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MACH1,
A ONE-DIMENSIONAL DIFFUSION-THEORY PACKAGE

by

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INTRODUCTION

The MACH1 diffusion-theory package embodies the basic features of the AIM-6¹ one-dimensional diffusion code, the DEL² perturbation code, and the 1188/RE³ delayed-neutron code, as well as several additional ancillary subroutines. MACH1 is the result of further modifications of and additions to the MAIM-6 code.⁴ The purpose of these modifications and additions was to allow single-step calculation of many reactor parameters of interest, with minimum required input data and at reasonably high speed.

The code is written in 3600-FORTRAN for a CDC-3600 computer with 64K core storage and at least six tape drives. The code itself requires approximately 50K core storage.

The storage structure of the code is the same as that of AIM-6; this layout has led to limitations on problem size, which would not otherwise be necessary. These limitations are not serious for fast-reactor problems, but preclude the use of the code for some classes of thermal reactor problems.

The program allows 20 regions, 150 mesh points, 30 energy groups, 15 groups of downscatter, and no upscatter. In addition, a special treatment of hydrogen scatter is used, allowing full downscatter for one hydrogen nuclide in each region. Microscopic cross sections for up to 20 nuclides may be read into core storage from a library tape or with the input data. Up to 20 homogenized materials, each made up of one to 20 nuclides, may be specified.

The main additions to MAIM-6 are the DEL perturbation code, beta-effective and lifetime calculations, inhour-equation solution, expanded reaction summary, group collapsing, point-by-point reaction rates and ratios, card flux dump, external-source calculation, alpha search, and microscopic cross-section modification at run time. Transfer may also be made to any subroutine written by a user. This subroutine would then have complete control of the MACH1 code.

Running time is strongly dependent on the type of core being calculated, the quality of the initial guess, and whether the problem is an initial case or a modification of a previous case. A k -calculation of a water-moderated system using 16 energy groups, five downscatter groups, 20 regions, and 130 mesh points, with a constant initial source guess, converged with 11 inner iterations to within $10^{-5} \Delta k/k$ in 46.5 sec. A composition search on a fast reactor core using 22 energy groups, 12 downscatter groups, 9 regions, and 150 mesh points, with a region-dependent initial source guess, converged with a total of 19 inner iterations and three trials to $10^{-6} \Delta k/k$, found the adjoint solution to the same convergence, and ran a single perturbation pass in 144.9 sec.

The code package may be obtained from the Argonne Code Center.

I. EQUATIONS

A. List of Symbols

<u>Symbol</u>	<u>Definition</u>
i	spatial-point index
j	energy-group index
n	regional index
m	material or nuclide index, depending on context
s	spatial distance from the problem origin
k	effective multiplication factor
ϕ	one-dimensional, real neutron flux
Φ	multidimensional, real neutron flux
ϕ^*	one-dimensional, adjoint neutron flux
Φ^*	multidimensional, adjoint neutron flux
σ_f	microscopic-fission cross section
σ_c	microscopic-capture cross section
$\sigma_{j \rightarrow k}$	sum of microscopic elastic and inelastic transfer cross sections from group j to group k
ν	number of neutrons emitted per fission
σ_{tr}	microscopic, transport cross section
D	diffusion coefficient
Σ_x	homogenized, macroscopic cross section of type x

<u>Symbol</u>	<u>Definition</u>
Σ_t	homogenized, macroscopic, total-removal cross section
$\nu \Sigma_f$	homogenized, macroscopic, fission-source cross section
B^2	transverse buckling
α	inverse of the asymptotic reactor period
v	neutron velocity
χ	energy distribution of prompt fission neutrons or external sources, depending on context
S_e	external source
ω	linear extrapolation length
$\Delta k/k$	fractional change in k due to perturbation of macroscopic cross section and/or buckling
S	normalized real fission source
S^*	normalized adjoint fission source
$\delta \Sigma_x$	perturbation in macroscopic cross section type x
δB^2	perturbation in transverse buckling
β_d	delayed fission spectrum
β^m	fraction of the fission neutrons produced by fission of nuclide m which are delayed
β_k	fraction of fission neutrons emitted into delayed group k , as defined by decay period
λ_k	decay constant of delayed group k
β_{eff}	effective delayed fission-neutron fraction
l_p	prompt-neutron lifetime
W_d	relative reactivity worth of a delayed fission neutron
W_p	relative reactivity worth of a prompt fission neutron
T	asymptotic reactor period
$\rho(T)$	reactivity corresponding to reactor period T
ρ_{ih}	reactivity, in inhours
k_{ex}	excess reactivity
$\beta_{eff,k}$	the effective delayed neutron fraction which is due to delayed group k

B. Solution of Diffusion Equation

1. Equation Set

The code solves the coupled set of one-dimensional, multigroup, diffusion equations in slab, cylindrical, or spherical coordinates, one of which is given by

$$D_j \nabla^2 \phi_j - \Sigma_{t,j} \phi_j + S_{s,j} + S_{f,j} + S_{e,j} = 0, \quad (\text{I.B.1})$$

where

$$D_j \text{ (diffusion coefficient)} = \frac{1}{3} \left\{ \sum_m \Sigma_{tr}^m \right\}^{-1},$$

$$\Sigma_{t,j} \text{ (total removal)} = D_j B_j^2 + \sum_{k>j} \Sigma_{j \rightarrow k} + \Sigma_{c,j} + \Sigma_{f,j} + \frac{\alpha}{v_j},$$

$$S_{s,j} \text{ (scattering source)} = \sum_{k<j} \Sigma_{k \rightarrow j} \phi_k,$$

$$S_{f,j} \text{ (fission source)} = \chi_{f,j} \left\{ \sum_k (\nu \Sigma_f)_k \phi_k \right\},$$

and

$$S_{e,j} \text{ (external source)} = \chi_{e,j} S_e.$$

The finite-difference approximations to the diffusion term at space point i are

$$\left. \frac{d\phi_i}{d\xi} \right|_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta\xi}, \quad (\text{I.B.2})$$

and

$$\nabla^2 \phi = \frac{1}{(\Delta\xi)^2} \left[\phi_{i+1} - 2\phi_i + \phi_{i-1} + \frac{(N-1)\Delta\xi}{2\xi} \{\phi_{i+1} - \phi_{i-1}\} \right]. \quad (\text{I.B.3})$$

In spherical geometry, trapezoidal integration of functions of the form $\xi^2\phi(\xi)$ leads to large errors near the origin. All such integrals in MACH1 are corrected by the first-order error term of the trapezoidal rule.

The reactor is divided into regions in which D_j , B_j^2 , all $\Sigma_{x,j}$, $\chi_{f,j}$ and $\chi_{e,j}$ are constant. The external source S_e is specified at each spatial mesh point.

The code provides for input of group-dependent transverse bucklings B_j^2 ; however, this procedure has no sound mathematical basis as is shown in Appendix C. Considerable caution should be exercised in use of this option.

Downscatter due to hydrogen is treated by the method described by H. H. Hummel.⁵ The user specifies a removal cross section for each energy group. The scattering source into group j from all groups k above j in energy is then calculated from

$$S_{s,j}^H = \Delta E_j \sum_{k > j} \frac{\Sigma_{rem,k} \phi_k}{E_k} \quad (\text{I.B.6})$$

where E_k is the lower energy bound of group k . To preserve neutron balance, the ΔE_j for the lowest energy group is set equal to E_{j-1} .

At interfaces between regions, the usual flux and current continuity conditions are satisfied using the gradient approximation given by Eq. (I.B.2). The arrangement of the difference scheme requires that each region contain at least two mesh intervals.

Four boundary conditions are available at each of the inner and outer boundaries. The general expression is

$$A\phi_j + B \frac{d\phi_j}{d\xi} = C. \quad (\text{I.B.7})$$

The options are as follows:

- a. $A = 0$, $B = 1$, $C = 0$ (zero gradient);
- b. $A = 1$, $B = 0$, $C = 0$ (zero flux);
- c. $A = 1$, $B = \omega_j$, $C = 0$ (homogeneous mixed);

where ω_j is the linear extrapolation length; it is negative at inner boundaries and positive at outer boundaries.

d. $A = 1, B = 0, C = \phi_j$ (constant flux).

