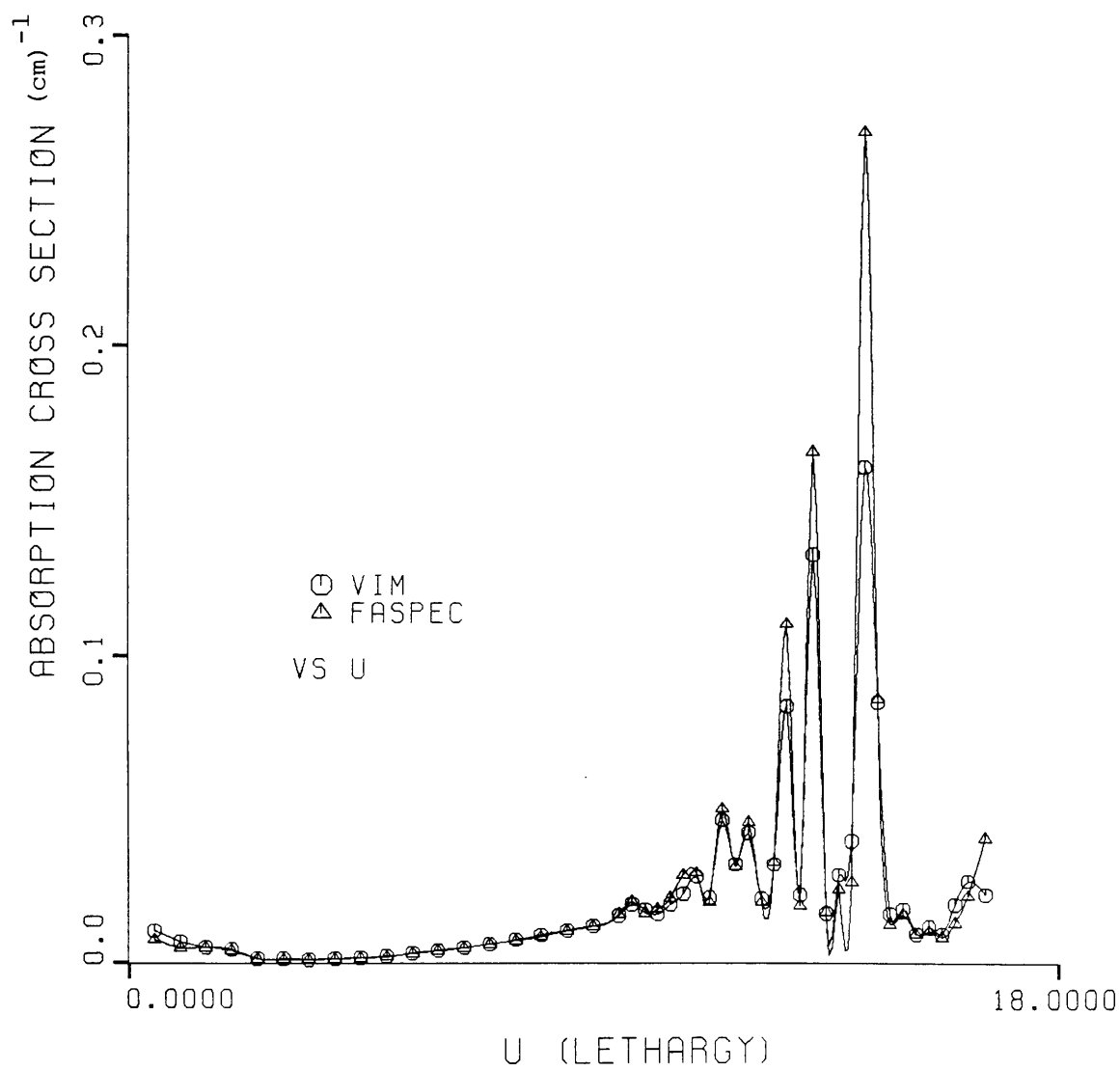


Figure 4.14  $\Sigma_a$  Comparison for Case B, BOL

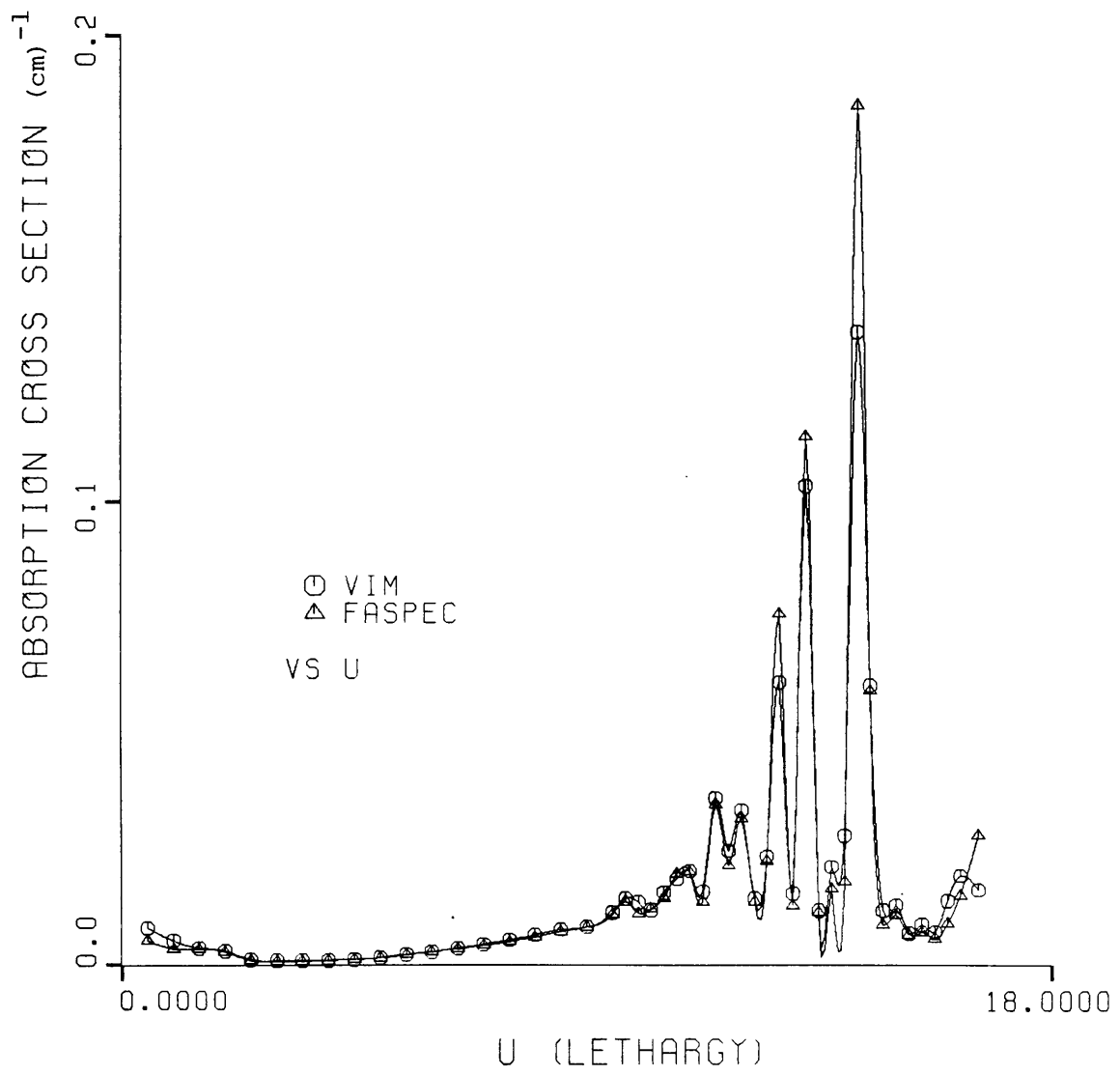


Figure 4.15  $\Sigma_a$  Comparison for Case C, BOL

Agreement is generally very good as to resonance locations within the spectrum.

Based on a rate of \$900 per hour of computer time, FASPEC averages in the vicinity of six dollars per run as opposed to approximately \$10 for a similar run on VIM. While much greater accuracy may be obtained with VIM, the cost of a single such run may range anywhere from \$10 to several hundred dollars. Obviously, using FASPEC to "ball park" a design and a large program like VIM to refine the design would be a benefit. It should also be noted that while FASPEC runs on a normal priority at the above mentioned rate, the larger programs such as VIM run on idle priority at a much reduced charge per minute of computer time. This fact alone, means that the designer or student's time is more efficiently used through FASPEC because he does not have to wait for the program to run and can see his results almost immediately.

Input is greatly simplified in FASPEC as compared to VIM. The only required input for FASPEC is atomic number density of each isotope and the macrogroup delimiters. FASPEC prompts user input where VIM does not. The VIM user gets a large, bulky printout from which he must try to extract the useful data and which he must generally leave his desk to pick up (sometimes in another building). The FASPEC user simply calls up the output files on his terminal and makes design changes based on those output data. This means that the FASPEC user can run several alternative or refined cor designs on FASPEC with an assurance of reasonable accuracy, then submit a single large program run in less time than the large program user takes to get the results of his first run-- which may or may not execute and may or may not give usable results.



#### 4.3 Possible Future Improvements

Improvements can be made in FASPEC in several different areas. One such area is the addition of terms to incorporate deuterium into the main equation. This would add more flexibility, increasing the utility of the program. An additional set of input data files generated for cases of a fast breeder design could be added, together with the appropriate input file switching function. This would allow the program to be used in both fast and thermal core design, again increasing utility. Another possible improvement is the incorporation of a short subroutine to determine atomic number densities from the input of lattice parameters. This simple change would eliminate all hand calculation of input while adding virtually nothing to the cost of operation.

While not exhausting the possibilities for improvements in the FASPEC program, the above seem worthwhile changes which would increase the utility of the program and further simplify its use without an appreciable increase in expense of operation.

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## APPENDICES

APPENDIX A  
The FASPEC Program

```

C*****
C
C                                     FASPEC                                     *
C                                     *                                     *
C                                     *                                     *
C          A PROGRAM TO DETERMINE GROUP CONSTANTS                         *
C          FOR UP TO 47 GROUPS IN A FAST NEUTRON SPECTRUM                 *
C                                     *                                     *
C          WRITTEN BY:                                                     *
C          ERNEST L. SETH, JR.                                             *
C                                     *                                     *
C          ADVISOR:                                                         *
C          DR. MILTON C. EDLUND                                            *
C                                     *                                     *
C*****
C
C          ***** SINGLE PRECISION *****
C
C          COMMON/DENUA/DEN(13),ESC(13,940),EU(940),SQUIG(13)
C          COMMON/DENUB/ALPHA(13),ESTOT(940),EPhi(940)
C
C          DIMENSION FC(13,47),ENERGY(47),VNU(47),FISBAR(47),SIGTR(47),
$          EYE(940),GNU(13,47),AMASS(13),SNUFIS(47),VBAR(47),ABAR(47),
$          CHI(47),E(47),U(47),D(47),CC(13,47),SIGFIS(47),ESREM(940),
$          ESTRAN(940),SI(13,47),ED(940),EE(940),EFC(13,940),ECC(13,940),
$          SIGREM(47),GNUBAR(47),GTRANS(47),ESI(13,940),ENU(13,940),
$          PHIBAR(47),DBAR(47),REMBAR(47),SIGABS(47),ECHI(940),JHIGH(47),
$          SC(13,47),PHI(47),JLOW(47)
C
C          CHARACTER QUEST*3
C
C          READ ELASTIC SCATTERING CROSS SECTIONS
C
C          DO 110 I=1,13
C             M=-5
C             DO 105 K=1,7
C                M=M+6
C                READ(1,155)SC(I,M),SC(I,M+1),SC(I,M+2),SC(I,M+3),
$                SC(I,M+4),SC(I,M+5)
105          CONTINUE
C             READ(1,160) SC(I,43),SC(I,44),SC(I,45),SC(I,46),SC(I,47)
110          CONTINUE
C
C          READ FISSION CROSS SECTIONS
C
C          DO 120 I=1,13
C             M=-5
C             DO 115 K=1,7
C                M=M+6
C                READ(2,155)FC(I,M),FC(I,M+1),FC(I,M+2),FC(I,M+3),
$                FC(I,M+4),FC(I,M+5)
115          CONTINUE

```

```

      READ(2,160) FC(I,43),FC(I,44),FC(I,45),FC(I,46),FC(I,47)
120  CONTINUE
C
C  READ CAPTURE CROSS SECTIONS
C
      DO 130 I=1,13
          M=-5
          DO 125 K=1,7
              M=M+6
              READ(3,155)CC(I,M),CC(I,M+1),CC(I,M+2),CC(I,M+3),
$              CC(I,M+4),CC(I,M+5)
125  CONTINUE
          READ(3,160) CC(I,43),CC(I,44),CC(I,45),CC(I,46),CC(I,47)
130  CONTINUE
C
C  READ NU
C
      DO 140 I=1,13
          M=-5
          DO 135 K=1,7
              M=M+6
              READ(4,155)GNU(I,M),GNU(I,M+1),GNU(I,M+2),GNU(I,M+3),
$              GNU(I,M+4),GNU(I,M+5)
135  CONTINUE
          READ(4,160) GNU(I,43),GNU(I,44),GNU(I,45),GNU(I,46),GNU(I,47)
140  CONTINUE
C
C  READ INELASTIC SCATTER CROSS SECTION
C
      DO 150 I=1,13
          M=-5
          DO 145 K=1,7
              M=M+6
              READ(13,155)SI(I,M),SI(I,M+1),SI(I,M+2),SI(I,M+3),
$              SI(I,M+4),SI(I,M+5)
145  CONTINUE
          READ(13,160)SI(I,43),SI(I,44),SI(I,45),SI(I,46),SI(I,47)
150  CONTINUE
C
155  FORMAT(6(2X,E10.5))
160  FORMAT(5(2X,E10.5))
C
C  ALPHA=[(A-1)/(A+1)]**2.0
C
      DO 170 I=1,13
          READ(7,165)ALPHA(I)
165  FORMAT(2X,E12.7)
170  CONTINUE
C
C  READ NUMBER DENSITY OF EACH ISOTOPE
C
      DO 180 I=1,13
          READ(8,175)DEN(I)
175  FORMAT(2X,E10.5)

```

```

180  CONTINUE
C
C  READ MASS OF EACH ISOTOPE
C      DO 190 I=1,13
          READ(9,185)AMASS(I)
185      FORMAT(2X,E12.7)
190  CONTINUE
C
C  READ LETHARGY GROUPS
C      DO 200 J=1,47
          READ(10,195)U(J)
195      FORMAT(2X,E11.6)
200  CONTINUE
C
C  READ SOURCE TERMS
C      DO 210 J=1,47
          READ(11,205)CHI(J)
205      FORMAT(2X,E13.8)
210  CONTINUE
C
C  READ LOG ENERGY DECREMENT
C      DO 230 I=1,13
          READ(12,220)SQUIG(I)
220      FORMAT(2X,E12.7)
230  CONTINUE
C
C  ASK, RECEIVE AND SET DEFAULT NUMBER DENSITIES
C      WRITE(6,700)
700  FORMAT(1X,'DO YOU WISH TO USE DEFAULT NUMBER DENSITIES?(YES/NO)')
      READ(5,710)QUEST
710  FORMAT(A3)
      IF(QUEST.EQ.'YES') GO TO 790
C
C  IF DEFAULT NUMBER DENSITIES ARE NOT TO BE USED, SET NEW VALUES
C      WRITE(6,715)
715  FORMAT(1X,'NUMBER DENSITY OF HYDROGEN?(EG. .46800E-01)')
      READ(5,720)DEN(1)
720  FORMAT(E10.5)
      WRITE(6,730)
730  FORMAT(1X,'NUMBER DENSITY OF PU-240?(EG. .46800E-01)')
      READ(5,720)DEN(2)
      WRITE(6,735)
735  FORMAT(1X,'NUMBER DENSITY OF PU-241?(EG. .46800E-01)')
      READ(5,720)DEN(3)
      WRITE(6,740)
740  FORMAT(1X,'NUMBER DENSITY OF U-235?(EG. .46800E-01)')
      READ(5,720)DEN(4)