This is an inhomogeneous boundary condition unless all ϕ_j are zero; a problem using this option is not an eigenvalue problem. This option is discussed further in Section I.B.3.

The linear extrapolation lengths of option c may either be input by the user or calculated by the code, according to the equations given by E. R. Cohen.⁶ These are simple interpolative formulas which have been fitted to most of the available data for black cylinders and spheres. The equations for extrapolation length on external surfaces are correct at zero radius and at infinite radius; however, the midrange dependence is not based on any detailed calculations (see Ref. 6). For practical radii (>10 cm), the calculated value is very near to the asymptote at infinite radius.

The equation set is described in detail in Ref. 6.

2. Procedure for Solution

With the input conditions of fission source, reactor size, concentrations, etc., the calculation proceeds from the reactor outer boundary to the inner boundary, starting with the highest energy group. After the sweep through all groups is completed, a new fission source is calculated from the resultant fluxes. Except in special cases (see Section I.B.3), this source is then normalized to a total of one fission neutron in the reactor in the direction of the calculation; that is, no integration is carried out over the transverse direction in slab or cylindrical geometry. This normalization is given in Section I.B.4.

For the first two inner iterations, the new normalized source distribution is used to calculate the fluxes in the following iteration. In the third and subsequent iterations, the starting source at a point for the following iteration is obtained by linear extrapolation from the two previous iterations. The equation is

$$S'_{f,l+1} = S_{f,l} + \theta_l(S_{f,l-1}), \quad (\text{I.B.8})$$

where

$S_{f,l}$ = the normalized resultant source from iteration l ,

$S'_{f,l+1}$ = the source guess for iteration $l + 1$,

$$\theta_l = \theta_0 \left\{ 1 - e^{-0.5(l-2)} \right\},$$

and

θ_0 = the source extrapolation factor $0 < \theta_0 < 1$.

$S'_{f,\ell+1}$ will not be extrapolated to a negative value. If a negative value is found it is replaced by zero.

Inner iterations are continued until one of two inner convergence criteria as selected by the user is met, or until the inner iteration limit is exceeded.

The eigenvalue criterion requires that

$$\left| \frac{k^\ell - k^{\ell-1}}{k^\ell} \right| < \epsilon_1. \quad (\text{I.B.9})$$

The pointwise criterion is satisfied when

$$\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max}} < \epsilon_1, \quad (\text{I.B.10})$$

where

$$\lambda_{\max} = \max_i (k S_{f,\ell} / S'_{f,\ell}),$$

and

$$\lambda_{\min} = \min_i (k S_{f,\ell} / S'_{f,\ell}).$$

This test is carried out only for mesh points with nonzero sources. By inserting a very small concentration of fissile atoms ($\sim 10^{-30}$) in nonfissioning regions, the fluxes in these regions may be tightly converged using this option.

When the inner iteration loop has converged, the code exits to one of several search or outer-loop options as specified by the user. These are described in Section I.B.5.

3. Inhomogeneous Problems

There are three possible classes of inhomogeneous problems. The first class is the case of option 4 boundary conditions (Section I.B.1) with no fissionable nuclides. Only one iteration is necessary for this case.

(One iteration may be run by setting N121 to zero. See Section II.B.4.) The second case is option d boundary conditions with fissionable nuclides present. This must be handled in the same way as an external source problem. (See below and Section II.B.3.i.)

The third class is the case in which external fixed sources are present, so that Eq. (I.B.1) is inhomogeneous. In this case, no normalization is done in the inner loop. The inner convergence test is on the ratio of the fission-source integrals from two successive iterations. (Either criterion may be used.) The reactor must be subcritical to obtain convergence, and if k is near unity, the convergence may be slow. The procedure used is as follows.⁷

The multiplication factor of the system with no external sources present is first calculated and tested to ensure that it is less than 1.0. Then the specified external source is added, and 20 inner iterations are carried out with no normalization or source extrapolation between iterations. The difference of sources at each point for the last two iterations is then multiplied by $1/(1 - k)$, and the result is added to the source from the last iteration.

Twenty more inner iterations are then carried out with zero extrapolation; this process is repeated until convergence is reached. The method sometimes overextrapolates, and a false result may be obtained as the following iterations begin to recover. It is advisable to run two problems, one containing a convergence criterion at least a factor of 10^2 smaller than the initial problem, in order to test this behavior.

4. Normalization

During the diffusion calculation the fission sources are normalized so that

$$\text{fission-source integral} = \int_0^{\xi_{\text{outer}}} \sum_k (\nu \Sigma_f)_k \phi_k d\xi = 1.0. \quad (\text{I.B.11})$$

Output resulting from this fission-source normalization is specified as source normalized or unnormalized output.

In slab geometry, this source integral has dimensions of $n/(\text{cm}^2 \cdot \text{sec})$; in cylindrical geometry, its dimensions are $n/(\text{cm} \cdot \text{sec})$; in spherical geometry, they are n/sec .

5. Outer Loop or Search Options

Three options that do not involve the outer loop are available. These are:

a. Inhomogeneous Problems. This is described in Section I.B.3. Normalization is determined by the magnitude of the external sources or boundary values.

b. One Iteration. A single sweep is made through the spatial mesh for all groups using input source values. The resultant sources are normalized before printing.

c. k-effective. The fission sources are converged within the inner-loop criterion; the sources are renormalized after each inner loop.

The following options involve successive trials of a search parameter to reach a specified value of k, which need not be equal to 1.0.

d. Dimension Search, Reactor Size Not Fixed. The thickness of one or more specified regions is varied, maintaining the position of the inner boundary of the innermost search region and the thickness of nonsearch regions.

e. Composition Search. The atom density of a specified fuel (which may consist of a number of nuclides) is varied either alone or inversely with the density of a specified diluent. A ratio may be input such that equal volumes of fuel and diluent are varied. In the general case, this ratio is:

$$R = \frac{N_d^{\text{tot}} \sum_f \frac{N_f A_f}{\rho_f}}{N_f^{\text{tot}} \sum_d \frac{N_d A_d}{\rho_d}} = \frac{N_d^{\text{tot}} \sum_f (V.F.)_f}{N_d^{\text{tot}} \sum_d (V.F.)_d}, \quad (\text{I.B.16})$$

where

N^{tot} = the total initial fuel or diluent atom density (a/cc),

A = atomic weight of a fuel or diluent nuclide,

ρ = full density (g/cc) of the fuel or diluent nuclide,

and

V.F. = volume fraction of the fuel or diluent nuclide.

If regions with different fuel concentrations are specified as search regions, the ratio of fuel atom density in one search region to fuel atom density in any other search region is maintained constant. The ratio R is specified for each material.

f. Dimension Search, Reactor Size Fixed. The thicknesses of specified search regions are varied, and the thickness of the first region outside the outermost search region is also varied so that its outer radius remains constant. If, for example, regions 1 and 3 of a four-region reactor were being varied, the outer radii of regions 2 and 4 would remain constant.

g. Buckling Search. The transverse buckling in specified regions is varied, under the assumption that the bucklings in the search regions are region- and group-independent.

h. Alpha Search. Either this option may be used as a constant input value in conjunction with any other search, or the value of alpha may be varied to achieve criticality.

The search procedure is the same as that described in Ref. 6, except that the second guess is calculated from

$$\left. \begin{array}{l} \Delta_2 = \Delta_1 \times \frac{1}{1 + T(k-1)} \text{ if } k < 1, \\ \text{or} \\ \Delta_2 = \Delta_1 \times [1 + T(1-k)] \text{ if } k > 1. \end{array} \right\} \quad (\text{I.B.17})$$

where T is a linear function of the percentage of the total fission source that is produced in search regions. If this percentage is more than 65%, T will be 1.75; if it is zero, T will be 5.0. These values have been found by trial to give reasonably good second guesses.

6. Adjoint Calculation

Options are available such that the user may specify real solution only, real and adjoint solutions, or adjoint solution only. If the adjoint is required for an ancillary routine, the second option will be set internally. No outer-loop options may be used on an adjoint solution.

When an adjoint is specified, the real parameters are stored on magnetic tape, the scattering matrix is transposed, χ and $\nu\Sigma_f$ are interchanged, and the group structure is inverted, so that the lowest energy group becomes group 1. All output information is restored to the normal group order before printing, with the exception of the adjoint cross sections, which are printed in the inverted order. The adjoint reaction summary is not available.

C. DEL Perturbation Equations

The perturbation calculation determines the fractional change in k due to a perturbation in the macroscopic cross sections of a particular nuclide, or of a material consisting of several nuclides, or in the buckling. Any section of the reactor may be perturbed in a given pass in the radial direction. Variation in the upper limit of integration in the transverse direction is also permitted, the lower limit being the midplane; and since the same region may be perturbed in consecutive passes and the results accumulated at the option of the user, results may be obtained, as pointed out below, for shells, discs, or rings of any size.

It can be shown from the presentation on perturbation analysis by D. Meneghetti⁹ that a first-order approximation to the fractional change in k due to a small perturbation in any system may be written as

$$\frac{\delta k}{k} = \sum_{\ell=1}^4 \int_{V_n} P_{\ell} dV / \int_V SS^* dV, \quad (\text{I.C.1})$$

where V_n is the volume of the region being perturbed, V is the volume of the entire reactor, with MP designating the nuclide or material being perturbed, and other quantities are defined as

$$kP_1 = S^* \sum_{j=1}^{NG} \Phi_j \delta(\nu \Sigma_f)_{j,MP}, \quad (\text{I.C.2})$$

$$kP_2 = - \sum_{j=1}^{NG} \Phi_j \Phi_j^* \delta \Sigma_{c+f,j,MP}, \quad (\text{I.C.3})$$

$$kP_3 = - \sum_{j=1}^{NG} \nabla \Phi_j \cdot \nabla \Phi_j^* \delta D_{j,MP}, \quad (\text{I.C.4})$$

$$kP_4 = - \sum_{j=1}^{NG-1} \Phi_j \sum_{k=j+1}^{NG} (\Phi_{i,j}^* - \Phi_{i,k}^*) \delta \Sigma_{j \rightarrow k,MP}, \quad (\text{I.C.5})$$

$$kS = \sum_{j=1}^{NG} (\nu \Sigma_f)_j \Phi_j, \quad (\text{I.C.6})$$

and

$$kS^* = \sum_{j=1}^{NG} \chi_{n,j} \Phi_j^*. \quad (\text{I.C.7})$$

The common factor is maintained in the numerator and denominator of Eq. (I.C.1) because the real and adjoint sources, S and S^* , respectively, are normalized by a factor of $1/k$ in MACH1.

In view of the quantities being perturbed in the expressions above, we define the four terms in Eq. (I.C.1) as the source, absorption, leakage, and scattering terms of $\Delta k/k$ according to $\ell = 1, 2, 3$, and 4 , respectively; so also, with the terms of the volumetrically weighted quantity $(\Delta k/k)/V_n$ and those of the quantity $(\Delta k/k)/cc$ at the midplane in the direction of the calculation, where the latter implies the application of Eq. (I.C.1) without integration of the numerator quantities P_ℓ . Both the radial distributions and the totals of all these quantities appear as normal output together with the radial distribution of the sources, source products, flux products, and integrals of these products together with their regional totals. Also available (see input option NPR1, p. 40) are the energy as well as radial distributions of the fluxes, gradients, and $(\Delta k/k)/cc$ at the midplane. (For a detailed description of the output, see Section IV.C.)

Since the neutron flux ϕ provided by MACH1 is the result of a one-dimensional solution, it is related, depending upon the geometry, to the neutron flux Φ in Eqs. (I.C.2)-(I.C.7) according to the list below (R.P. indicates a rectangular parallelepiped):

Geometry	$\phi(\xi)$
R.P. Slab	$\phi(z) \cos \gamma_{Xx} \cos \gamma_{Yy}$
Cylindrical Slab	$\phi(z) J_0(\gamma_R r)$
Cylinder	$\phi(r) \cos \gamma_H z$
Sphere	$\phi(r)$

In the above list, for a given region,

$$\gamma_X = \pi/(X + 2\Delta X), \quad (I.C.8)$$

$$\gamma_Y = \pi/(Y + 2\Delta Y), \quad (I.C.9)$$

$$\gamma_R = 4.8096/(D + 2\Delta R), \quad (I.C.10)$$

and

$$\gamma_H = \pi/(H + 2\Delta H). \quad (I.C.11)$$

Figures 1-3 provide a visual conception of the quantities X , ΔX , Y , ΔY , etc. Since integration of the numerator of Eq. (I.C.1) is not performed over ΔX , ΔY , etc., appropriate changes in these quantities in successive modification problems (see N125 = 2, p. 35) and/or changes in the radial limits of integration allow the user to obtain results for shells, discs, or rings.

Fig. 1. Rectangular Parallelepiped Slab

Finite: $\begin{cases} D_n = H_n < 10^{10} \\ Y_n \leq 10^{-10} \end{cases}$

Infinite: $D_n = H_n \geq 10^{10}$

Flux Relation: $\Phi = \phi(z) J_0(\gamma_n r)$
 $\gamma_n = 4.8096 / (D_n + 2\Delta R_n)$

Fig. 2. Cylindrical Slab

Finite: $H_n < 10^{10}$

Infinite: $H_n \geq 10^{10}$

Flux Relation: $\Phi = \phi(r) \cos \gamma_n z$
 $\gamma_n = \pi / (H_n + 2\Delta H_n)$

Fig. 3. Cylinder

Since the flux relationship varies with geometry, so also does the vector-dot product indicated in Eq. (I.C.4). In all but the spherical case, there results two components in the leakage term of Eq. (I.C.1). The radial component involves the product of the real- and adjoint-flux derivatives, and the transverse component involves the product of the real and adjoint fluxes. At the midplane, the transverse component is zero and the radial component reduces to the product of the derivatives by itself. In the spherical case, the dot product reduces directly to the product of the derivatives.²

The perturbation in the diffusion coefficient is calculated under the option NTR2 = 0 (p. 40) from the differential expression

$$\delta D_j = -\delta \Sigma_{tr,j,MP} / (3 \Sigma_{tr,j,H_1}^2), \quad (I.C.12)$$

where H_1 implies the original homogenized, macroscopic, transport cross section. If NTR2 = 1, however, the change in the homogenized transport cross section is noted, so that

$$\delta D_j = -\delta \Sigma_{tr,j,MP} / (3 \Sigma_{tr,j,H_1} \Sigma_{tr,j,H_2}), \quad (I.C.13)$$

where H_2 refers to the resultant (perturbed) homogenized, macroscopic, transport cross section. The magnitude of D_j will be larger under the latter option than under the former option if the material is removed, and smaller if it is added. This effect will be reflected in the radial and transverse components of the leakage term.

In addition to the transverse and radial components of the leakage term, if the user specifies a change in the transverse buckling, B^2 (see DB2, p. 41, the component P'_3 is added to the leakage term, where P'_3 is defined by

$$kP'_3 = -\delta B^2 \sum_{j=1}^{NG} D_j \Phi_j \Phi_j^*. \quad (I.C.14)$$

The unperturbed diffusion coefficient is used here.

The neutron-flux derivative for a given energy group is evaluated according to the location of the reference point. At the inner and outer edges of the reactor, values are assigned according to the input options in MACH1 of N3 and N4, respectively (see pp. 31 and 32). For N3 = 1 and 3, application of the divergence theorem to the diffusion equation

$$D \nabla^2 \Phi - \Sigma_t \Phi + \chi S = 0 \quad (I.C.15)$$

yields, for the derivative of the flux at the innermost boundary,

$$\left. \frac{d\Phi}{d\xi} \right|_{\xi_1} = \left(1 + \frac{G\Delta\xi}{\xi_1} \right) \left[\frac{\Phi(\xi_3) - \Phi(\xi_1)}{2\Delta\xi} \right] + \left(1 + \frac{G\Delta\xi}{2\xi_1} \right) \frac{\bar{A}\Delta\xi}{D}, \quad (\text{I.C.16})$$

where $G = 0, 1$, or 2 for slabs, cylinders, and spheres, respectively, and $\bar{A}$ is a linear average value of the quantity $\chi S - \Sigma_t \Phi$ on the interval (ξ_1, ξ_2) . When $N_4 = 0$ or 3 , a similar application yields, for the derivative of the flux at the outermost boundary,

$$\left. \frac{d\Phi}{d\xi} \right|_{\xi_i} = \left(1 - \frac{G\Delta\xi}{\xi_i} \right) \left[\frac{\Phi(\xi_i) - \Phi(\xi_{i-2})}{2\Delta\xi} \right] - \left(1 - \frac{G\Delta\xi}{2\xi_i} \right) \frac{\bar{A}\Delta\xi}{D}, \quad (\text{I.C.17})$$

where G is as above and $\bar{A}$ this time is on the interval (ξ_{i-1}, ξ_i) . Equation (I.C.17) also applies to the derivative of the flux on the inside of all interior boundaries. On the outside of an interior boundary,

$$\left. \frac{d\Phi}{d\xi} \right|_{\xi_0} = \frac{D_i}{D_0} \left. \frac{d\Phi}{d\xi} \right|_{\xi_i}. \quad (\text{I.C.18})$$