```

```

      WRITE(6,745)
745  FORMAT(1X,'NUMBER DENSITY OF U-238?(EG. .46800E-01)')
      READ(5,720)DEN(5)
      WRITE(6,750)
750  FORMAT(1X,'NUMBER DENSITY OF PU-239?(EG. .46800E-01)')
      READ(5,720)DEN(6)
      WRITE(6,755)
755  FORMAT(1X,'NUMBER DENSITY OF PU-242?(EG. .46800E-01)')
      READ(5,720)DEN(7)
      WRITE(6,760)
760  FORMAT(1X,'NUMBER DENSITY OF CR(IN SS-CLAD)?(EG. .46800E-01)')
      READ(5,720)DEN(8)
      WRITE(6,765)
765  FORMAT(1X,'NUMBER DENSITY OF NI(IN SS-CLAD)?(EG. .46800E-01)')
      READ(5,720)DEN(9)
      WRITE(6,770)
770  FORMAT(1X,'NUMBER DENSITY OF FE(IN SS-CLAD)?(EG. .46800E-01)')
      READ(5,720)DEN(10)
      WRITE(6,775)
775  FORMAT(1X,'NUMBER DENSITY OF O-16 IN FUEL?(EG. .46800E-01)')
      READ(5,720)DEN(11)
      WRITE(6,780)
780  FORMAT(1X,'NUMBER DENSITY OF O-16 IN MODERATOR?(EG. .46800E-01)')
      READ(5,720)DEN(12)
      WRITE(6,785)
785  FORMAT(1X,'NUMBER DENSITY OF ZIRCALLOY CLAD?(EG. .46800E-01)')
      READ(5,720)DEN(13)
      GO TO 800
790  WRITE(6,795)
795  FORMAT(1X,'DEFAULT NUMBER DENSITIES WILL BE USED. SEE USER'S GUID
      $E FOR DEFAULT VALUES.')
800  CONTINUE
C
C  START MAIN PROGRAM *****
C
C
C  SET HEADINGS FOR MICROGROUP FILES
C
      WRITE(14,300)
      WRITE(14,305)
      WRITE(15,311)
      WRITE(15,312)
300  FORMAT(2X,'GP',4X,'LOWEST',6X,'SIGMA',7X,'SIGMA',9X,'D',10X,'FLUX'
      $
      )
305  FORMAT(2X,'NO',4X,'ENERGY',5X,'REMOVAL',4X,'ABSORPTION')
311  FORMAT(2X,'GP',4X,'LOWEST',5X,'NU SIGMA',5X,'SIGMA',9X,'NU')
312  FORMAT(2X,'NO',4X,'ENERGY',5X,'FISSION',5X,'FISSION')
C
C  SET NECESSARY ARRAYS TO ZERO
C
      L=0
      DO 308 J=1,47
          E(J)=(1.0E+07)/EXP(U(J))
          SNUFIS(J)=0.0

```

```

SIGREM(J)=0.0
SIGABS(J)=0.0
SIGTR(J)=0.0
SIGFIS(J)=0.0
VNU(J)=0.0
D(J)=0.0
PHI(J)=0.0

```

C  
C  
C

BEGIN SUB-DIVISION OF THE 47 GROUPS TO 940 MICROGROUPS

```

DO 307 M=1,20
  L=L+1
  IF(J.EQ.1) THEN
    DU=U(1)/20.0
    EU(L)=M*DU
    DCHI=CHI(1)/20.0
    ECHI(L)=M*DCHI
  ELSE
    DU=(U(J)-U(J-1))/20.0
    EU(L)=U(J-1)+(M*DU)
    DCHI=(CHI(J)-CHI(J-1))/20.0
    ECHI(L)=CHI(J-1)+(M*DCHI)
  END IF
  DO 306 I=1,13
    IF(J.EQ.1) THEN
      DSC=SC(I,1)/20.0
      ESC(I,L)=M*DSC
      DFC=FC(I,1)/20.0
      EFC(I,L)=M*DFC
      DCC=CC(I,1)/20.0
      ECC(I,L)=M*DCC
      DNU=GNU(I,1)/20.0
      ENU(I,L)=M*DNU
      DSI=SI(I,1)/20.0
      ESI(I,L)=M*DSI
    ELSE
      DSC=(SC(I,J)-SC(I,J-1))/20.0
      ESC(I,L)=SC(I,J-1)+(M*DSC)
      DFC=(FC(I,J)-FC(I,J-1))/20.0
      EFC(I,L)=FC(I,J-1)+(M*DFC)
      DCC=(CC(I,J)-CC(I,J-1))/20.0
      ECC(I,L)=CC(I,J-1)+(M*DCC)
      DNU=(GNU(I,J)-GNU(I,J-1))/20.0
      ENU(I,L)=GNU(I,J-1)+(M*DNU)
      DSI=(SI(I,J)-SI(I,J-1))/20.0
      ESI(I,L)=SI(I,J-1)+(M*DSI)
    END IF
  306   CONTINUE
  307   CONTINUE
  308   CONTINUE

```

C  
C  
C

BEGIN CALCULATIONS USING 940 MICROGROUPS BY ZEROING ARRAYS

```

DO 310 J=1,940

```



```

      EE(J)=(1.0E+07)/EXP(EU(J))
      EYE(J)=0.0
      ESTOT(J)=0.0
      ESTRAN(J)=0.0
      ED(J)=0.0
      EPHI(J)=0.0
      ESREM(J)=0.0
310  CONTINUE
C
C  CALCULATE GROUP CONSTANTS OTHER THAN FLUX & REMOVAL X-SECTION
C
C  ***** MAIN CALCULATION LOOP *****
C
      DO 340 J=1,940
        SUMSTR=0.0
        SUMSTO=0.0
        DO 315 I=1,13
          SIGTJ=DEN(I)*(ESC(I,J)+ECC(I,J)+EFC(I,J)+ESI(I,J))
          IF(DEN(I).LE.0.0)THEN
            V=0.0
          ELSE
            V=1.0/(DEN(I)*ESC(I,J)*(1.0-(2.0/(3.0*AMASS(I)))))
            SIGTRN=1.0/V
          END IF
          SUMSTO=SUMSTO+SIGTJ
          SUMSTR=SUMSTR+SIGTRN
315  CONTINUE
        ESTOT(J)=SUMSTO
        ESTRAN(J)=SUMSTR
        ED(J)=1.0/(3.0*SUMSTR)
C
C  BEGIN FLUX CALCULATION
C
C  CALCULATE DENOMINATOR OF FLUX EQUATION
C
        SUMO=0.0
C
C  ISOTOPES OTHER THAN HYDROGEN
C
        DO 316 I=2,13
          OTERM=DEN(I)*ESC(I,J)
          SUMO=SUMO+OTERM
316  CONTINUE
        ALP=ESTOT(J)-SUMO
C
C  HYDROGEN TERM
C
        IF(J.EQ.1) THEN
          DELU=EU(1)
          DEC=(1.0-EXP(-EU(J)))*DEN(1)*(ESC(1,J)/DELU)*(EXP(EU(J))-1)
        ELSE
          DELU=EU(J)-EU(J-1)
          DEC=(EXP(-EU(J-1))-EXP(-EU(J)))*(DEN(1)*ESC(1,J)/DELU)*
            (EXP(EU(J))-EXP(EU(J-1)))
        END IF
      END DO

```

```

      END IF
C
C      DENOMINATOR == BOTT
C
      BOTT=ALP-DEC
C
C      CALCULATE NUMERATOR OF FLUX EQUATION
C
C      NOTE THAT ALL TERMS EXCEPT SOURCE ARE ZERO IN FIRST GROUP
C
      IF (J.EQ.1) THEN
        EPHI(1)=ECHI(1)/BOTT
      ELSE
        SUMH=0.0
C
C      HYDROGEN TERM
C
        DO 319 K=1,J-1
          IF(K.EQ.1)THEN
            HTERM=DEN(1)*ESC(1,1)*EPHI(1)*(EXP(EU(1))-1.0)/DELU
          ELSE
            HTERM=(EXP(EU(K))-EXP(EU(K-1)))*DEN(1)*ESC(1,K)*
$           EPHI(K)/DELU
          END IF
          SUMH=SUMH+HTERM
319      CONTINUE
          HYD=(EXP(-EU(J-1))-EXP(-EU(J)))*SUMH
C
C      FLUX
C
          EPHI(J)=(ECHI(J)+EYE(J)+HYD)/BOTT
        END IF
C
C      END FLUX CALCULATION
C
C      *****
C      *
C      *   NOTE:  SEE PROGRAM USER'S GUIDE FOR LOCATION AND   *
C      *                   USE OF THE FOLLOWING FILES          *
C      *
C      *****
C
C      ADD FOR DEBUG OR ADDITIONAL DATA *****TESTOUT DAT*****
C      WRITE(24,321) J,ECHI(J),EYE(J),SUMH,HYD
C321      FORMAT(2X,I3,4(2X,E12.5))
C
C      ADD FOR DEBUG OR ADDITIONAL DATA *****TEST DATA*****
C      WRITE(25,322) J,ESTOT(J),SUMO,ALP,DEC,EPHI(J)
C322      FORMAT(2X,I3,5(2X,E12.5))
C
C      CALCULATE FLUX CONTRIBUTION FROM INELASTIC SCATTER AND STORE
C      IN APPROPRIATE ARRAY LOCATIONS
C
      DO 325 I=2,7

```

```

        IF(J.GE.400) GO TO 325
        H=(6.4/SQRT(AMASS(I)))*SQRT(EE(J)*1.0E-06)
        F=H*1.0E+06
        DO 320 K=1,940
            IF((F.GE.EE(K+1)).AND.(F.LT.EE(K)))THEN
                EYE(K)=EYE(K)+(DEN(I)*ESI(I,J)*EPHI(J))
            END IF
320      CONTINUE
325      CONTINUE
C
C      USE SUBROUTINE "REMOVL" TO CALCULATE REMOVAL CROSS SECTIONS
C
        CALL REMOVL(J,REMOV)
        ESREM(J)=REMOV
340      CONTINUE
C
C      END OF MAIN CALCULATION LOOP, BEGIN COLLAPSING ROUTINES
C
C      ***** COLLAPSE BACK TO 47 GROUPS *****
        L=0
        DO 350 J=1,47
            SIREM=0.0
            SIABS=0.0
            SITR=0.0
            SIPHI=0.0
            SDEUK=0.0
            DO 345 M=1,20
                L=L+1
                IF (L.EQ.1) THEN
                    DEUK=EU(L)
                ELSE
                    DEUK=EU(L)-EU(L-1)
                END IF
                GIREM=ESREM(L)*EPHI(L)*DEUK
                SIREM=SIREM+GIREM
                GITR=ESTRAN(L)*EPHI(L)*DEUK
                SITR=SITR+GITR
                GIPHI=EPHI(L)*DEUK
                SIPHI=SIPHI+GIPHI
                SDEUK=SDEUK+DEUK
345      CONTINUE
            SIGREM(J)=SIREM/SIPHI
            SIGTR(J)=SITR/SIPHI
            D(J)=1.0/(3.0*SIGTR(J))
            PHI(J)=SIPHI/SDEUK
            SUMNSF=0.0
            SUMFIS=0.0
            SUMABS=0.0
            DO 360 I=1,13
                SIGMAF=DEN(I)*FC(I,J)
                SUMFIS=SUMFIS+SIGMAF
                SIGNU=GNU(I,J)*DEN(I)*FC(I,J)
                SUMNSF=SUMNSF+SIGNU
                SIABS=DEN(I)*(CC(I,J)+FC(I,J))

```

```

        SUMABS=SUMABS+SIABS
360    CONTINUE
        DELU=U(J)-U(J-1)
        SNUFIS(J)=SUMNSF*PHI(J)*DELU/(PHI(J)*DELU)
        SIGFIS(J)=SUMFIS*PHI(J)*DELU/(PHI(J)*DELU)
        VNU(J)=SNUFIS(J)/SIGFIS(J)
        SIGABS(J)=SUMABS*PHI(J)*DELU/(PHI(J)*DELU)
C
C    SET UP MICROGROUP FILES FOR PRINT OR DIRECT USE
C
C    ***** AMICRO GROUP FILE *****
C
        WRITE(14,347)J,E(J),SIGREM(J),SIGABS(J),D(J),PHI(J)
347    FORMAT(2X,I2,2X,E10.4,2X,E10.4,2X,E10.4,2X,E10.4,2X,E10.4)
C
C    ***** BMICRO GROUP FILE *****
C
        WRITE(15,348)J,E(J),SNUFIS(J),SIGFIS(J),VNU(J)
348    FORMAT(2X,I2,2X,E10.4,2X,E10.4,2X,E10.4,2X,E10.4)
C
C    ANOTHER COPY OF THE TEST FILES--SEE USER'S GUIDE BEFORE USING
C
C ADD FOR DEBUG *****TESTOUT DAT *****
C    WRITE(24,358) J,E(J),CHI(J),EYE(J),PHI(J)
C358    FORMAT(2X,I2,6(2X,E12.5))
C
C ADD FOR DEBUG *****TEST DATA *****
C    WRITE(25,359) J,HYD,SUMO,DEC
C359    FORMAT(2X,I2,5(2X,E12.5))
C
350    CONTINUE
C
C    END FIRST COLLAPSE, BEGIN COLLAPSE TO USER SPECIFIED GROUPS
C
C    ***** COLLAPSING ROUTINE *****
C    SET HEADINGS FOR MACROGROUP FILES
C
        WRITE(16,900)
        WRITE(16,910)
        WRITE(17,911)
        WRITE(17,912)
900    FORMAT(2X,'GP',4X,'LOWEST',6X,'SIGMA',7X,'SIGMA',9X,'D',10X,'FLUX'
$      )
910    FORMAT(2X,'NO',4X,'ENERGY',5X,'REMOVAL',4X,'ABSORPTION')
911    FORMAT(2X,'GP',4X,'LOWEST',5X,'NU SIGMA',5X,'SIGMA',9X,'NU')
912    FORMAT(2X,'NO',4X,'ENERGY',5X,'FISSION',5X,'FISSION')
C
C    SET N FROM USER
C
        WRITE(6,915)
915    FORMAT(1X,'ENTER NUMBER OF MACRO GROUPS DESIRED(EG. 05).')
        READ(5,920)N
920    FORMAT(I2)
        DO 940 I=1,N

```

```

        WRITE(6,925)I
925  FORMAT(1X,'ENTER LOWER GROUP NO. AND UPPER GROUP NO. FOR MACRO GRO
      $UP ',I2)
        WRITE(6,930)
930  FORMAT(1X,'(EG. 05 16)')
        READ(5,935)JLOW(I),JHIGH(I)
935  FORMAT(I2,1X,I2)
940  CONTINUE
C
C  BEGIN COLLAPSE
C
      DO 955 M=1,N
        LL=JLOW(M)
        KK=JHIGH(M)
        GFIS=0.0
        GBS=0.0
        ABS=0.0
        GTR=0.0
        GPHI=0.0
        USUB=0.0
        GRE=0.0
        DO 945 J=LL,KK
          IF(J.EQ.1) THEN
            GPFSN=SNUFIS(J)*U(1)
            GV=SIGFIS(J)*U(1)
            BS=SIGABS(J)*U(1)
            GFLUX=PHI(J)*U(1)
            GNTR=SIGTR(J)*PHI(J)*U(1)
            GPREM=SIGREM(J)*PHI(J)*U(1)
            USUB=USUB+U(1)
          ELSE
            GPFSN=SNUFIS(J)*(U(J)-U(J-1))
            GV=SIGFIS(J)*(U(J)-U(J-1))
            BS=SIGABS(J)*(U(J)-U(J-1))
            GFLUX=PHI(J)*(U(J)-U(J-1))
            GNTR=SIGTR(J)*PHI(J)*(U(J)-U(J-1))
            GPREM=SIGREM(J)*PHI(J)*(U(J)-U(J-1))
            USUB=USUB+(U(J)-U(J-1))
          END IF
          GFIS=GFIS+GPFSN
          GPHI=GPHI+GFLUX
          ABS=ABS+BS
          GTR=GTR+GNTR
          GRE=GRE+GPREM
          GBS=GBS+GV
945  CONTINUE
        GNUBAR(M)=GFIS/USUB
        FISBAR(M)=GBS/USUB
        VBAR(M)=GNUBAR(M)/FISBAR(M)
        GTRANS(M)=GTR/GPHI
        PHIBAR(M)=GPHI/USUB
        ABAR(M)=ABS/USUB
        DBAR(M)=1.0/(3.0*GTRANS(M))
        REMBAR(M)=GRE/GPHI

```

```

ENERGY(M)=E(KK)
C
C   END COLLAPSE TO USER SPECIFIED GROUPS
C   SET UP MACROGROUP FILES
C
C   *****AMACRO GROUP FILE *****
C
      WRITE(16,950)M,ENERGY(M),REMBAR(M),ABAR(M),DBAR(M),PHIBAR(M)
950    FORMAT(2X,I2,2X,E10.4,2X,E10.4,2X,E10.4,2X,E10.4,2X,E10.4)
C
C   *****BMACRO GROUP FILE *****
C
      WRITE(17,951)M,ENERGY(M),GNUBAR(M),FISBAR(M),VBAR(M)
951    FORMAT(2X,I2,2X,E10.4,2X,E10.4,2X,E10.4,2X,E10.4)
955    CONTINUE
      STOP
      END
C
C
C   SUBROUTINE "REMOVL" CALCULATES REMOVAL CROSS SECTIONS
C   FOR EACH ENERGY MICROGROUP
C
      SUBROUTINE REMOVL(J,REMOV)
C
      COMMON/DENUA/DEN(13),ESC(13,940),EU(940),SQUIG(13)
      COMMON/DENUB/ALPHA(13),ESTOT(940),EPhi(940)
C
C
      IF(J.EQ.1) GO TO 30
      SUMH=0.0
      SUMO=0.0
C
C   HYDROGEN TERM
C
      DO 10 K=1,J
        IF(K.EQ.1)THEN
          DELUH=EU(1)
          HTERM=DEN(1)*ESC(1,K)*EPhi(1)*(EXP(EU(K))-1.0)/DELUH
        ELSE
          DELUH=EU(K)-EU(K-1)
          HTERM=DEN(1)*ESC(1,K)*EPhi(K)*(EXP(EU(K))-EXP(EU(K-1)))/
$              DELUH
        END IF
        SUMH=SUMH+HTERM
10    CONTINUE
      HREM=SUMH*(EXP(-EU(J-1))-EXP(-EU(J)))
C
C   ISOTOPES OTHER THAN HYDROGEN
C
      DO 20 I=2,13
        OTERM=SQUIG(I)*DEN(I)*ESC(I,J)*EPhi(J)
        SUMO=SUMO+OTERM
20    CONTINUE
C