At all points interior to a given region,

$$\left. \frac{d\Phi}{d\xi} \right|_{\xi} = \frac{\Phi(\xi + \Delta\xi) - (\xi - \Delta\xi)}{2\Delta\xi}. \quad (\text{I.C.19})$$

Since Φ appears in every term of Eqs. (I.C.15)-(I.C.19), it may be replaced by ϕ with an appropriate change in the definition of $\bar{A}$, since the latter contains S , whose definition by Eq. (I.C.6) involves Φ .

Integration over a given interval is carried out using the trapezoidal rule,

$$\int_{\xi}^{\xi+\Delta\xi} f(\xi) d\xi = \frac{\Delta\xi}{2} [\xi^G f(\xi) + (\xi + \Delta\xi)^G f(\xi + \Delta\xi)], \quad (\text{I.C.20})$$

where G is as defined above, depending on geometry. For a sphere, however, an error term arising from the Newton-Cotes method of quadratures is included, namely,

$$\text{ERR} = \frac{(\Delta\xi)^2}{6} [\xi f(\xi) - (\xi + \Delta\xi) f(\xi + \Delta\xi)]. \quad (\text{I.C.21})$$

D. Reaction Summaries

In general, the summaries are given as regional integrals; some groupwise and some pointwise information is also given. Values will be defined below as necessary in the order in which they appear in the output

list. The three types of summary available are total power normalized, sums over a specified number of groups, and sums over all groups.

If a value of total power has been entered, the sources and fluxes will be renormalized to that power and printed before the reaction summary is started. The expression used for total power is

$$\text{Power} = A \times \text{Fission Integral} / (3.1 \times 10^{10})$$

where

$$\text{Fission Integral} = C\pi R_{\text{PHYSICAL}}^2 \int_{\xi} \Sigma_f(\xi) \phi(\xi) d\xi \quad \text{for slabs}$$

$$= H_{\text{PHYSICAL}} \int_{\xi} 2\pi\xi \Sigma_f(\xi) \phi(\xi) d\xi \quad \text{for cylinders}$$

$$= \int_{\xi} 4\pi\xi^2 \Sigma_f(\xi) \phi(\xi) d\xi \quad \text{for spheres,}$$

and

A = total power normalization factor.

Also, C is 1.0 for nonreflective slabs and 2.0 for reflective slabs, and $\phi(\xi)$ is the unnormalized flux from the diffusion calculation. This procedure implies that the $\phi(\xi)$ have been calculated at the average transverse power position.

The user may specify that the summary be calculated for all groups only, or for group j to the last group as well as for all groups. The following quantities are printed (unless otherwise stated, the quantities refer to the direction of calculation only):

1. Physical height or radius.
2. Peak to average source in core (as specified by user).
3. Median energies in core-source, absorption, flux.
4. Core conversion ratio, defined by

$$\text{C.R.} = \frac{\text{fertile captures in core}}{\text{fissile absorption in core}}$$

5. Reactor breeding ratio, defined by

$$\text{B.R.} = \frac{\text{fertile captures in reactor}}{\text{fissile absorption in reactor}}$$

6. Fissile material-core/reactor absorption, defined by

$$F.C. = \frac{\text{fissile absorption in core}}{\text{fissile absorption in reactor}}$$

The following quantities are given for each region:

7. Flux integrals.
8. Effective buckling in direction of calculation, calculated from

$$B_j^2 = \frac{\int \nabla^2 \phi(\xi) d\xi}{\int \phi(\xi) d\xi}$$

9. Transverse leakages, defined by

$$\text{Transverse leakage} = D_j B_j^2 \int \phi(\xi) d\xi$$

10. Outer radius of region.
11. Volume. This is the actual volume, using the physical height or radius in a cylinder or slab.
12. Fission source/ k effective.
13. Conversion ratio, defined by

$$C.R. = \frac{\text{fertile captures in region}}{\text{fissile absorption in region}}$$

14. Leakage in.
15. Leakage out.
16. Transverse leakage; sum of item 9 over energy groups.
17. Peak fission density.
18. Average fission density.

Items 19 through 23 are given for each nuclide that has been mixed into a material.

19. Mass (kg). This is item 11, multiplied by the density of the nuclide in kg/liter.
20. Captures. This is item 7, multiplied by the macroscopic capture cross section and summed over groups.
21. Fissions. This is the same as item 20, with the fission cross section.
22. Number of source neutrons. This is the same as item 20, with ν times the fission cross section.

23. Alpha, capture-to-fission ratio.

24. Pointwise fission densities.

E. Beta Effective, Lifetime, and Inhour Equations

Using the radial distribution of the real and adjoint fluxes, ϕ and ϕ^* , respectively, provided by MACH1, subroutine BAILIFF determines the corresponding effective delayed fission neutron fraction,

$$\beta_{\text{eff}} = \frac{\sum_m \int_V \left[\sum_j (\nu \Sigma_f)_j^m \phi_j \right] \left[\beta^m \sum_j \beta_{d,j}^m \phi_j^* \right] dV}{\sum_m \int_V \left[\sum_j (\nu \Sigma_f)_j^m \phi_j \right] \left[\beta^m \sum_j \beta_{d,j}^m \phi_j^* + (1 - \beta^m) \sum_j \chi_{j,n} \phi_j^* \right] dV}, \quad (\text{I.E.1})$$

the prompt-neutron lifetime,

$$\ell_p = \frac{k \int_V \left[\sum_j \phi_j \phi_j^* / v_j \right] dV}{\sum_m \int_V \left[\sum_j (\nu \Sigma_f)_j^m \phi_j \right] \left[\sum_j \chi_{j,n} \phi_j^* \right] dV}, \quad (\text{I.E.2})$$

the worth of a delayed fission neutron emitted by nuclide m in region n (relative),

$$w_{d,n}^m = \frac{\int_{V_n} \left[\sum_j (\nu \Sigma_f)_j^m \phi_j \right] \left[\sum_j \beta_{d,j}^m \phi_j^* \right] dV}{\int_{V_n} \left[\sum_j (\nu \Sigma_f)_j^m \phi_j \right] dV}, \quad (\text{I.E.3})$$

and the worth of a prompt fission neutron emitted by nuclide m in region n (relative),

$$w_{p,n}^m = \frac{\int_{V_n} \left[\sum_j (\nu \Sigma_f)_j^m \Phi_j \right] \left[\sum_j \chi_{j,n} \Phi_j^* \right] dV}{\int_{V_n} \left[\sum_j (\nu \Sigma_f)_j^m \Phi_j \right] dV}, \quad (\text{I.E.4})$$

where V_n is the volume of region n , and V is the volume of the entire reactor. In the evaluation of the expressions^{3,9,10} defined in Eqs. (I.E.1)-(I.E.4), the relationships between the real fluxes Φ and ϕ and the adjoint fluxes Φ^* and ϕ are as in Section I.C. The trapezoidal rule for integration illustrated in that section is also employed here. Although the prompt-fission spectrum χ is assumed to be materially independent, it is possible within the input structure of MACH1 (See A(11644) p. 38), to specify regionally dependent values.

In addition to the total effective delayed fission neutron fraction as defined in Eq. (I.E.1), nuclide and delayed family-dependent distributions of this quantity are provided. The same denominator is employed in all cases. The family-dependent value is obtained by replacing the fraction of fission neutrons emitted by nuclide m which are delayed, β^m , in the numerator of Eq. (I.E.1) with one of six family-dependent fractions β_k^m which satisfy the relation

$$\beta^m = \sum_{k=1}^6 \beta_k^m. \quad (\text{I.E.5})$$

The values β_k^m are taken from the cross-section library (see Appendix A). The family-dependent value $\beta_{\text{eff},k}$, the nuclide-dependent value β_{eff}^m , and the family- and nuclide-dependent value $\beta_{\text{eff},k}^m$ are defined such that

$$\beta_{\text{eff}} = \sum_k \beta_{\text{eff},k} = \sum_m \beta_{\text{eff}}^m = \sum_m \sum_k \beta_{\text{eff},k}^m. \quad (\text{I.E.6})$$

Another quantity provided by BAILIFF is the inhours per percent reactivity, $0.01/\rho$ (3600 sec), where the reactivity ρ is expressed as a function of reactor period T for a given lifetime by the inhour equation,¹¹

$$\rho(T) = \frac{1}{\ell_p + T} \left(\ell_p + T \sum_m \sum_k \frac{\beta_{\text{eff},k}^m}{1 + T\lambda_{k,m}} \right). \quad (\text{I.E.7})$$

The decay constants $\lambda_{k,m}$ are taken from the cross-section library (see Appendix A).

At the option of the user (see Section II.C.3), the inhour equation can be evaluated for up to 1000 asymptotic reactor periods. In addition to the reactivity, there are provided for each period T the excess reactivity,

$$k_{\text{ex}} = \rho / (1 - \rho), \quad (\text{I.E.8})$$

$$\text{Dollars 1} = \rho / \beta_{\text{eff}}, \quad (\text{I.E.9})$$

$$\text{Dollars 2} = k_{\text{ex}} / \beta_{\text{eff}}, \quad (\text{I.E.10})$$

and the reactivity of the reactor in inhours,¹²

$$\rho_{\text{ih}} = \rho (T) / \rho (3600 \text{ sec}). \quad (\text{I.E.11})$$

F. Group Collapsing

Macroscopic cross sections collapsed by flux integral weighting in each region may be printed and punched on cards in DDF-2, MACH1, or standard Argonne format. The group collapsing may be made degenerate; that is, if the number of collapsed groups is equal to the number of initial groups, the flux integrals will be set equal to one and the cards punched immediately. This provides a technique for translating microscopic cross sections from one format to another, by running a degenerate MACH1 with a single nuclide of unit concentration in each region.

The equations used are the standard linear-weighting set. The average neutron yield per fission in collapsed groups is calculated from the averaged source cross section and the averaged fission cross section.

G. Point-by-Point Reaction Rates and Ratios

Point-by-point reaction rates and regional integrals may be calculated for capture, fission, or source reactions. Options are provided for microscopic or macroscopic rates, summed over all groups or specified groups and for individual groups. Any nuclide that is in core storage may be treated.

Reaction ratios may be calculated for any two nuclides in any combination of the three cross sections listed above. The individual rates may be summed over all groups or over specified groups.

II. INPUT DATA

There are two basic types of problem decks. The first, the initial problem, includes complete specifications for a reactor. The second includes only modifications of previous problems. During running of a problem, series data that have been set once will remain until modified by subsequent problems. Option arrays are set to zero only at the start of a problem series.

A. Deck Structure

For every problem, four card sets are necessary and two sets are optional. One additional card set is required at the start of a problem series. These are given below in the order in which they must appear. Ancillary subroutine data must appear in each problem deck if the option is operative.

A typical problem series is listed in Appendix D.

B. Card Formats; Required Data

1. Scope Control Cards

See 3600 Scope and FORTRAN manuals. (All these cards except the accounting card require a 7 and 9 punch in column 1.)

CardIdentification

- a Sequence card. This card is added when the job is submitted for running.
- b Job card
- c Accounting card
- d Comment cards listing the program and cross-section library tapes to be mounted. Refer to Satcops II documentation for formats.
- e Equip card for the program library tape. The BCD title enclosed in parentheses must agree exactly with the title on the program library tape whose number is given in card d.
- f Equip card for cross-section library tape 7 (same requirements as for card e)
- g Loadmain card. This card loads the program overlay tape and initiates execution.

2. Title Card

This is one card containing up to 80 columns of BCD problem identification.

3. Cross-section Data

The format and meanings of the cross-section data cards depend on the type of problem being run. Card descriptions for the two types will be listed separately for an initial problem and for a modification problem.

- a. Initial Problem. For an initial problem, nuclide cross sections are to be read into core storage.

CardFormatData Description

a	A3	Alphanumeric cue for operation.

<u>Blank:</u> Nuclide cross sections are to be read from library tape 7 and/or directly with the input data.

<u>NTP:</u> A complete cross-section set will be read with the input data, starting with the next card. No cross-section tape 7 is required. Card formats and order are described in Appendix A (MACH1 format only).

<u>LST:</u> List cross-section tape and proceed as if this field were blank. |
| | I3 | Number of regions in the reactor. |
| | I3 | Number of homogenized materials to be specified. |

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
	20I3	A3 field blank. These are the nuclide numbers to be read into core storage. If a nuclide number is positive, it will be read from tape 7; if negative, it will be read with the input data. Numbers must be arranged in increasing numerical order. A3 field = NTP; field not used.

If there are negative nuclide numbers in the 20I3 field of this card, the program expects one of two types of data to follow this card in the same order as the order of the negative nuclide numbers.

The first type of data is complete microscopic cross-section decks for the specified nuclides. The formats of these cards are described in Appendix A.

The second possible type of data is specification of the energy distribution of external sources. Up to 15 different energy spectra may be assigned to different reactor regions. The card formats for this type are also described in Appendix A.

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
b	I6	Dummy field. This may be used as a material-numbering field. Materials are numbered internally in the order of their position in the deck.
	I6	Number of nuclides in this material.
	A60	Alphanumeric material identifier.
c	I3	Dummy field.
	I3	Nuclide number to be mixed into the material.
	I6	Composition search flag -1: fuel 0: structural +1: diluent.
	E12.5	Concentration of this nuclide.

The above group of four formats on card set c is repeated, three per card, up to the number of nuclides given in card set b. The nuclide numbers may appear in any order and any number of times with the same or different composition search flags. Negative concentrations are permissible.

Card sets b and c are then repeated to the number of materials given in card set a.

b. Modification Problem. For a modification problem, no nuclide cross sections will be read.

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
a	A3	MOD.
	I3	Number of materials to be modified. This may be zero, in which case no cards of set b or c are required.
b	I6	Material number to be modified.
	I6	Number of nuclides in this material to be modified or added.
	10A6	Alphanumeric material identifier.
c	I3	Blank if the nuclide is being added or if its search flag and/or concentration is being changed. If a replacement is to be made, this field is equal to the nuclide number that is to replace the nuclide given in the next I3 field. A nuclide may replace itself.
	I3	The nuclide number being modified. If the positive value is given, the nuclide will be added to the list of nuclides in this material; or, if the nuclide is already in the list, the flag and concentration will be changed to those given in the next two fields. If a nuclide appears more than once in a material, the flags and concentrations will be modified in the order of their appearance in the list. If the negative value of the nuclide number is given, this nuclide will be replaced by the one given in the first I3 field of this group.
	I6	Composition search flag. See card c above for initial problem.
	E12.5	If the nuclide is being added or its concentration changed, this is the new atom density. If the nuclide is being replaced, this is the ratio of the new to the old atom density. For example, to remove 40% sodium from a material it would be replaced by itself and this field would be set equal to 0.6.

The above group of four formats is repeated, three per card, up to the number of nuclides being modified in the specified material.

Card sets b and c are repeated to the number of materials to be modified, as given in card set a.

4. Fixed-point Data

When the first entry to the program is made at the start of a problem series, the fixed-point data array and the floating-point data array described in Section 5 below are set equal to zero. Thus all options that are not set will be zero. (Note: At least one fixed-point card is required on every problem.)

The user specifies the number of data words on a card and the relative address of the first word of the data. Following words on the card are stored sequentially in increasing order. The N numbers associated with the option descriptions are the relative addresses of those options.