```

C     REMOVAL CROSS SECTION

C

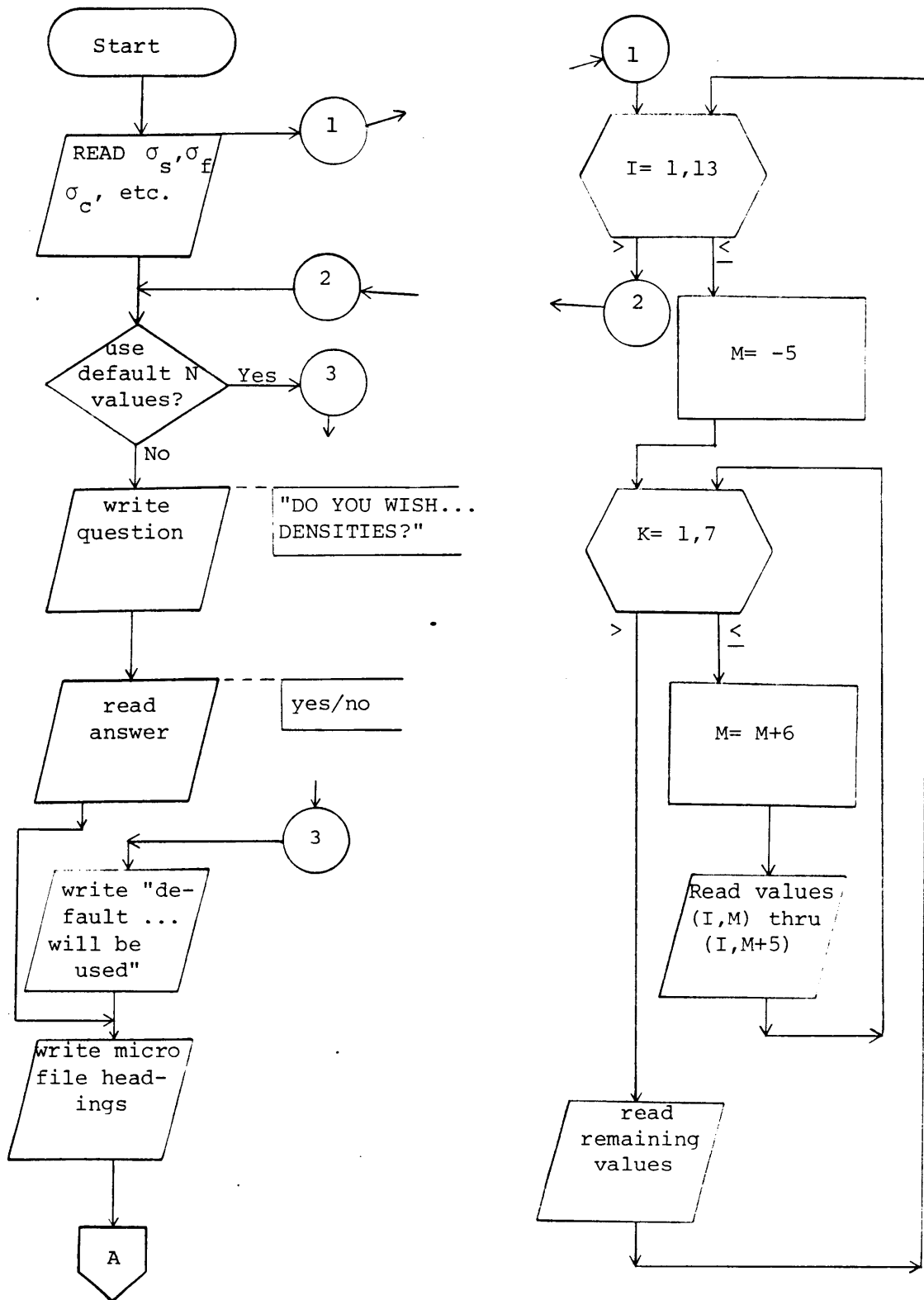
     REMOV=(HREM+SUMO)/EPI(J)