<u>Card Format</u>	<u>Data Description</u>
--------------------	-------------------------

I2	Number of data words on the card.
I2	Set equal to one to identify the last card of fixed-point data; otherwise set to zero.
I8	Relative address of first data word.
10I6	Fixed-point data words

<u>Fixed-point Data Word</u>	<u>Data Description</u>
----------------------------------	-------------------------

N1	<u>Geometry</u> . This must be specified. 1: Slab. 2: Cylinder. 3: Sphere.
N2	<u>Type of Search</u> 0: No search. 1: Dimension search, reactor size not fixed. 2: Composition search. 3: Dimension search, reactor size fixed. 4: Buckling search. 5: Alpha search.
N3	<u>Inner Boundary Condition</u> 0: $\text{grad } \phi_j = 0.$ 1: $\phi_j = 0.$ 2: $\phi_j + \omega_j \text{ grad } \phi_j = 0.$ 3: $\phi_j = \omega.$ 4: Same as 2, except that ω_j is calculated by the code.

Fixed-point
Data Word

Data Description

N4	<u>Outer Boundary Condition</u> 0: $\phi_j = 0$. 1: $\text{grad } \phi_j = 0$. 2: $\phi_j + \omega_j^i \text{grad } \phi_j = 0$. 3: $\phi_j = \omega_j^i$. 4: Same as 2, except that ω_j^i is calculated by the code.
N5	<u>Convergence</u> 0: Eigenvalue. 1: Pointwise.
N6	<u>Adjoint</u> 0: Real solution only. 1: Real and adjoint; will be selected if N19 or N20 $\neq 0$. 2: Adjoint only.
N7	<u>Height/radius or Buckling by Region</u> 0: Constant in all regions. 1: Region-dependent.
N8	<u>Buckling by Group</u> 0: Constant in all groups. 1: Group-dependent.
N9	<u>Starting Source</u> 0: By region. 1: By point. 2: From previous case.
N10	<u>Mesh Doubling Option</u> 0: No doubling. >0: Converge search with input mesh; then double the number of intervals in regions 1 to N10.
N11	<u>Number of Control Regions</u> 0: Search in all regions. >0: Search in N11 regions (see N60).
N12	<u>Input Data Print</u> 0: Print problem specifications only. 1: Input specifications and initial cross sections.

Fixed-point
Data Word

Data Description

N12

Input Data Print (Contd.)

- 2: Input specifications and final cross sections.
- 3: Input specifications and initial and final cross sections.

The last two options are pertinent only to concentration searches.

N13

Flux Normalization

- 0: Source normalized (see Section I.B.4).
- 1: Divide flux at each point by the flux in group N14 at point N15.
- 2: Normalize to the maximum flux over all groups and points.
- 3: Sum of flux over all groups at each point normalized to 100.0. Source normalized fluxes will also be printed.
- 4: Normalize to 1.0 in each group at the center of the reactor. Source normalized fluxes will also be printed.

N14

Group Number for Normalization (N13 = 1 only)

N15

Point Number for Normalization (N13 = 1 only)

N16

Flux Multiplication

- 0: Not used.
- 1: Multiply all fluxes by number entered in A(12374).

N17

Output Print

- 0: Print eigenvalue and fluxes.
- 1: Print eigenvalue only.

N18

Reaction Summary (see Section I.D)

- 0: Not used.
- 1: Sum over all groups only.
- >1: Sum from group N18 to last group; then sum over all groups.

N19

Perturbation Theory (DEL)

- 0: Not used.
- >0: Set equal to the number of perturbation "passes" (see Section II.C.2).

Fixed-point
Data Word

Data Description

N20 Beta Effective and Lifetime (BAILIFF)
 0: Not used.
 1: Calculate β_{eff} and ℓ_p ; print only regional integrals and final results.
 2: Same as 1, plus pointwise summations (see Section IV.D).

N21 Inhour Curve (If N20 = 0 and N21 = 1, N20 is set to 1 by the code.)
 0: Not used.
 1: Calculate curve (see Section I.E).

N22 Group Collapsing (see Section I.F)
 0: Not used.
 >0: Set equal to number of collapsed groups.

N23 Card Flux Dump
 0: Not used.
 1: Punch point-by-point, group-by-group fluxes in standard ANL format.

 Note: For input to SNARG,¹⁵ the last value in each group must be deleted.

N24 Dummy Option
 0: Not used.
 >0: Call Overlay 7 (see Section III.C).

N25 Point-by-point Reaction Rates and Ratios
 0: Not used.
 >0: Equal to the number of reaction rate cards (see Section II.C.5).
 <0: Same as previous option. Negative sign indicates cards are to be punched.

N40-N59 Number of Intervals in Each Region

N60-N79 Control Region Numbers
 N11 region numbers.

N80-N99 Core Region Identifiers
 0: Noncore region.
 1: Core region.

(Used only for reaction summaries.)

<u>Fixed-point Data Word</u>	<u>Data Description</u>
N100-N119	<u>Material Number in Each Region</u>
N120	<u>Source Extrapolation Factor</u> (see Section I.B.2) 0: Use built-in factor (0.2). 1: Input extrapolation factor ($0 < \theta < 1.0$).
N121	<u>Limit on Number of Inner Iterations</u> If no value is entered, the limit will be 40.
N122	<u>Limit on Number of Outer Iterations</u> If no value is entered, the limit will be 10.
N123	<u>Converge to k-effective from Previous Problem</u> 0: Not used. 1: All $\nu\Sigma_f$ is divided by the k-effective of the previous problem, and this problem is run to convergence. The $\nu\Sigma_f$ is then restored.
N124	<u>Adjoint Cross-section Print</u> 0: Not used. 1: Print adjoint cross sections.
N125	<u>Problem Skip</u> 0: Not used. 1: Skip this problem. 2: Do ancillary subroutines only, using fluxes from previous problem.

(Option 1 can be employed when the nth problem in a deck has failed and must be rerun. All previous problems can be skipped when the job is rerun; all their information will be stored. N125 can then be set to zero for the problem. Under option 2, any problem parameter may be changed.)

N126	<u>Number of Groups</u> This is not required unless the user wishes to change the number of groups from that on the cross-section tape.
N127	<u>Number of Downscatters</u> Do not enter this quantity except in special circumstances. Normally this value is taken from the cross-section tape.
N128	<u>Number of Regions</u> This may be entered to change the number of regions in a modification problem. In an initial problem, it is to be entered on the second card, as described in Section II.B.3.

Fixed-point
Data Word

Data Description

N129

External Source Cue

When an external-source "nuclide" is encountered, this register is set to the position of the external-source "nuclide" in the nuclide array. Thus, if the external-source "nuclide" is the fourth item in the nuclide list, N129 is set to 4. On an initial problem, this value is set by the code. If the current problem does not contain an external source, enter a zero in this location.

5. Floating-point Data

(Note: At least one floating-point data card is required on every problem.)

Card Format

Data Description

I2

Number of data words on card.

I2

Set to nonzero to identify the last card of floating-point data; otherwise set to zero.

If this I2 is negative, microscopic change cards will be expected to follow (see Section II.C.1).

I8

Relative address of first data word.

5E12.5

Floating-point data words.

Floating-point
Data Word

Data Description

A(1)

Inner-convergence Criterion

A(2)

Outer-convergence Criterion

A(3)

Extrapolation Factor

If N120 = 1, enter θ here.

A(23)

Inner Radius of Reactor

Initially set to zero in the code.

A(24)-A(53)

Extrapolated Height (Cylinder) or Radius (Slab)

Group-independent Height or Radius

If N7 and N8 are both zero, enter one number.

If N7 = 1 and N8 = 0, enter M (number of regions) numbers.