     GO TO 40

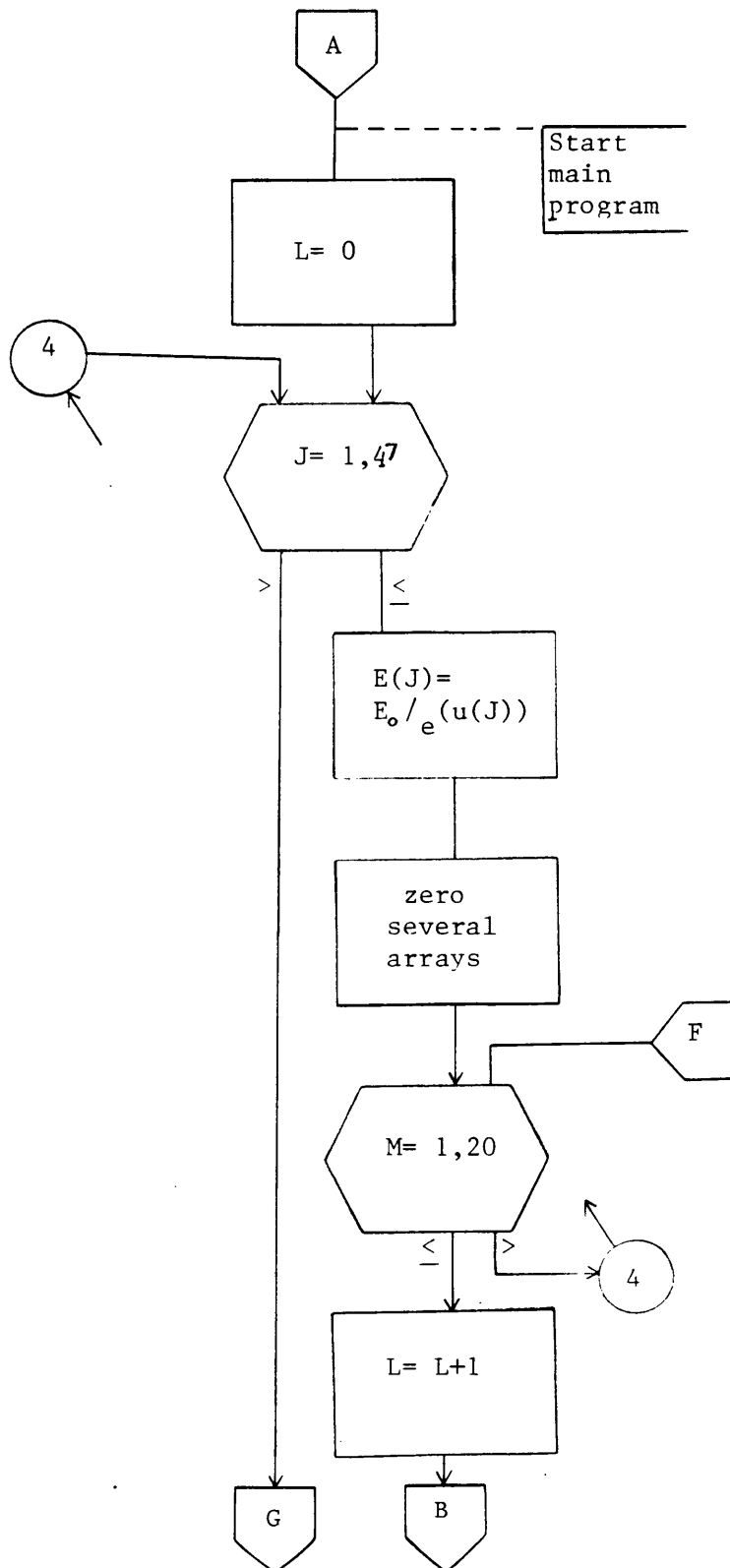
30     REMOV=0.0

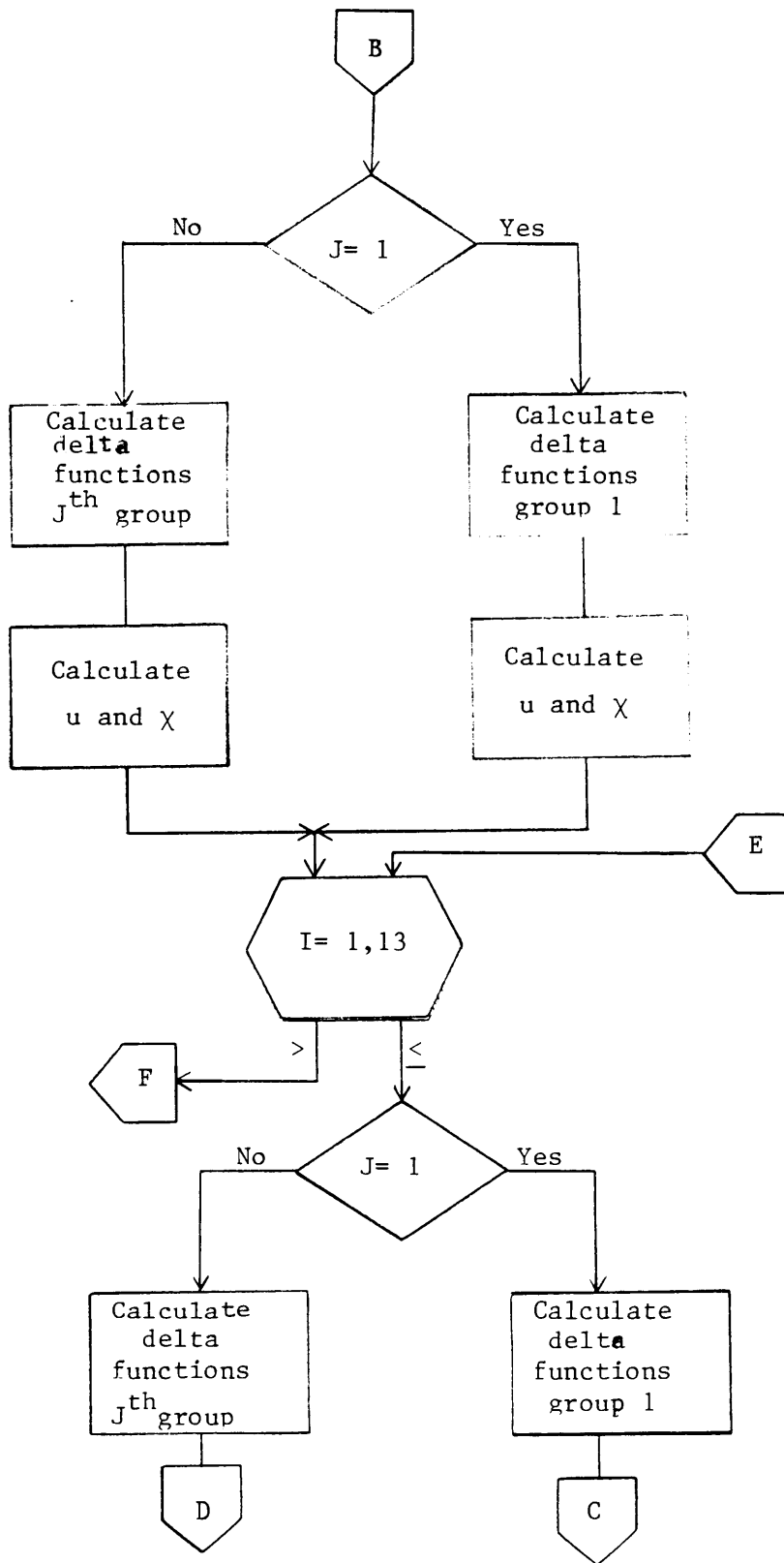
40     RETURN

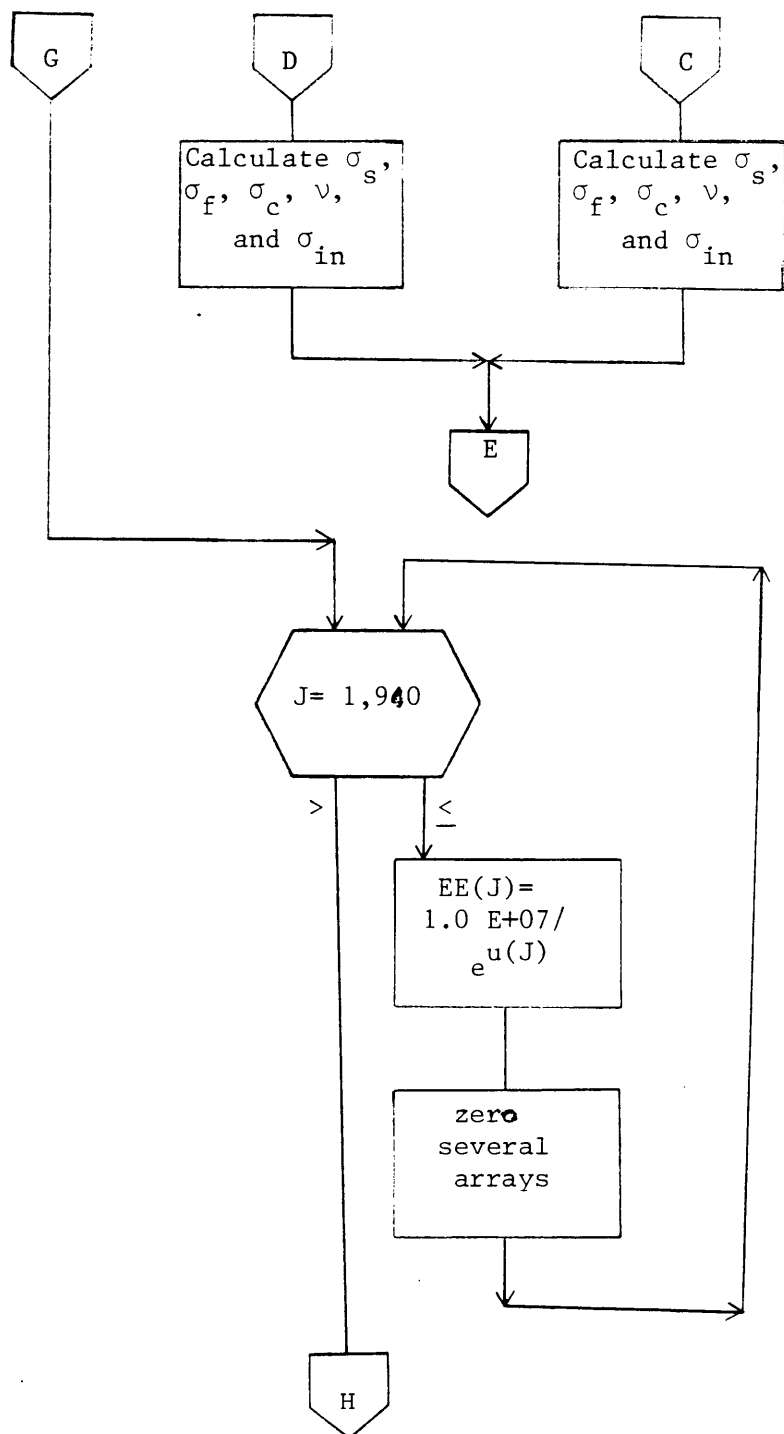
     END

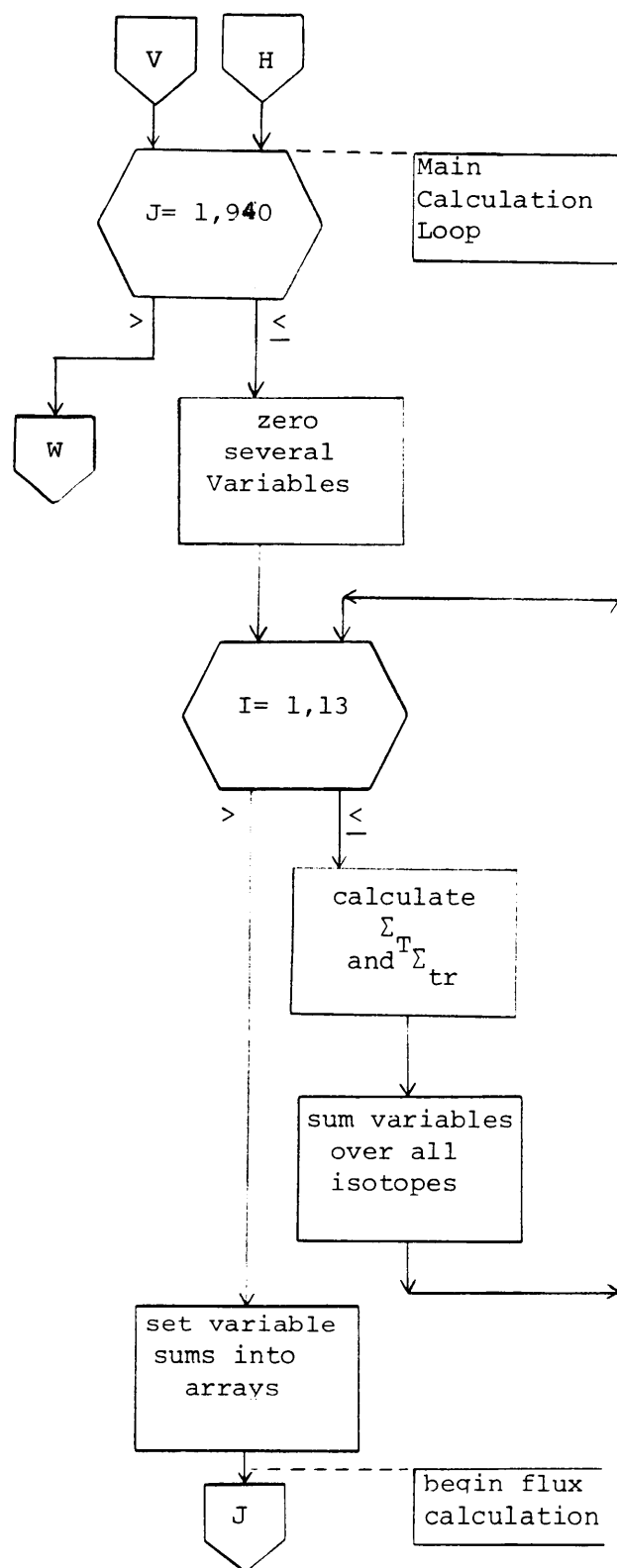


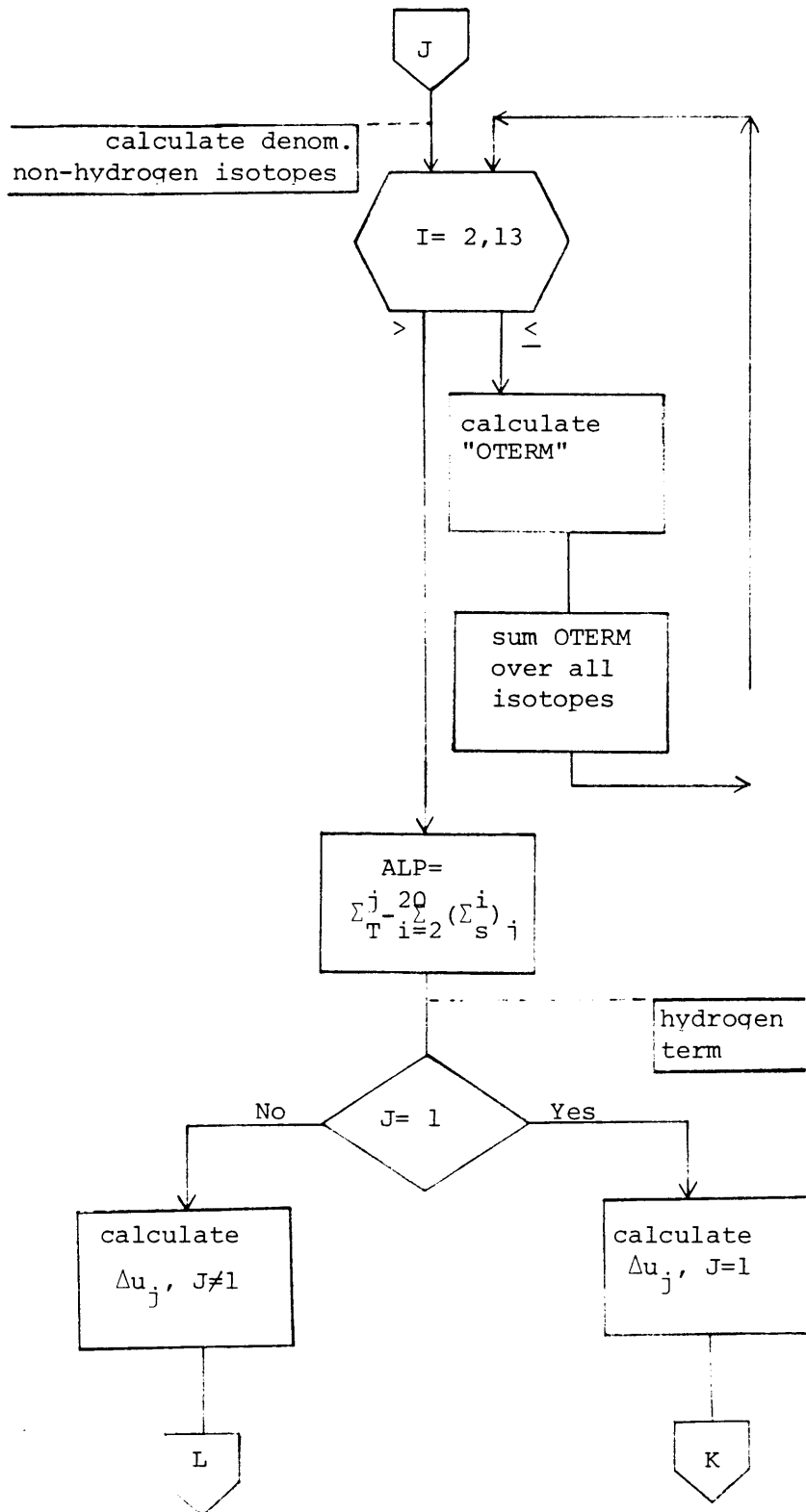


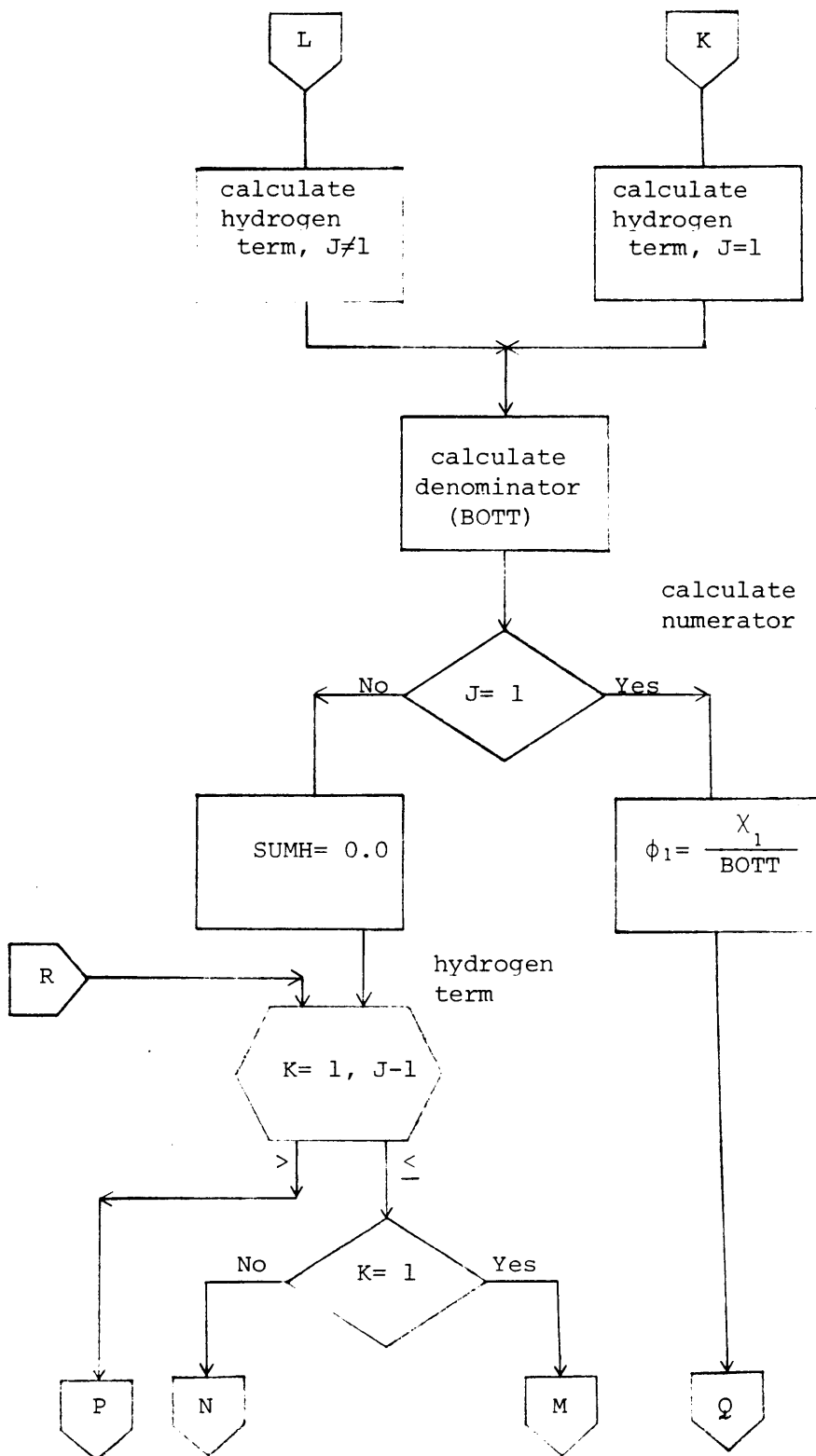


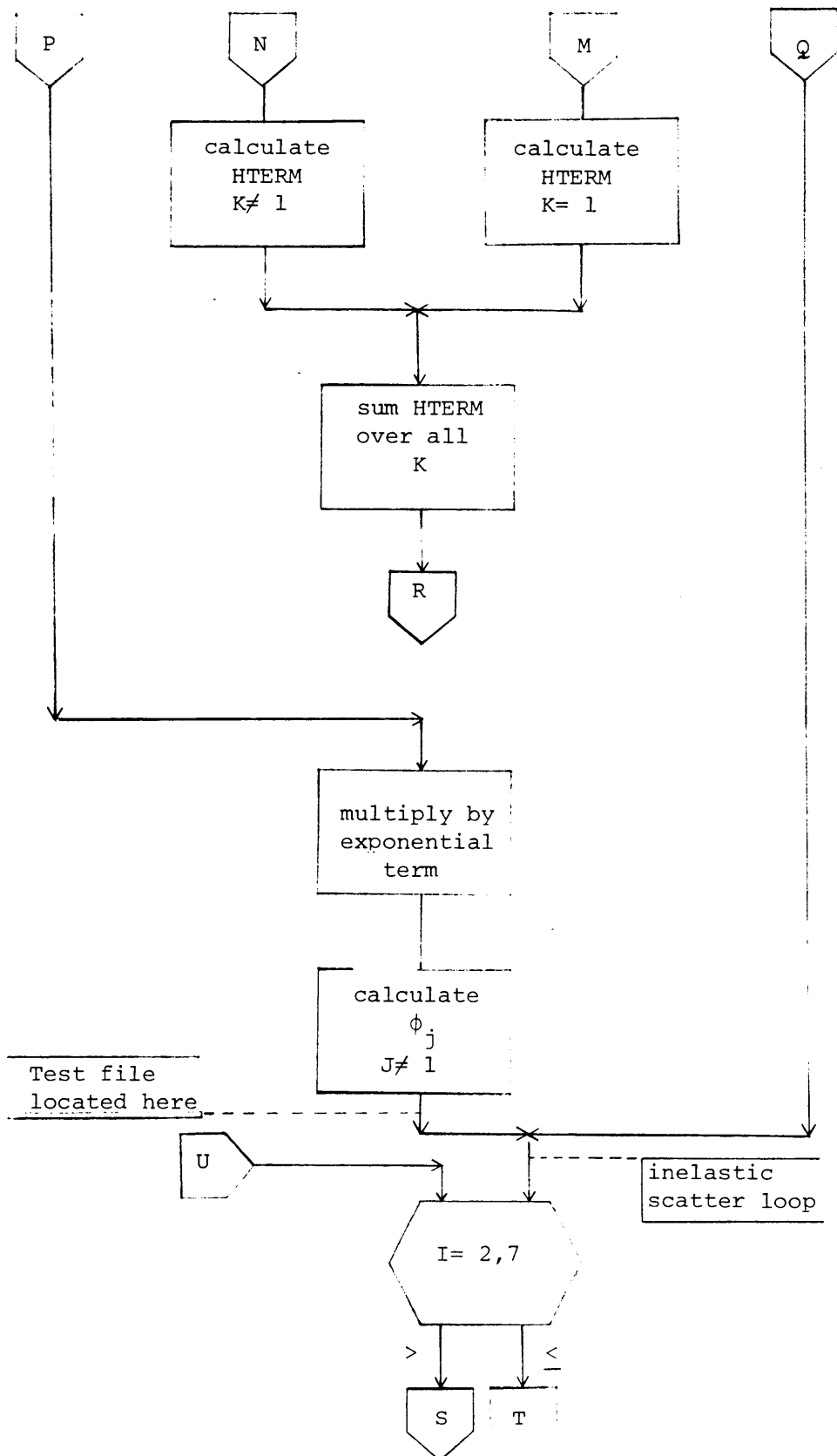


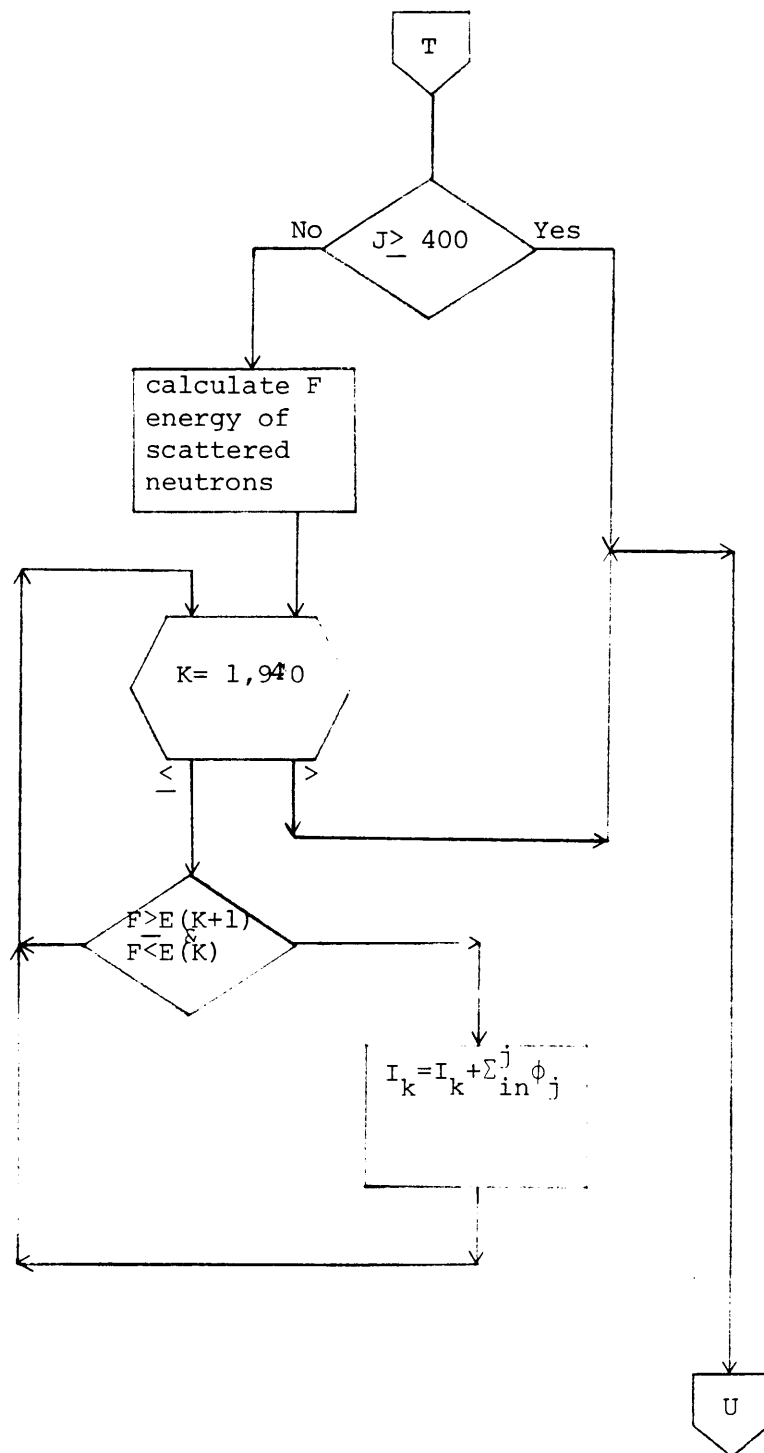




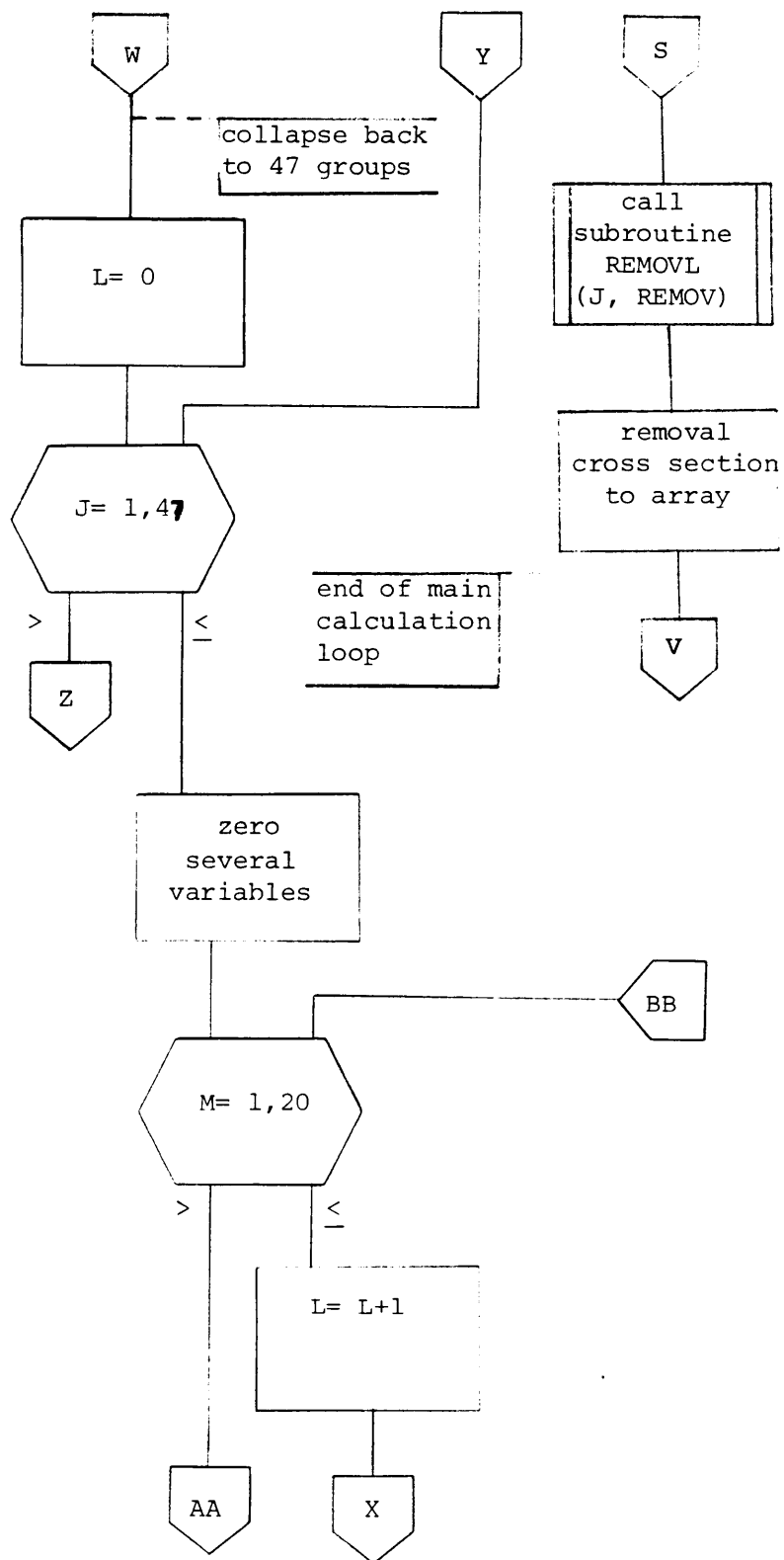


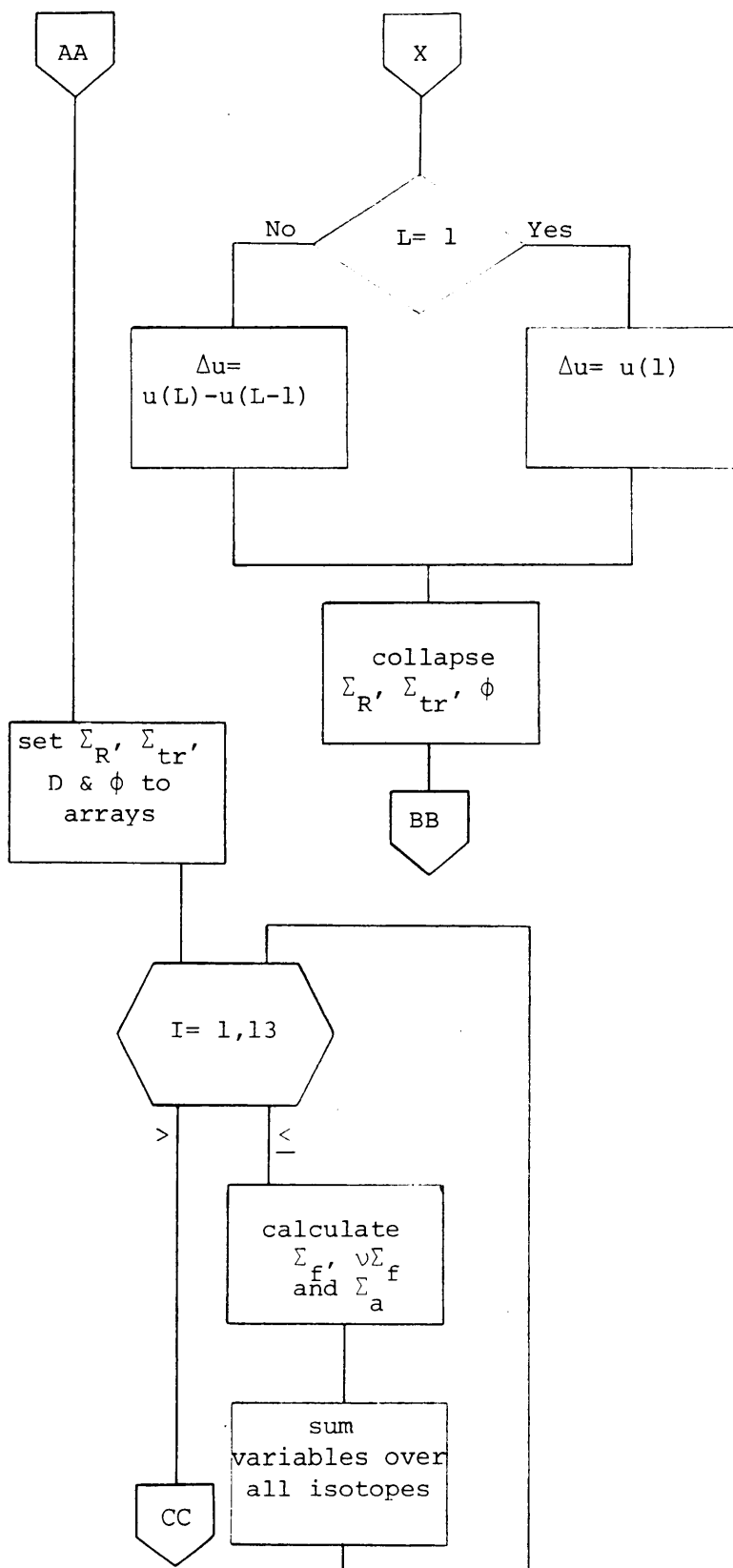


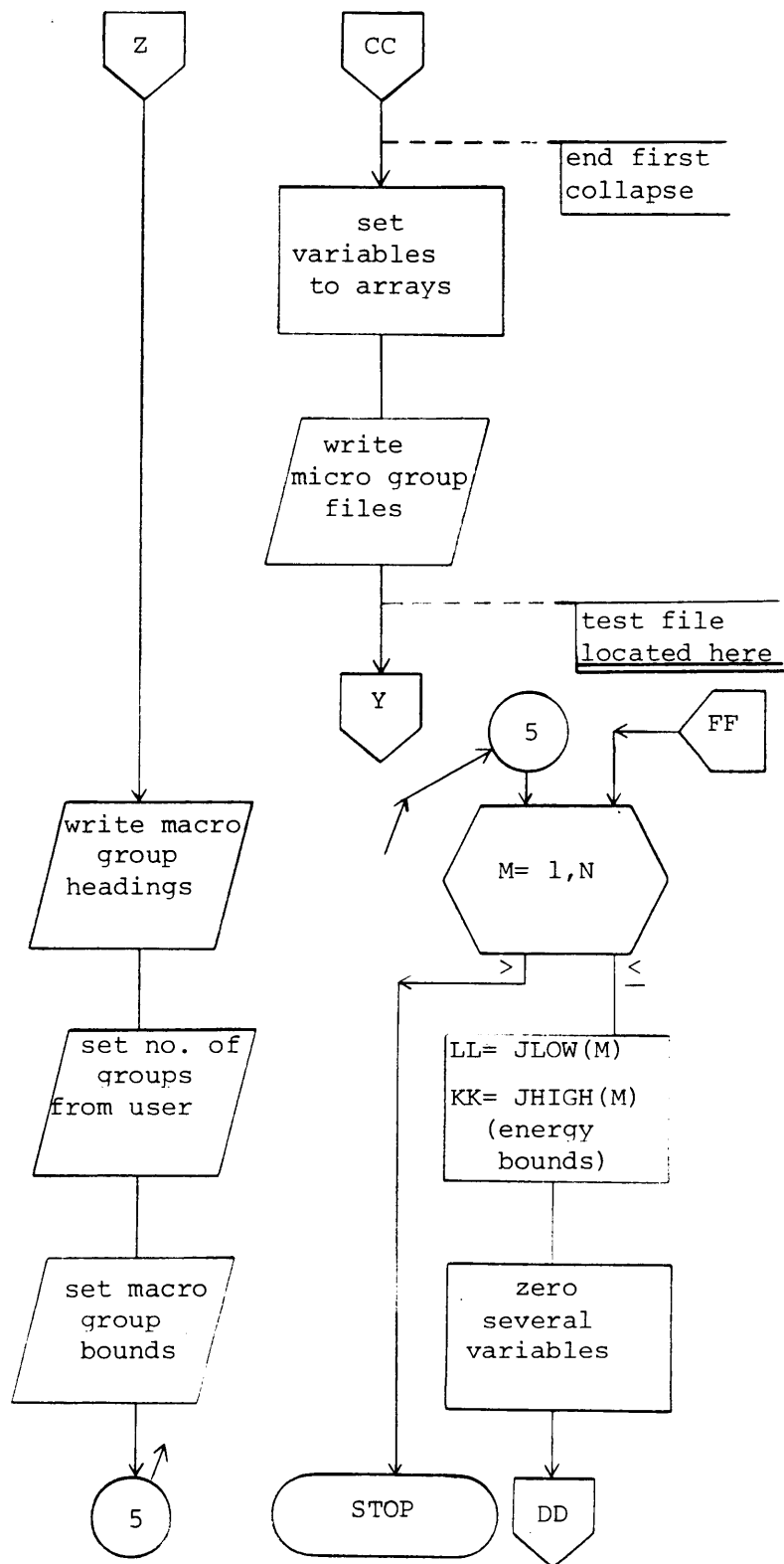


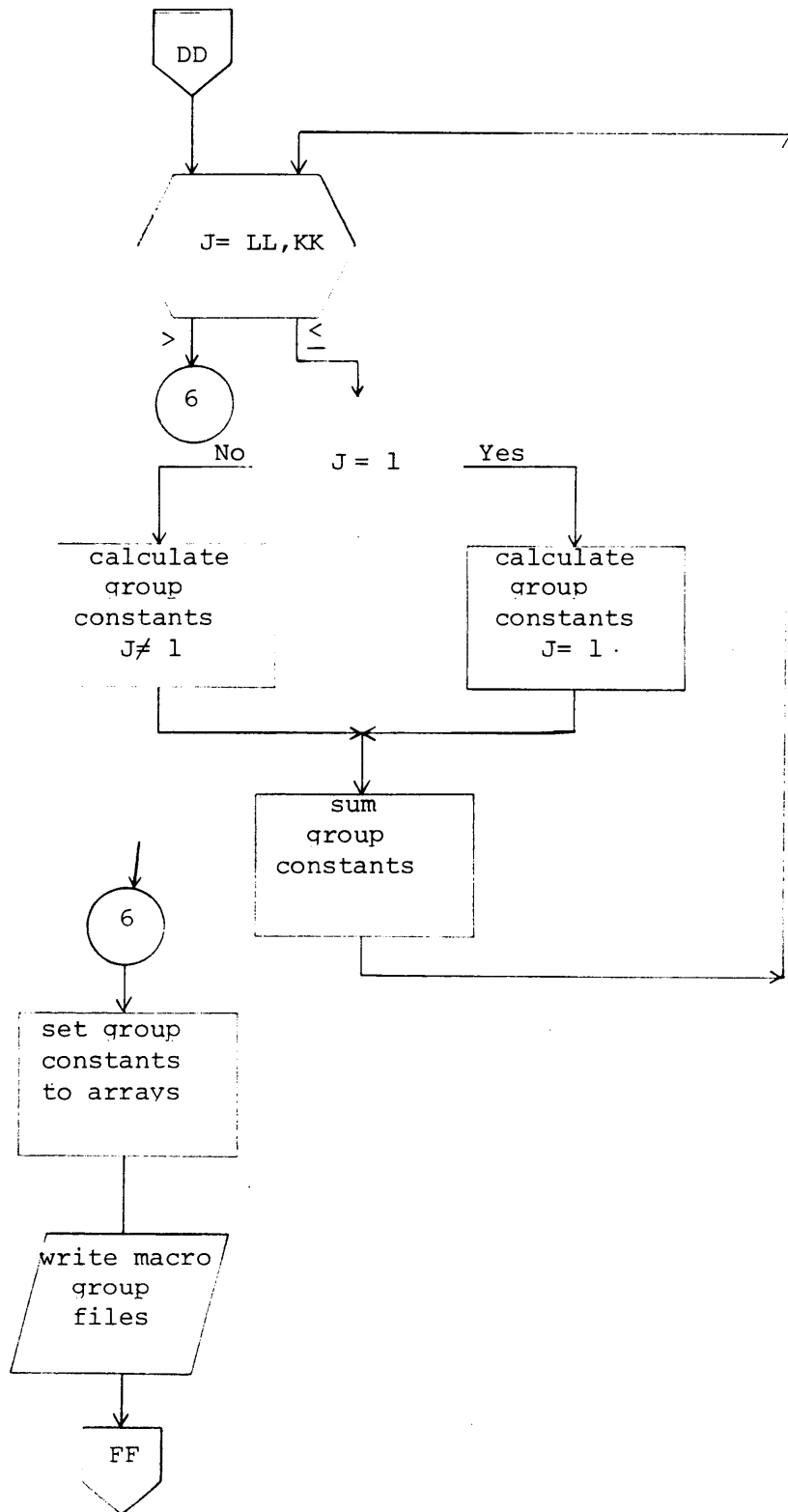


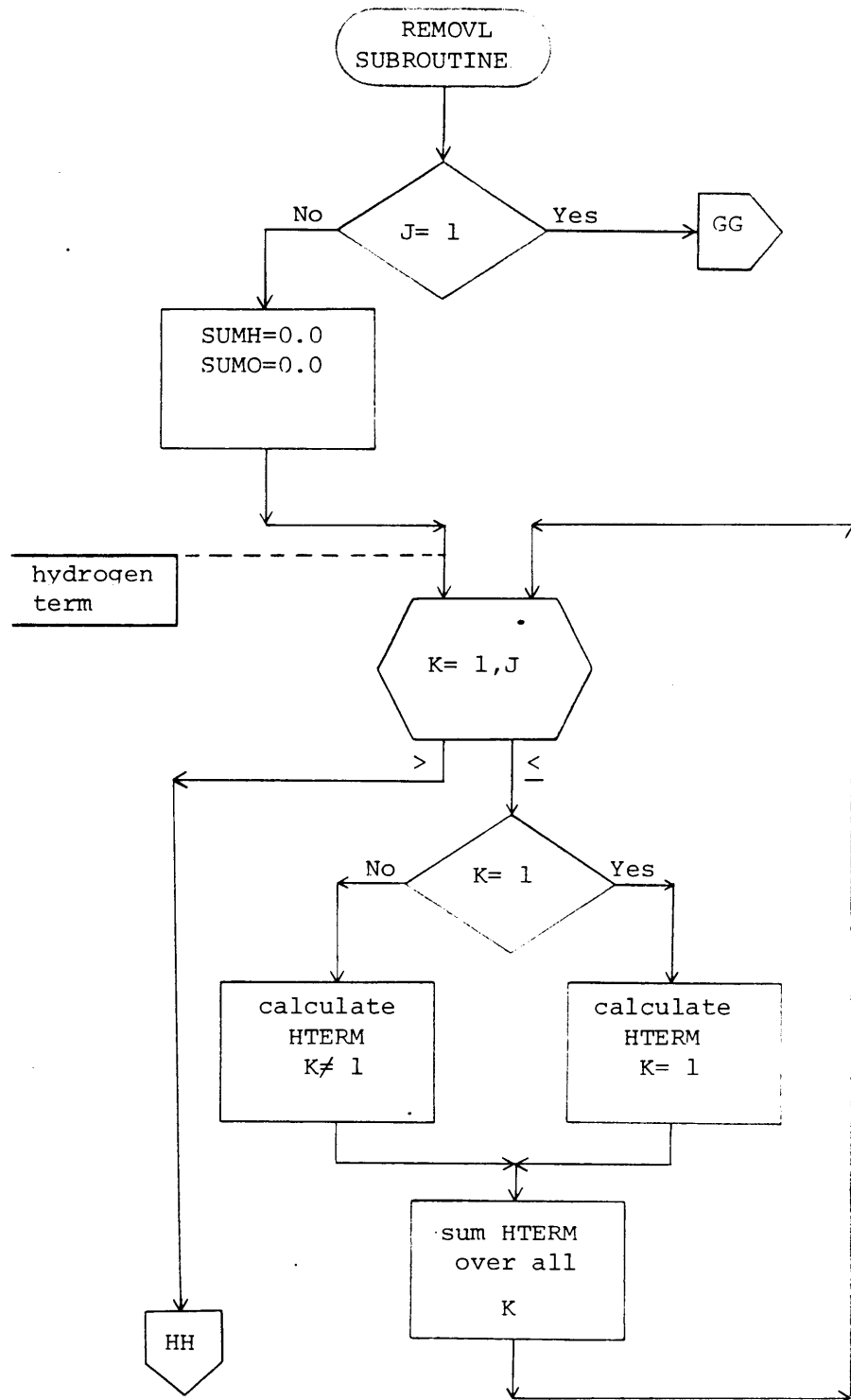


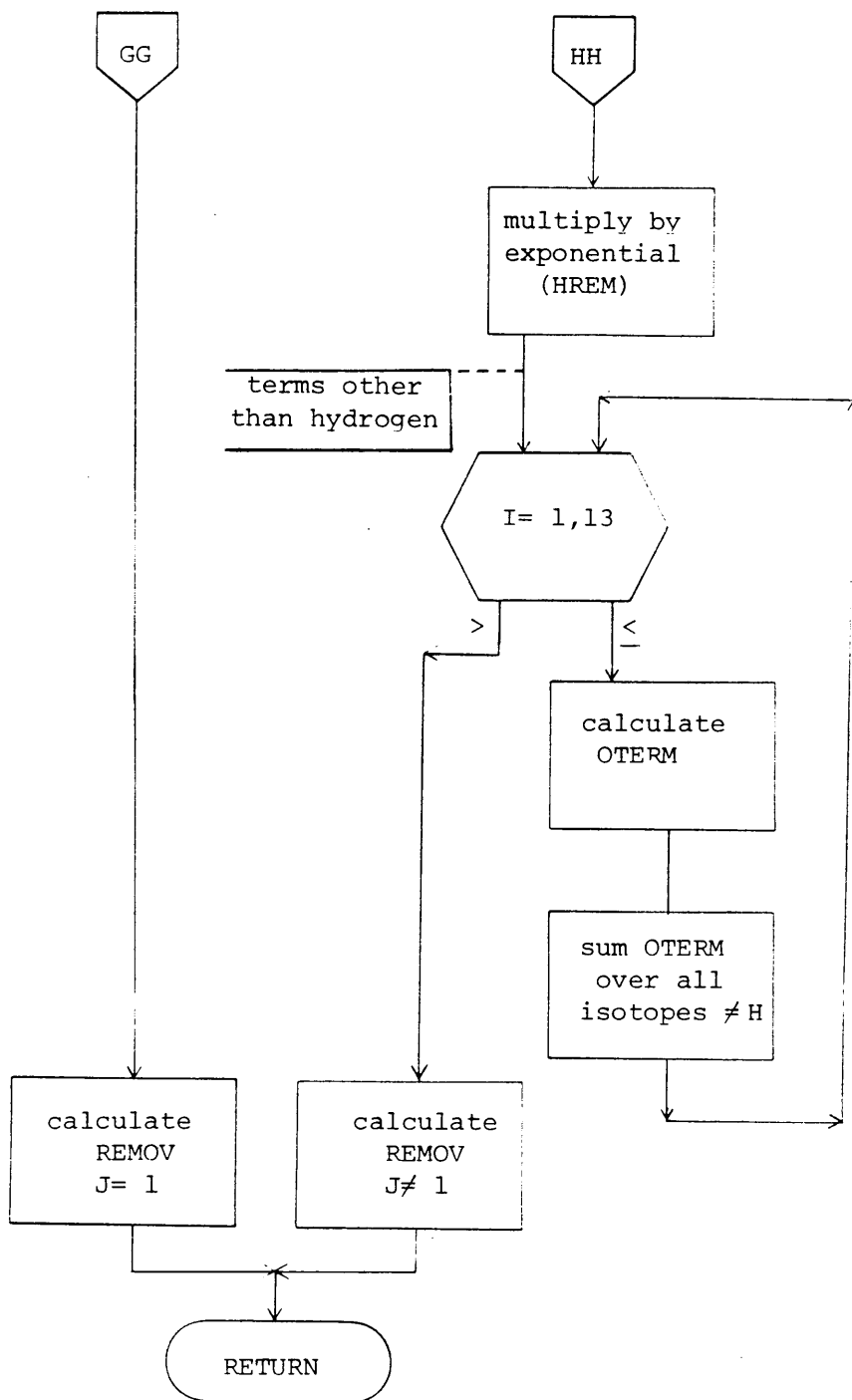












## FASPEC Execution Driver

```
&CONTROL OFF
GLOBAL TXTLIB VFORTLIB
GLOBAL LOADLIB VFLODLIB
FILEDEF 1 DISK SCATTER DATA A
FILEDEF 2 DISK FISSION DATA A
FILEDEF 3 DISK CAPTURE DATA A
FILEDEF 4 DISK NU DATA A
FILEDEF 7 DISK ALPHA DATA A
FILEDEF 8 DISK DENSITY DATA A
FILEDEF 9 DISK MASS DATA A
FILEDEF 10 DISK LETHARGY DATA A
FILEDEF 11 DISK SOURCE DATA A
FILEDEF 12 DISK LOGSLOW DATA A
FILEDEF 13 DISK INELAST DATA A
FILEDEF 14 DISK AMICRO GROUP A
FILEDEF 15 DISK BMICRO GROUP A
FILEDEF 16 DISK AMACRO GROUP A
FILEDEF 17 DISK BMACRO GROUP A
FILEDEF 24 DISK TESTOUT DAT A (LRECL 133 BLKSIZE 133
FILEDEF 25 DISK TEST DATA A
LOAD FASPEC(START NOMAP
```

Table A.I Scatter Data File

.12620D+01	.17446D+01	.24189D+01	.31922D+01	.41762D+01	.53782D+01
.70795D+01	.89794D+01	.11180D+02	.13378D+02	.15364D+02	.16977D+02
.18147D+02	.18983D+02	.19549D+02	.19895D+02	.20111D+02	.20242D+02
.20324D+02	.20350D+02	.20364D+02	.20377D+02	.20389D+02	.20403D+02
.20416D+02	.20429D+02	.20442D+02	.20449D+02	.20449D+02	.20449D+02
.20449D+02	.20449D+02	.20449D+02	.20449D+02	.20449D+02	.20449D+02
.20449D+02	.20449D+02	.20465D+02	.20510D+02	.20526D+02	.20546D+02
.20624D+02	.20885D+02	.21114D+02	.21435D+02	.28289D+02	
.36047D+01	.42450D+01	.41839D+01	.36741D+01	.38770D+01	.50909D+01
.70414D+01	.84809D+01	.96603D+01	.10923D+02	.12168D+02	.12885D+02
.13740D+02	.14412D+02	.15292D+02	.15058D+02	.17119D+02	.18283D+02
.20158D+02	.16618D+02	.12556D+02	.19437D+02	.28164D+02	.11985D+02
.18662D+02	.20223D+02	.34047D+02	.14397D+02	.81371D+02	.67282D+01
.68836D+02	.50140D+01	.69925D+01	.89108D+01	.75367D+01	.82790D+01
.89271D+01	.95779D+01	.10744D+02	.12000D+02	.13723D+02	.16707D+02
.22892D+02	.42773D+02	.13801D+03	.56350D+03	.63985D+01	
.31028D+01	.40591D+01	.39595D+01	.39036D+01	.43959D+01	.53275D+01
.65537D+01	.80186D+01	.92723D+01	.10141D+02	.10673D+02	.10889D+02
.11162D+02	.11463D+02	.11983D+02	.12476D+02	.12766D+02	.12659D+02
.12658D+02	.13099D+02	.13297D+02	.14073D+02	.14114D+02	.13967D+02
.13693D+02	.13123D+02	.13048D+02	.13985D+02	.13413D+02	.13152D+02
.11627D+02	.13328D+02	.11628D+02	.17343D+02	.15738D+02	.10193D+02
.10508D+02	.11220D+02	.85526D+01	.95276D+01	.67988D+01	.79261D+01
.84232D+01	.10295D+02	.10779D+02	.11182D+02	.11678D+02	
.40549D+01	.47832D+01	.46158D+01	.39762D+01	.41127D+01	.51083D+01
.64597D+01	.75787D+01	.86382D+01	.96649D+01	.10489D+02	.10988D+02
.11310D+02	.11605D+02	.11828D+02	.11825D+02	.11928D+02	.12082D+02
.12437D+02	.12495D+02	.12318D+02	.12136D+02	.12427D+02	.12769D+02
.12510D+02	.12429D+02	.12288D+02	.12343D+02	.12460D+02	.12789D+02
.11907D+02	.12185D+02	.11558D+02	.11816D+02	.10844D+02	.11965D+02
.11398D+02	.10240D+02	.10600D+02	.10913D+02	.11353D+02	.11530D+02
.11986D+02	.12335D+02	.12820D+02	.12867D+02	.13937D+02	
.36433D+01	.46676D+01	.46208D+01	.40782D+01	.47461D+01	.60432D+01
.77067D+01	.92214D+01	.10534D+02	.11818D+02	.12479D+02	.12695D+02
.13221D+02	.13793D+02	.13905D+02	.15048D+02	.14984D+02	.13920D+02
.13089D+02	.13038D+02	.10728D+02	.11011D+02	.12962D+02	.14053D+02
.19010D+02	.90196D+01	.22261D+02	.58117D+01	.14191D+02	.90567D+01
.19167D+02	.15112D+02	.96550D+01	.14527D+02	.71465D+01	.84911D+01
.95793D+01	.14864D+02	.59351D+01	.77269D+01	.81827D+01	.84333D+01
.85962D+01	.87066D+01	.87687D+01	.88348D+01	.88943D+01	
.37388D+01	.44351D+01	.42414D+01	.37763D+01	.41343D+01	.52260D+01
.66156D+01	.76803D+01	.87008D+01	.95411D+01	.10219D+02	.10727D+02
.10970D+02	.11282D+02	.11918D+02	.12288D+02	.13540D+02	.12713D+02
.13649D+02	.12856D+02	.15524D+02	.12078D+02	.16395D+02	.18323D+02
.12264D+02	.14037D+02	.15762D+02	.14252D+02	.15271D+02	.13754D+02
.11920D+02	.80587D+01	.97142D+01	.11406D+02	.10204D+02	.10339D+02
.60664D+01	.94189D+01	.85254D+01	.87283D+01	.90550D+01	.93613D+01
.96055D+01	.98458D+01	.10055D+02	.10520D+02	.10939D+02	
.32053D+01	.36691D+01	.37557D+01	.39416D+01	.45725D+01	.58017D+01
.72050D+01	.84381D+01	.98159D+01	.11196D+02	.12668D+02	.14016D+02
.15321D+02	.16416D+02	.18551D+02	.20068D+02	.21367D+02	.25176D+02
.28927D+02	.30454D+02	.33799D+02	.28842D+02	.42080D+02	.12035D+02



.28091D+02	.16835D+02	.22841D+02	.27234D+02	.14805D+02	.19467D+03
.73864D+01	.92236D+01	.99454D+01	.10070D+02	.10488D+02	.10843D+02
.11245D+02	.11720D+02	.12848D+02	.14789D+02	.21459D+02	.12850D+03
.18938D+01	.52182D+01	.63497D+01	.72655D+01	.78606D+01	
.19987D+01	.24127D+01	.26965D+01	.27613D+01	.29882D+01	.31660D+01
.32854D+01	.38066D+01	.59496D+01	.63500D+01	.61919D+01	.32102D+01
.30527D+01	.61683D+01	.24571D+02	.25912D+02	.99025D+01	.58032D+01
.49389D+01	.46749D+01	.45782D+01	.45151D+01	.44709D+01	.44384D+01
.44150D+01	.43977D+01	.43850D+01	.43752D+01	.43676D+01	.43617D+01
.43574D+01	.43538D+01	.43515D+01	.43493D+01	.43478D+01	.43466D+01
.43457D+01	.43450D+01	.43444D+01	.43440D+01	.43438D+01	.43435D+01