<u>Floating-point Data Word</u>	<u>Data Description</u>
A(24)-A(53)	<u>Extrapolated Height (Cylinder) or Radius (Slab) (Contd.)</u> <u>Group-dependent Buckling</u> If $N7 = 0$ and $N8 = 1$, enter buckling values here. If $N7 = 1$ and $N8 = 1$, enter values later.
A(54)-A(223)	<u>Starting Source</u> If $N9 = 0$, enter by region. If $N9 = 1$, enter for each point. Enter two values sequentially at each region interface. (If no values are entered, the initial source will be set to one at all points.)
A(224)-A(243)	<u>Outer Radius of Each Region</u>
A(244)-A(843)	<u>Buckling Values if $N7 = 1$ and $N8 = 1$</u> Stored as $B^2(I, J)$, where $I = \text{region}$, $J = \text{group}$. B^2 for group j in region n is entered at $Y = 244 + 20(j - 1) + n - 1$.
A(844)-A(1013)	<u>External Sources</u> Point-by-point values. Enter two values sequentially at each region interface. (Note: Source discontinuities may occur only at region interfaces.)
A(1141)	<u>Alpha (the inverse asymptotic reactor period)</u> This is the initial value of alpha if the search option $N2 = 5$ is used, or the fixed value of alpha if some other option is in operation. If not set, its value is zero.
A(2915)	<u>Physical Height (Cylinder) or Radius (Slab)</u> This is used only in the reaction summary for the calculation of core volumes necessary for the total power normalization.
A(3404)-A(3423)	<div style="display: flex; align-items: center;"> <div style="margin-right: 10px;"> <u>H</u> <u>DX</u> <u>Y</u> <u>DY</u> </div> <div style="font-size: 3em; margin-right: 10px;">}</div> <div> These four items are required only if $N19$ or $N20$ is nonzero (see Section II.C.2). These items are given for each region if $N7 = 1$; one value only is required if $N7 = 0$. Ignore these items for spheres. </div> </div>
A(3484)-A(3503)	
A(3504)-A(3523)	
A(3524)-A(3543)	

<u>Floating-point Data Word</u>	<u>Data Description</u>
A(11644)-A(12243)	<u>Regionwise Fission Spectrum</u> These data are stored in a two-dimensional array of size 20 x 30. Thus the chi for group j of region n is stored at address Y, where Y is given by $Y = 11644 + 20(j - 1) + n - 1$.
A(12244)-A(12273)	<u>Inner-boundary Extrapolation Lengths or Flux Values</u> One value is entered for each energy group. If N3 = 2, extrapolation lengths are given. (These values must be negative.) If N3 = 3, flux values are given.
A(12274)-A(12303)	<u>Outer-boundary Extrapolation Lengths or Flux Values</u> One value is entered for each energy group. If N4 = 2, extrapolation lengths are given. (These values must be positive.) If N4 = 3, flux values are given.
A(12304)-A(12323)	The ratio R for each material (composition search option only; see Section I.B.5.v). If no value is entered for a given material, R is set to unity.
A(12370)	The total power in watts to which the reaction summary is to be normalized. If this item is not entered, no total power normalization is done.
A(12374)	The number by which the sources and fluxes are to be multiplied under the option N16 = 1.
A(12375)	The k-effective to be searched for. If no value is entered here, the search is to a k-effective of 1.0.

C. Card Formats; Optional Data

The order of the data in this section must be maintained; for example, if the inhour equation and group-collapsing cues are operative, the group-collapse data must follow the inhour data.

1. Microscopic Cross-section Changes

This card set is cued by setting the second I2 field of the last floating-point card to a negative value.

<u>Card Format</u>	<u>Data Description</u>
I2	Number of data words on card.
I2	Nonzero for last cross-section change card.
I2	The group number of the first microscopic change word.
I2	If the downscatter matrix is being modified, this is the index of the group from which the scatter occurs for the first word. Subsequent words on this card will be stored in increasing final-group number, and the number of groups between initial and final groups will be maintained. If any cross section other than the downscatter matrix is being modified, this field is not used.
I2	Nuclide number of the nuclide being changed.
I2	The index number of the cross section being changed. These index numbers are as follows: 1: Capture + fission 2: Sigma transport 3: Nu sigma fission 4: Nu 5: Scattering matrix.
5E12.5	The values of the cross section to be inserted in the positions specified by the above index set.

The removal cross section for hydrogen is stored in the nu sigma fission array, and is accessible for changes.

2. DEL (Perturbation) and BAILIFF (Beta Effective)

The first four items in the list below consist of regional data, which are required input for both DEL and BAILIFF and are to be included in the floating-point input of Section II.B.5. No additional input is required for BAILIFF. For DEL, however, there are to be N19 (see Section II.B.4) additional cards, one for each perturbation pass, each containing the information listed below in order of appearance after the A-data. The format of the pass card is (8I3, 3E12.5, 6I3).

<u>Symbol</u>	<u>Explanation</u>
	(Note: See Figs. 1-3 for a visual depiction of the A-data. Ignore A-data for spheres.)
H,A(3404)	$\geq 10^{10}$ for all infinite geometries. $< 10^{10}$ for all finite geometries and the semi-infinite rectangular parallelepiped.

Symbol	Explanation
DX,A(3484)	Used in perturbation analysis.
Y,A(3504)	Used for slabs when $H < 10^{10}$. $>10^{10}$ for semi-infinite rectangular parallelepipeds. $<10^{-10}$ for finite cylindrical slabs. $>10^{-10}$ and $<10^{10}$ for finite rectangular parallelepipeds.
DY,A(3524)	Used in perturbation analysis.
INTS	Begin perturbation in this interval.
INTF	Finish perturbation in this interval, not restricted to same region as INTS.
MATP	Number of the material to be perturbed in this pass.
ISOP	Number of the nuclide to be perturbed in this pass. Both ISOP and MATP can be perturbed in one pass.
NTR2	= 0: Ignore change in the homogenized, macroscopic, transport cross section. = 1: Do not ignore this change (see Section I.C).
KLRT	= 0: Accumulate grand totals (see Section IV.C). = 1: Clear grand totals.
NPR1	= 1: Print radial and energy distribution of fluxes, gradients, and $(\Delta k/k)/cc$ at the midplane in the direction of the calculation from INTS through INTF. (If energy-dependent perturbations are to be punched, NPR1 must be 1.) = 0: Suppress this printing.
NPU	= 0: Do not exercise punch option. = 16: Punch central fluxes, adjoints only. = 1: Punch DK/K per cc. = 2: Punch DK/K . = 4: Punch DK/K per DV. } Interval-dependent = 3, 5, 6, 7: Punch appropriate combinations of the above, as indicated by this entry.
	Note: With $NPU = 16$ and $INTS = 0$, no other perturbations will be done.
	Note: With $NPU > 0$, central fluxes and adjoints will be punched.
MFRAC	The fraction of material MATP to be perturbed. This number multiplies the homogenized macroscopic cross sections of the isotopes of which MATP is comprised to obtain the cross-section perturbations indicated by $\delta(\nu\Sigma_f)_j^{MP}$, etc., in Section I.C. If $ISOP > 0$, the perturbations used in the calculation include those indicated below under IDENS.

<u>Symbol</u>	<u>Explanation</u>
IDENS	Change in volume fraction or atom density depending on whether library cross sections for ISOP are macroscopic or microscopic, respectively. This number multiplies the library cross sections of ISOP to obtain the cross-section perturbations indicated by $\delta(\nu\Sigma_f)_j^{MP}$, etc., in Section I.C. If MATP > 0, the perturbations used in the calculation include those indicated above under MFRAC.
DB2	Perturbation, δB^2 , in the transverse buckling [see Eq. (I.C.14)].
6I3	Punch energy-dependent perturbations. Three pairs of entries are allowed. Begin punching energy-dependent perturbations in the interval denoted by the first entry, and continue through all intervals inclusive of the interval denoted by the following entry. Three pairs of intervals are allowed. If these are blank or zero, no energy-dependent perturbations are punched. If punching is desired in one interval only, it is necessary to put in a pair of entries, each entry being equal to that interval number where punching is desired. Note: To punch energy-dependent perturbations, NPR1 must be 1, and at least two (one pair) of the above 6I3 fields (columns 61 through 78) must be >0. Other perturbation punching depends on the contents of NPU. If only energy-dependent perturbations are to be punched, the above is done and NPU is set to zero. This is the only way punching can be activated while NPU = 0.

3. Inhour Curve

Two cards are required when the inhour option (see Section II.B.4, N21) is exploited. It is necessary for BAILIFF to be executed (see Section II.B.4, N20) before the inhour calculation. Both cards with inhour data have the same format (6E12.5). The first contains from two to six reactor periods, in seconds. The second contains from one to five time increments, in seconds, to be used in stepping between the periods indicated on the first card. The first increment is used between the first and second periods; the second increment is used between the second and third periods; etc. The calculation begins with the first reactor period and ends when a zero period is encountered, the sixth period has been used, or 1000 calculations have been made, whichever comes first.