.43433D+01	.43431D+01	.43430D+01	.43430D+01	.43448D+01	
.21197D+01	.20535D+01	.21355D+01	.25980D+01	.29170D+01	.30758D+01
.43977D+01	.61620D+01	.56852D+01	.70215D+01	.80394D+01	.10941D+02
.38668D+02	.32626D+02	.11984D+02	.26513D+02	.16408D+02	.16001D+02
.16563D+02	.16944D+02	.17141D+02	.17295D+02	.17416D+02	.17513D+02
.17590D+02	.17650D+02	.17697D+02	.17734D+02	.17764D+02	.17786D+02
.17803D+02	.17818D+02	.17828D+02	.17837D+02	.17843D+02	.17848D+02
.17853D+02	.17856D+02	.17858D+02	.17860D+02	.17862D+02	.17863D+02
.17864D+02	.17865D+02	.17866D+02	.17867D+02	.17882D+02	
.20119D+01	.21581D+01	.23468D+01	.22712D+01	.22809D+01	.30073D+01
.35877D+01	.38353D+01	.34887D+01	.53608D+01	.46376D+01	.16896D+02
.14385D+01	.40883D+01	.12294D+02	.62747D+01	.70109D+01	.84246D+01
.93136D+01	.99832D+01	.10417D+02	.10739D+02	.10982D+02	.11161D+02
.11273D+02	.11354D+02	.11389D+02	.11399D+02	.11400D+02	.11400D+02
.11400D+02	.11400D+02	.11400D+02	.11400D+02	.11400D+02	.11400D+02
.11400D+02	.11400D+02	.11400D+02	.11400D+02	.11400D+02	.11400D+02
.11400D+02	.11400D+02	.11400D+02	.11400D+02	.11400D+02	.11400D+02
.11400D+02	.11400D+02	.11400D+02	.11400D+02	.11414D+02	
.89812D+00	.17256D+01	.14141D+01	.20217D+01	.39140D+01	.29970D+01
.63786D+01	.34768D+01	.35165D+01	.35927D+01	.36493D+01	.36875D+01
.37105D+01	.37251D+01	.37341D+01	.37395D+01	.37429D+01	.37449D+01
.37461D+01	.37468D+01	.37471D+01	.37473D+01	.37475D+01	.37476D+01
.37477D+01	.37478D+01	.37479D+01	.37479D+01	.37480D+01	.37480D+01
.37480D+01	.37480D+01	.37481D+01	.37481D+01	.37481D+01	.37481D+01
.37481D+01	.37481D+01	.37481D+01	.37481D+01	.37481D+01	.37481D+01
.37481D+01	.37481D+01	.37481D+01	.37481D+01	.37573D+01	
.88946D+00	.17254D+01	.14071D+01	.20104D+01	.39354D+01	.29984D+01
.63521D+01	.34768D+01	.35166D+01	.35930D+01	.36495D+01	.36873D+01
.37105D+01	.37251D+01	.37341D+01	.37396D+01	.37429D+01	.37449D+01
.37461D+01	.37468D+01	.37471D+01	.37473D+01	.37475D+01	.37476D+01
.37477D+01	.37478D+01	.37479D+01	.37479D+01	.37480D+01	.37480D+01
.37480D+01	.37480D+01	.37481D+01	.37481D+01	.37481D+01	.37481D+01
.37481D+01	.37481D+01	.37481D+01	.37481D+01	.37481D+01	.37481D+01
.37481D+01	.37481D+01	.37481D+01	.37481D+01	.37712D+01	
.23838D+01	.21278D+01	.29152D+01	.45626D+01	.66001D+01	.89136D+01
.93992D+01	.91031D+01	.91227D+01	.94934D+01	.10566D+02	.69716D+01
.10082D+02	.75423D+01	.11161D+02	.91355D+01	.10389D+02	.72907D+01
.60098D+01	.70720D+01	.61247D+01	.62347D+01	.10586D+02	.59893D+01
.61196D+01	.61375D+01	.61583D+01	.61714D+01	.61804D+01	.61868D+01
.61919D+01	.61958D+01	.61982D+01	.62003D+01	.62019D+01	.62032D+01
.62041D+01	.62047D+01	.62053D+01	.62057D+01	.62063D+01	.62068D+01
.62049D+01	.62000D+01	.62000D+01	.62000D+01	.62000D+01	

Table A.II Alpha Data File

.1580000D-04  
.9834750D+00  
.9835394D+00  
.9831258D+00  
.9833372D+00  
.9834064D+00  
.9836108D+00  
.9259468D+00  
.9341315D+00  
.9308735D+00  
.7784845D+00  
.7784845D+00  
.9571583D+00

Table A.III Lethargy Data File

.500000D+00  
.100000D+01  
.150000D+01  
.200000D+01  
.250000D+01  
.300000D+01  
.350000D+01  
.400000D+01  
.450000D+01  
.500000D+01  
.550000D+01  
.600000D+01  
.650000D+01  
.700000D+01  
.750000D+01  
.800000D+01  
.850000D+01  
.900000D+01  
.950000D+01  
.975000D+01  
.100000D+02  
.102500D+02  
.105000D+02  
.107500D+02  
.110000D+02  
.112500D+02  
.115000D+02  
.117500D+02  
.120000D+02  
.122500D+02  
.125000D+02  
.127500D+02  
.130000D+02  
.132500D+02  
.135000D+02  
.137500D+02  
.140000D+02  
.142500D+02  
.145000D+02  
.147500D+02  
.150000D+02  
.152500D+02  
.155000D+02  
.157500D+02  
.160000D+02  
.162500D+02  
.165876D+02

Table A.IV Amicro Group File

GP NO	LOWEST ENERGY	SIGMA REMOVAL	SIGMA ABSORPTION	D	FLUX
1	0.6065E+07	0.4668E-02	0.7024E-02	0.8646E+01	0.4531E+00
2	0.3679E+07	0.1515E-01	0.4609E-02	0.3547E+01	0.1085E+01
3	0.2231E+07	0.2383E-01	0.4632E-02	0.3114E+01	0.2295E+01
4	0.1353E+07	0.3831E-01	0.3760E-02	0.2765E+01	0.3146E+01
5	0.8208E+06	0.6322E-01	0.1272E-02	0.1944E+01	0.3338E+01
6	0.4979E+06	0.8594E-01	0.1085E-02	0.1601E+01	0.3578E+01
7	0.3020E+06	0.1280E+00	0.1023E-02	0.1223E+01	0.3236E+01
8	0.1832E+06	0.1903E+00	0.1188E-02	0.1087E+01	0.2488E+01
9	0.1111E+06	0.2696E+00	0.1459E-02	0.1128E+01	0.1769E+01
10	0.6738E+05	0.3312E+00	0.1831E-02	0.1018E+01	0.1448E+01
11	0.4087E+05	0.3884E+00	0.2773E-02	0.9314E+00	0.1238E+01
12	0.2479E+05	0.4369E+00	0.3522E-02	0.8920E+00	0.1103E+01
13	0.1503E+05	0.4747E+00	0.4391E-02	0.8563E+00	0.1017E+01
14	0.9119E+04	0.5023E+00	0.5373E-02	0.8262E+00	0.9628E+00
15	0.5531E+04	0.5223E+00	0.6380E-02	0.8033E+00	0.9264E+00
16	0.3355E+04	0.5356E+00	0.7587E-02	0.7815E+00	0.9028E+00
17	0.2035E+04	0.5445E+00	0.9300E-02	0.7717E+00	0.8864E+00
18	0.1234E+04	0.5503E+00	0.1031E-01	0.7834E+00	0.8741E+00
19	0.7485E+03	0.5549E+00	0.1365E-01	0.8096E+00	0.8627E+00
20	0.5829E+03	0.3192E+00	0.1670E-01	0.8153E+00	0.8450E+00
21	0.4540E+03	0.3713E+00	0.1334E-01	0.8341E+00	0.8398E+00
22	0.3536E+03	0.4116E+00	0.1467E-01	0.8522E+00	0.8368E+00
23	0.2754E+03	0.4476E+00	0.1783E-01	0.8157E+00	0.8245E+00
24	0.2145E+03	0.4768E+00	0.2405E-01	0.7957E+00	0.8104E+00
25	0.1670E+03	0.4983E+00	0.2465E-01	0.7665E+00	0.7997E+00
26	0.1301E+03	0.5099E+00	0.1557E-01	0.8066E+00	0.7985E+00
27	0.1013E+03	0.5320E+00	0.4481E-01	0.7754E+00	0.7764E+00
28	0.7889E+02	0.5462E+00	0.2737E-01	0.8079E+00	0.7579E+00
29	0.6144E+02	0.5534E+00	0.4239E-01	0.8612E+00	0.7484E+00
30	0.4785E+02	0.5504E+00	0.1084E-01	0.8374E+00	0.7507E+00
31	0.3727E+02	0.5495E+00	0.2771E-01	0.7946E+00	0.7536E+00
32	0.2902E+02	0.5935E+00	0.9226E-01	0.7594E+00	0.6908E+00
33	0.2260E+02	0.5840E+00	0.1046E-01	0.8309E+00	0.6869E+00
34	0.1760E+02	0.6186E+00	0.1510E+00	0.8320E+00	0.6378E+00
35	0.1371E+02	0.6162E+00	0.1424E-01	0.8576E+00	0.6173E+00
36	0.1068E+02	0.5563E+00	0.1554E-01	0.9052E+00	0.6782E+00
37	0.8315E+01	0.5579E+00	0.1492E-01	0.8833E+00	0.6739E+00
38	0.6476E+01	0.6760E+00	0.2553E+00	0.8312E+00	0.5424E+00
39	0.5043E+01	0.7028E+00	0.7746E-01	0.8663E+00	0.4898E+00
40	0.3928E+01	0.5892E+00	0.1371E-01	0.9227E+00	0.5672E+00
41	0.3059E+01	0.5584E+00	0.8931E-02	0.9013E+00	0.5947E+00
42	0.2382E+01	0.5585E+00	0.1157E-01	0.8923E+00	0.5930E+00
43	0.1855E+01	0.5593E+00	0.7249E-02	0.8878E+00	0.5904E+00
44	0.1445E+01	0.5628E+00	0.8669E-02	0.8831E+00	0.5852E+00
45	0.1125E+01	0.5785E+00	0.2468E-01	0.8740E+00	0.5668E+00
46	0.8764E+00	0.6608E+00	0.1582E+00	0.8568E+00	0.4858E+00
47	0.6253E+00	0.9938E+00	0.4525E-01	0.7919E+00	0.3993E+00

Table A.V Bmicro Group File

GP NO	LOWEST ENERGY	NU SIGMA FISSION	SIGMA FISSION	NU
1	0.6065E+07	0.2414E-01	0.6990E-02	0.3454E+01
2	0.3679E+07	0.1378E-01	0.4526E-02	0.3045E+01
3	0.2231E+07	0.1218E-01	0.4405E-02	0.2765E+01
4	0.1353E+07	0.8507E-02	0.3247E-02	0.2620E+01
5	0.8208E+06	0.1071E-02	0.4012E-03	0.2669E+01
6	0.4979E+06	0.5069E-03	0.1842E-03	0.2752E+01
7	0.3020E+06	0.4444E-03	0.1641E-03	0.2708E+01
8	0.1832E+06	0.4468E-03	0.1669E-03	0.2677E+01
9	0.1111E+06	0.4791E-03	0.1803E-03	0.2657E+01
10	0.6738E+05	0.5169E-03	0.1956E-03	0.2642E+01
11	0.4087E+05	0.5549E-03	0.2112E-03	0.2628E+01
12	0.2479E+05	0.5909E-03	0.2258E-03	0.2617E+01
13	0.1503E+05	0.6381E-03	0.2445E-03	0.2609E+01
14	0.9119E+04	0.7445E-03	0.2867E-03	0.2597E+01
15	0.5531E+04	0.8942E-03	0.3442E-03	0.2598E+01
16	0.3355E+04	0.1129E-02	0.4358E-03	0.2590E+01
17	0.2035E+04	0.1437E-02	0.5524E-03	0.2602E+01
18	0.1234E+04	0.1833E-02	0.7065E-03	0.2594E+01
19	0.7485E+03	0.2396E-02	0.9188E-03	0.2608E+01
20	0.5829E+03	0.2842E-02	0.1110E-02	0.2560E+01
21	0.4540E+03	0.4142E-02	0.1583E-02	0.2616E+01
22	0.3536E+03	0.3541E-02	0.1358E-02	0.2608E+01
23	0.2754E+03	0.4202E-02	0.1602E-02	0.2623E+01
24	0.2145E+03	0.5677E-02	0.2175E-02	0.2610E+01
25	0.1670E+03	0.5353E-02	0.2038E-02	0.2627E+01
26	0.1301E+03	0.5984E-02	0.2282E-02	0.2622E+01
27	0.1013E+03	0.6164E-02	0.2343E-02	0.2630E+01
28	0.7889E+02	0.8758E-02	0.3245E-02	0.2699E+01
29	0.6144E+02	0.1016E-01	0.3769E-02	0.2697E+01
30	0.4785E+02	0.1658E-01	0.6298E-02	0.2633E+01
31	0.3727E+02	0.7743E-02	0.3017E-02	0.2566E+01
32	0.2902E+02	0.9292E-02	0.3665E-02	0.2536E+01
33	0.2260E+02	0.1076E-01	0.4139E-02	0.2599E+01
34	0.1760E+02	0.1399E-01	0.5282E-02	0.2649E+01
35	0.1371E+02	0.1986E-01	0.7220E-02	0.2751E+01
36	0.1068E+02	0.2070E-01	0.7578E-02	0.2732E+01
37	0.8315E+01	0.1711E-01	0.6507E-02	0.2630E+01
38	0.6476E+01	0.1775E-01	0.6321E-02	0.2809E+01
39	0.5043E+01	0.1096E-01	0.3970E-02	0.2762E+01
40	0.3928E+01	0.9709E-02	0.3366E-02	0.2884E+01
41	0.3059E+01	0.6922E-02	0.2687E-02	0.2576E+01
42	0.2382E+01	0.5059E-02	0.1934E-02	0.2616E+01
43	0.1855E+01	0.4800E-02	0.1811E-02	0.2651E+01
44	0.1445E+01	0.5581E-02	0.2092E-02	0.2668E+01
45	0.1125E+01	0.8180E-02	0.3118E-02	0.2623E+01
46	0.8764E+00	0.1563E-01	0.6063E-02	0.2578E+01
47	0.6253E+00	0.6291E-01	0.2308E-01	0.2726E+01

Table A.VI Amacro Group File

GP NO	LOWEST ENERGY	SIGMA REMOVAL	SIGMA ABSORPTION	D	FLUX
1	0.8208E+06	0.3923E-01	0.4259E-02	0.2612E+01	0.2063E+01
2	0.5531E+04	0.2569E+00	0.2902E-02	0.1095E+01	0.1777E+01
3	0.6253E+00	0.5472E+00	0.3540E-01	0.8211E+00	0.7189E+00

Table A.VII Bmacro Group File

GP NO	LOWEST ENERGY	NU SIGMA FISSION	SIGMA FISSION	NU
1	0.8208E+06	0.1194E-01	0.3914E-02	0.3050E+01
2	0.5531E+04	0.5817E-03	0.2204E-03	0.2640E+01
3	0.6253E+00	0.9794E-02	0.3658E-02	0.2678E+01

## APPENDIX B

### User's Guide

#### B.1 Notes on Program Use

It should be stated at the outset that if the user intends to use this program for anything other than the default value run, he should read this section first. In fact, if no other section of the User's Guide is of any use whatsoever, this section contains information necessary to the operation of the program.

##### B.1.1 Input and Input Files

All the input files for the FASPEC program are in isotope and/or energy order with the isotope order predominant. For example, using the elastic scatter cross section file (Table A.I), the cross sections are given in barns with the first group of 47 those of each lethargy group (1 through 47) for hydrogen. The next group of 47 is then for plutonium 240, and so on down through the final entry, group 47 for zircalloy.

When energy is not a factor, as in the ALPHA DATA file, alpha of each isotope is listed in isotope order, as in Table A.II, from isotope number one through number 13. When the isotope plays no part, as in lethargy (LETHARGY DATA file), the entries are in order of ascending lethargy, groups one through 47.

If the user wishes to change existing cross section data, he need only change those portions of the files in need of change. For example, the elastic scatter cross sections for hydrogen may be changed without necessarily changing others. Grouping of lethargy may be changed



without changing all the cross sections, etc. It should be remembered, however, that cross sections are somewhat energy-dependent and changes should not be made to data input files without considerable thought being given to the extent of the required changes and the ramifications of such changes.

Those who wish to change input data should take care to maintain the same format. This also applies to number density input. When the program prompts with an example, that example should be followed explicitly. For example, the entry "(e.g., .46800E-01)" will function in FASPEC. Any other entry format may or may not function properly and is not guaranteed to yield similar or correct results. When entering group numbers for macrogroup selection, the program expects to see two digit numbers. The two groups 1 and 5 must be entered as 01 05 with a single space between.

If the user wishes to insert different isotopes in place of existing isotopes, the position of the isotope to be replaced must be the same in each data file which is isotope-dependent. If adding a 14th isotope, for example, not only must the additional data be added to each isotope dependent file, even if the additional data is all zeros (such as  $\nu$  of hydrogen) but the loop control parameters of every isotope loop (I) must be raised to the appropriate total number of isotopes. For example, when adding one isotope, any loop containing loop parameters of 1,13 or 2,13 must be changed to 1,14 and 2,14 respectively. The approximate program locations of these loops may be found easily by referring to the program listing and flow chart, both of which are included within these appendices.

### B.1.2 Test Files

Two special use files, TESTOUT DAT and TEST DATA, have been written into the FASPEC program. These two files were originally written to aid in debugging the program by allowing the user to "take a peek" at various non-output variables within the program without changing the output files or rearranging the program proper. These two files were left in the program to allow the user to see interim results and portions of equations if desired. They may be used singly or together and are activated by removing the comment signs (C in column 1) from the "WRITE" and "FORMAT" statement of each file to be activated. The appropriate desired variables are placed after the write statement and the format statement is changed as necessary.

It should be noted that although the files may be placed anywhere the user desires within the program to get the desired results, some care should be taken to place the files in a position which will give the desired results (after a variable is calculated, for example, rather than before). Some thought should be exercised before putting a file entry in to readout macroscopic cross sections, such as placing this inside an isotope loop nested within an energy loop. The result may then be  $940 \times 13 = 12220$  entries for each variable. This may tax your budget in addition to being an annoyance.

The test files are located at the end of the flux calculation and again at the end of the first collapsing routine. In each case, they are deactivated by making them appear as comments. They are also noted in each instance with a comment advising the user to see this user's guide.

### B.1.3 Changing the Number of Micro and Macro Groups

In some instances the user may wish to change the number of groups into which the initial 47 groups are subdivided. This may be done by locating the comment which notes the subdivision in the program listing and changing the loop control parameter of the loop numbered 307. The original loop parameter is  $M = 1,20$ , subdividing the initial 47 into 20 microgroups each for a total of 940 groups. By making the loop control  $M = 1,1$ , for example, the original 47 groups will result.  $M = 1,2$  results in two microgroups for each original group, or 94 microgroups, and so on. Within the subdividing loops, 306 and 307, the divisor of each delta function statement (for example,  $DU = (u(J) - u(J-1))/20.0$ ) must equal the largest value of the loop control parameter. For example, if the loop control is changed to  $M = 1,2$  as above, each delta function statement denominator must then be changed to 2.0. Note that this is a real number while the loop control is an integer.

When the number of microgroups is changed, the collapsing routine control parameters must also be changed to agree with the total number of groups to be written into the MICRO output files. This is done in the same way that is used to change the number of groups in the first collapse.

To collapse to more than or less than 47 groups in the initial collapsing routine, to change loop control parameters in loops numbered 345 and 350. Loop number 350 sets the final number of groups and the number of groups written to the MICRO output files, while loop 345 controls the number of microgroups to be collapsed into each output microgroup.

#### B.1.4 Deuterium

It should be noted that the slowing down properties of deuterium do not fit either the equation governing hydrogen or that for heavier elements. The introduction of deuterium into the program may therefore be expected to yield incorrect results unless the proper equation terms are correctly integrated with the existing program.

#### B.2 Data files

The data input files available for program and user call and user modification are as shown in Table B.I. The output data files are shown in Table B.II

The default number densities and isotope numbers are shown in Table B.III. These number densities indicate an "end of life" core originally composed of enriched  $\text{UO}_2$  fuel, zircalloy cladding and light water moderator.

Table B.IV shows the lethargy groups, lethargies and associated energies. Energies associated with the group numbers are also found in the output files.

#### B.4 Lattice Parameters and Determination of Number Density

This section is intended simply to refresh the users memory. No attempt is made to prove the methods involved or to teach new material. For a more complete explanation of the calculation of number density, refer to Reference 10. For proof of unit cell geometry, a plane geometry text will help the student.

Table B.1 Input Data Files

<u>FILE NAME</u>		<u>Variable Name</u>	<u>Variable</u>	<u>File Size</u>	
SCATTER	DATA	SC(I,J)	$\sigma_s$	13x47	Elastic scatter cross section
FISSION	DATA	FC(I,J)	$\sigma_f$	13x47	Fission cross section
CAPTURE	DATA	CC(I,J)	$\sigma_c$	13x47	Capture cross section
NU	DATA	GNU(I,J)	$\nu$	13x47	Avg. neutrons per fission
INELAST	DATA	SI(I,J)	$\sigma_{in}$	13x47	Inelastic scatter cross section
ALPHA	DATA	ALPHA(I)	$\alpha$	13	
DENSITY	DATA	DEN(I)	N	13	Number density
MASS	DATA	AMASS(I)	A	13	Isotopic mass
LETHARGY	DATA	U(J)	u	47	Lethargy
SOURCE	DATA	CHI(J)	X	47	source terms
LOGSLOW	DATA	SQUIG(I)	$\xi$	13	Log. energy decrement

Table B.II Output Files

<u>FILENAME</u>	<u>Variables</u>	<u>Length</u>
AMICRO GROUP	Group Number, Energy, $\Sigma_R, \Sigma_a, D, \phi$	47
BMICRO GROUP	Group Number, Energy, $v\Sigma_f, \Sigma_{f1} v$	47
AMACRO GROUP	same as AMICRO	set by user (1-46)
BMACRO GROUP	same as BMICRO	set by user (1-46)

Table B.III Default Number Densities

<u>Number</u>	<u>Isotope</u>	<u>Default Number Density</u>
1	Hydrogen	.26034D-01
2	Pu-240	.18299D-04
3	Pu-241	.95147D-05
4	U-235	.64847D-04
5	U-238	.76290D-02
6	Pu-239	.41708D-04
7	Pu-242	.36598D-05
8	Chromium {in stainless	.00000D+00
9	Nickel {steel	.00000D+00
10	Iron {clad	.00000D+00
11	O-16 in fuel	.16053D-01
12	O-16 in water	.13017D-01
13	Zircalloy clad	.36132D-02

Table B.IV Group Lethargy and Energy Values

GROUP NUMBER	UPPER LETHARGY	LOWER ENERGY
0	0.00	1.0000E+07
1	0.50	6.0653E+06
2	1.00	3.6788E+06
3	1.50	2.2313E+06
4	2.00	1.3534E+06
5	2.50	8.2085E+05
6	3.00	4.9879E+05
7	3.50	3.0197E+05
8	4.00	1.8316E+05
9	4.50	1.1109E+05
10	5.00	6.7379E+04
11	5.50	4.0868E+04
12	6.00	2.4788E+04
13	6.50	1.5034E+04
14	7.00	9.1188E+03
15	7.50	5.5308E+03
16	8.00	3.3546E+03
17	8.50	2.0347E+03
18	9.00	1.2341E+03
19	9.50	7.4852E+02
20	9.75	5.8295E+02
21	10.00	4.5400E+02
22	10.25	3.5358E+02
23	10.50	2.7536E+02
24	10.75	2.1445E+02
25	11.00	1.6702E+02
26	11.25	1.3007E+02
27	11.50	1.0130E+02
28	11.75	7.8893E+01
29	12.00	6.1442E+01
30	12.25	4.7851E+01
31	12.50	3.7267E+01
32	12.75	2.9023E+01
33	13.00	2.2603E+01
34	13.25	1.7603E+01
35	13.50	1.3710E+01
36	13.75	1.0677E+01
37	14.00	8.3153E+00
38	14.25	6.4760E+00
39	14.50	5.0435E+00
40	14.75	3.9279E+00
41	15.00	3.0590E+00
42	15.25	2.3824E+00
43	15.50	1.8554E+00
44	15.75	1.4450E+00
45	16.00	1.1254E+00
46	16.25	8.7640E-01
47	16.585	6.2530E-01



Since there are only two fuel lattice types among light water reactors in common use today, square and hexagonal, these will be the only types considered here. The unit cell is composed of the smallest number of rods which still maintains the geometric unit of the lattice. The distance between rod centers is the rod or lattice pitch,  $p$ . The area of the cell,  $A_c$ , may be considered numerically equal to the volume by assuming a unit cell height of one unit of measure; for example, one centimeter in the cgs system.

#### B.4.1 Unit Cell Areas

In the square lattice arrangement, four adjacent rods define the unit cell; one rod-center at each corner of a square of side  $p$ . Since each corner contains one-fourth of a rod, the cell contains one rod and the cell may be considered a square of side  $p$  centered about each rod (see Fig. B-1). The area of the unit cell is then

$$A_c = p^2$$

The hexagonal lattice consists of six rods arranged in a regular equilateral hexagon with one rod-center at each apex of the hexagon plus a central rod. The simplest way to determine the area of the cell is to divide it into six equilateral triangles of side  $p$ . Each apex of one triangle subtends an angle of  $60^\circ$  (see Fig. B-2). The area of the triangle is  $\frac{1}{2} \times \text{base} \times \text{height}$ . The base is  $p$ , the height,  $h$ , from Fig. B-2 is

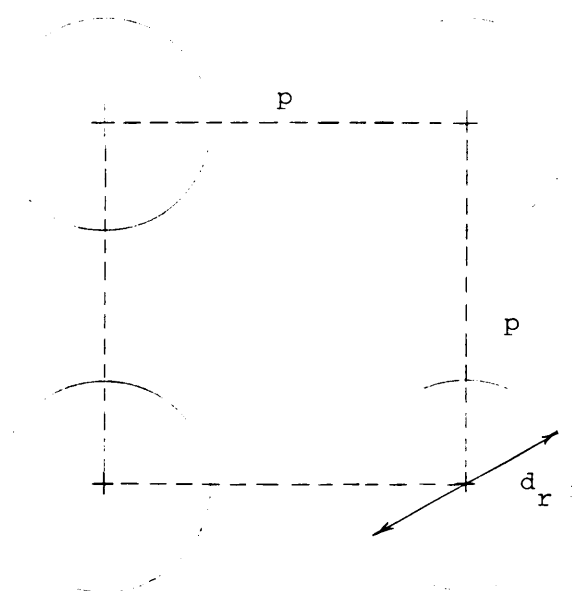


Figure B.1 The Square Unit Cell

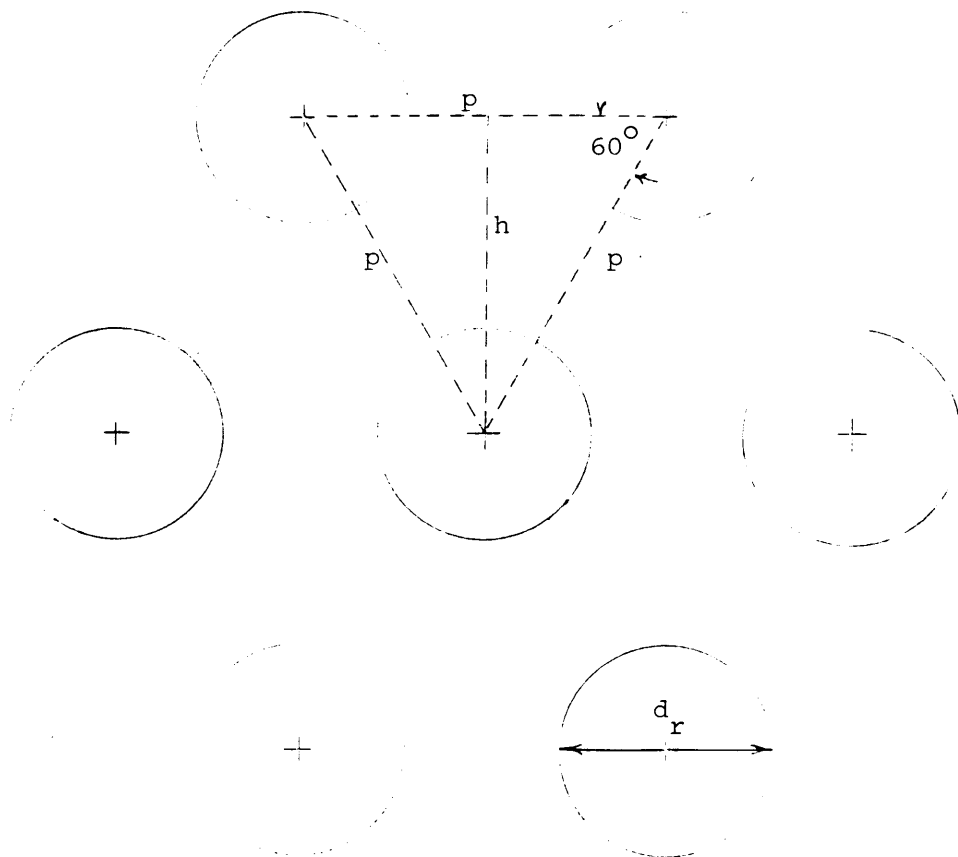


Figure B.2 The Hexagonal Cell

$$h = p \sin 60^\circ = \frac{\sqrt{3}}{2} p .$$

Since there are three rods in the above cell, and, the area of the unit cell is

$$A_c = \frac{6(1/2 hp)}{3} = hp = \frac{\sqrt{3}}{2} p^2 .$$

#### B.4.2 Area Ratios

Since the fuel rods are circular in cross section, the areas are simple to determine (see Fig. B-3). Using subscripts f for fuel, r for rod, cl for clad, and m for moderator, the areas are then

$$\begin{aligned} A_f &= \frac{\pi}{4} d_f^2 & A_r &= \frac{\pi}{4} d_r^2 \\ A_{cl} &= A_r - A_f & A_m &= A_c - A_r \end{aligned}$$

The various area ratios are then  $A_f/A_c$ ,  $A_{cl}/A_c$  and  $A_m/A_c$ . Fuel to water, FTWR, is then simply  $A_f/A_m$ . These ratios do not change with lattice type. Only the area of the cell changes.

#### B.4.3 Number Densities

The number density of a pure isotope is written as

$$N_i = \frac{\rho_i N_A}{A_i} \quad (B.1)$$

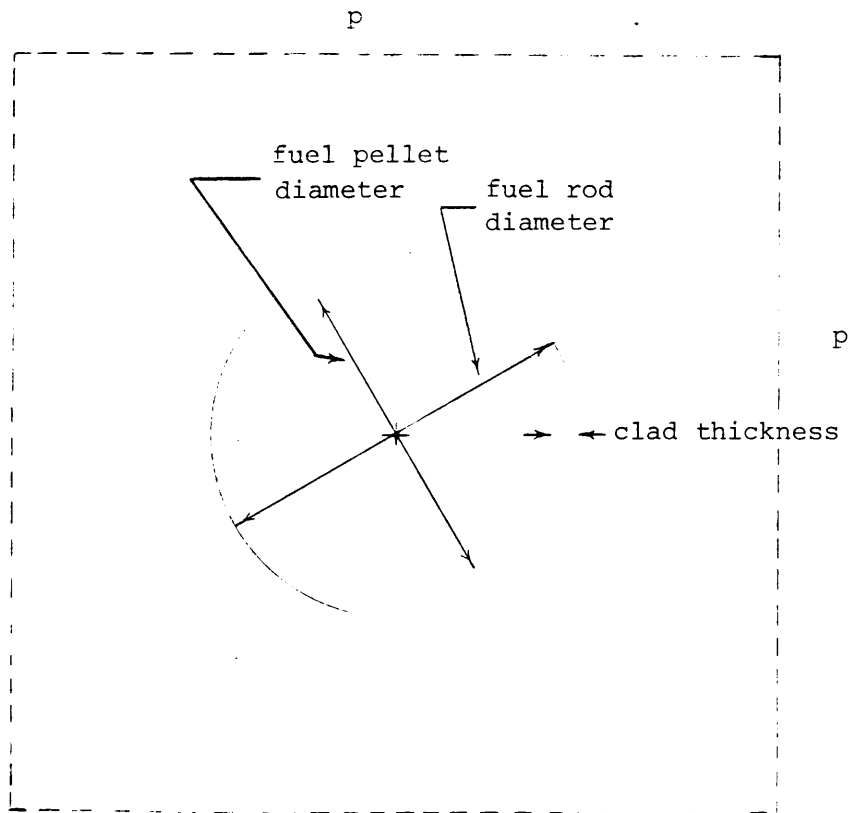


Figure B.3 Unit Cell Area Parameters

where

$N_i$  = number density of the isotope,  $i$ ,

$\rho_i$  = density of the isotope in the system,

$N_A$  = Avogadro's number,  $0.6022 \times 10^{24}$  atoms/mole,

$A_i$  = atomic weight (mass) of the isotope.

This is fine for pure isotopes, but pure isotopes are seldom found. We may, however, use this method to find the number densities of the constituent atoms in a molecular substance by using  $\rho$  and  $A$  in B.1 above and then multiplying by the number of atoms per molecule.

For example, consider a light water moderator at operating temperature. The density is approximately  $0.7 \text{ gm/cm}^3$ . The atomic mass is

$$A = 2(M_H) + M_O$$

assuming pure  $H^1$  and  $O^{16}$ , which is generally a good assumption, the atomic mass is then

$$A = 2(1.00797) + 15.9994 = 18.01534 \text{ gm/mole}$$

and the number density becomes

$$N_{H_2O} = \frac{0.7 \text{ gm/cm}^3 (0.6022 \times 10^{24} \text{ molecules/mole}) \times (1 \times 10^{-24} \text{ cm}^2/\text{barn})}{18.01534 \text{ gm/mole}}$$

where the number density of B.1 has been multiplied by the conversion from centimeters to barns,  $1 \times 10^{-24} \text{ cm}^2/\text{b}$ . This is done for convenience. Not only does it avoid cumbersome exponents, but the cross section data provided in FASPEC data files is in barns and the data required for number densities must be in units of  $(\text{b-cm})^{-1}$ , the units resulting from the above equation. The number density above is

$$N_{\text{H}_2\text{O}} = 2.3399 \times 10^{-2} (\text{b-cm})^{-1}$$

The number density for O-16 in the moderator is then the same,  $2.3399 \times 10^{-2} (\text{b-cm})^{-1}$  while that of hydrogen is

$$N_{\text{H}} = 2N_{\text{H}_2\text{O}} = 4.6798 \times 10^{-2} (\text{b-cm})^{-1} .$$

The number densities must then be multiplied by the moderator area ratio for the cell under consideration.

For mixtures of isotopes, including enrichments, the atomic mass of the mixture must first be determined. If it is the percent enrichment (or percent of the lesser isotope),  $m$ , the mass of the lesser and  $M$  the mass of the more dominant isotope,

$$\frac{1}{A} = \frac{1}{100} \left( \frac{i}{m} + \frac{100 - i}{M} \right) . \quad (\text{B.2})$$

For example, in a 25 percent enriched uranium mixture of  $\text{UO}_2$  fuel

$$\frac{1}{A_u} = \frac{1}{100} \left( \frac{25}{235.0439} + \frac{75}{238.0508} \right)$$

$$A_u = 237.2924$$

This result may then be applied as was earlier done for H<sub>2</sub>O.



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FASPEC  
A Program to Determine Group Constants  
for up to 47 Groups in a Fast Neutron Spectrum

by

Ernest L. Seth, Jr.

(ABSTRACT)

In reactor core design, a gap exists between the manual calculation of few-group constants and the many-group calculation, by large computer programs. A method is needed by which group constants may be calculated easily and quickly. The FASPEC program is designed to reduce the amount of manual calculation and to complement the large program by reducing the number of times the large program must be run to achieve desired results.

The program calculates group constants from 940 microgroups, collapsing to any user-specified number of macrogroups up to 47. FASPEC is based on group-averaged flux calculations by a solution of the infinite medium neutron transport equation. Flux contributions from inelastic scatter are included while those from neutron up-scatter are not. The energy spectrum considered is from 10 MeV to 0.625 eV. Required input is the atomic number density of each isotope, the number of macrogroups desired and the upper and lower microgroup numbers of each macrogroup. Input is facilitated by prompting in each case. Cross section look-up tables were provided by the Very Improved Monte Carlo code (VIM) for a mid-range infinite hexagonal lattice. Self-shielding effects are included indirectly. A brief user's guide is provided.

Group constants calculated and stored for either terminal display

or printed output are group number, lowest energy of the group, macroscopic removal cross section, macroscopic absorption cross section, diffusion coefficient, flux, macroscopic fission cross section,  $\nu$ , the average number of neutrons emitted per fission, and  $\nu\Sigma_f$ .