4. Group Collapsing

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
a	I3	Punch format cue. 1: XLIBIT ¹³ format 2: MACH1 format 3: DDF-2 ¹⁴ format.
	I3	Transport cross-section collapsing method. 0: Find coarse-group $\bar{\Sigma}_{tr}$ by averaging fine-group Σ_{tr} (SIGTR weighting). 1: Find coarse-group $\bar{\Sigma}_{tr}$ by averaging fine-group $1/\Sigma_{tr}$ (D weighting).
	1X	Space.
	A5	New collapsed cross-section set name if XLIBIT format has been selected. If blank, the original set name is used. Not operative if the collapsed format is not XLIBIT.
	24I3	Initial group indices of the lower energy bound of the final group structure. Enter N22 numbers.
b		

5. Point-by-Point Reaction Rates and Ratios

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
a	16	Rate nuclide number. This nuclide will be the denominator of any specified ratios.
	I3	Groupwise rates and ratios cue. 0: Sum over all groups. 1: Calculate rates and ratios for individual groups over the specified range and for the sum over this range as well as the sum over groups.
	I3	Initial group number of range when previous I3 field is 1.
	I3	Final group number of range.
	I3	0: Microscopic rates and ratios. 1: Macroscopic rates and ratios using the atom density in each region.
	I3	Reaction type for the rate nuclide (ratio denominator).
		Ratio-numerator nuclide number.
		Reaction type for the ratio-numerator nuclide.
	Reaction types:	
	1: Capture	
	2: Fission	
	3: Source ($\nu\sigma_f$ or $\nu\Sigma_f$).	

Repeated
up to
six times

{
{
{

Thus up to six ratios may be formed for any given rate nuclide. The first zero or blank value of the reaction type for the rate nuclide in the ratio list terminates the list. Up to 20 cards may be run on any one problem; the number of cards must agree with the value of N25. (See Sample Problem 5, Appendix D.)

III. PROGRAM OPERATION

A. Library Tapes

1. Program Tape System

The program overlay tape consists of a main program and six overlays, stored in absolute binary on a 556 bpi tape. The tape is labeled with the current version label. It is loaded by the SCOPE control order LOADMAIN, n. No RUN card is required by the current version of SCOPE.

Because of continuing problems of tape damage during use, a source tape is also saved in the library. This consists of relocatable binary subprograms plus suitable loader control cards for preparation of a new overlay tape. If the current overlay tape fails, the user should prepare a new overlay tape by referencing the source tape, loading it, then running the problem by means of the control cards LOAD, n and RUN, t, l. The new overlay tape may be saved for later use.

A deck of relocatable binary cards is also available from the authors in the event of failure of the source tape. A new source tape should first be prepared from the cards by use of FILE, n and FILE END. A new overlay tape is then prepared from the source tape; both of these tapes may be saved.

All the above recovery operations may be carried out by the user at problem running time.

2. Cross-section Tape

The binary library tape is prepared by the program MACHLIB. (Appendix A). It consists of two identical files each containing the same cross-section set. MACH1 is arranged to skip to the second file in case of a parity check in the first file. An appropriate error message is printed. When the user encounters this message in his output list, he should obtain the BCD cross-section cards from their author and remake the cross-section tape using MACHLIB.

B. Data and Running Errors

MACH1 will detect most, but not all, errors of commission and omission usually found in input data. Self-explanatory error messages are

printed, and in general the code will proceed to the next case of the series. This procedure can at times produce spectacular behavior of the following problems; however, it was felt that something of value may be salvaged by this method.

Running errors are handled in the same fashion as input errors. They include such failures as no convergence and impossible requirements in search options.

A separate class of running errors is parity failure on cross-section or scratch tapes. As already mentioned, the program will attempt a recovery from parity on the cross-section library tape. If this fails, an exit to monitor will be made. As for scratch tapes, the action depends on the position of the parity and its relation to later calculations. An error message is printed in any case.

C. Overlay 7 Feature

The program contains a call to a nonexistent Overlay 7, on logical Unit 48, cued by setting $N24 \neq 0$. The call is placed after all other ancillary subroutine calls.

This option can be used as follows: By copying the standard common and equivalence blocks from a subroutine of the program, the user gains access to all the data input to and calculated by the code. He may then write his own subroutine or subroutines up to a total length of approximately 10,000 octal words, in order to calculate values not now produced by the code or to change data for subsequent problems on the basis of results from the current problem.

The user's routines are compiled and made up as an overlay, which must be number 7 on logical Unit 48. This tape is then mounted along with the MACH1 overlay tape and the cross-section tape for the job. The first MACH1 problem in the job which contains $N24 \neq 0$ will transfer control to the user's routine at the end of its specified operations. The user's routine may carry out any operations within the limitations of the code, such as change any internal data, read new input, print, punch, or plot output, or rewrite the MACH1 input tape for the next problem. By use of the problem skip ($N125$), he may specify that the next problem only do ancillary routines such as DEL, BAILIFF, and so on, with only the changes made in his routines. The user's routine may call segments of its own or any subroutine or entry point in the main program of MACH1. A normal return transfers control back to MACH1 for the next problem.

IV. OUTPUT

The printed output is divided into three blocks, namely input data edit, diffusion solution output, and ancillary subroutine output. Since the information printed is largely self-descriptive, it will be described here only in general terms. The reaction-summary printing is described in Section I.D.

A. Input Data Edit

The first item of output is a direct listing of the input cards, followed by a check on the cross-section tape mounting time.

The program then reads and checks the data for the first problem. Most parameters that would produce a meaningless result if incorrect are tested, and appropriate error prints are made. If there are error prints, exit to the next problem is made.

The next item is a list of the input conditions for the first problem, including the nuclide data, input options, geometric configurations, microscopic cross sections modified (if any), and the type of problem to be solved. The initial macroscopic cross sections are then printed, if requested.

B. Diffusion Solution Results

Following the input data edit, the solution routines are entered; the eigenvalues from the last two inner iterations are printed after each outer iteration, along with inner and outer iteration counts and the value of the search parameter in the first search region. Problem failure prints, if any, appear here. When the problem is converged, the final macroscopic cross sections are listed, if specified, along with point-by-point sources and fluxes. These are subject to the various normalization options already described. The above process is then repeated for the adjoint solution, if this option is operative.

If parity errors are encountered during program operation, an error print is made; operation may continue after the print. If this is the case, the information derived from output following the parity print should be examined carefully.

C. DEL

1. Printed Output

The perturbation output for each pass begins with the heading MACH1 DEL RESULTS, followed by the general problem description and an edit of pertinent input data, starting with the pass and region numbers.

The descriptive heading for each succeeding section appears below in capital letters and is followed by a list of the information presented in that section.

<u>FORTTRAN</u> <u>Symbol</u>	<u>Math</u> <u>Symbol</u>	<u>Definition of Symbol or Section Title</u>
		POINTWISE SOURCES, SOURCE AND FLUX PRODUCTS, AND INTEGRALS OF THE PRODUCTS.
		(This section occurs only on the first pass. The information below is given for each point in the reactor after which the regional totals of ISS* and IPP* appear.)
I	i	Spatial-point index.
R	ξ	Radial distance from origin.
S	$S(\phi)$	The normalized real source obtained with MACH1 fluxes.
S*	$S^*(\phi^*)$	The normalized adjoint source obtained with MACH1 fluxes.
SS*		Product of S and S* defined above.
PP*		$\sum_j \phi_j \phi_j^*$
ISS*		Integral over (I, I+1) of $S(\phi)S^*(\phi)^*$.
IPP*		Integral over (I, I+1) of $\sum_j \phi_j \phi_j^*$.
		ENERGY DISTRIBUTION AT THE MIDPLANE OF FLUXES, GRADIENTS, AND DK/K PER CC IN THE DIRECTION OF THE CALCULATION AT R =
		(This section occurs when NPR1 = 1. The data are given for all energy groups at each point within the radial limits of perturbation for the given pass.)
EGRP	j	Energy-group index.
PHI	ϕ	Real flux in the radial direction at the midplane.
PHI*	ϕ^*	Adjoint flux in the radial direction at the midplane.

<u>FORTTRAN Symbol</u>	<u>Math Symbol</u>	<u>Definition of Symbol or Section Title</u>
R	ξ	Radial distance from midplane to I.
DV	ΔV	Increment in volume over (I, I+1).
DK/K	$\Delta k/k$	Fractional change in k over (I, I+1).
TOTAL		Accumulated fractional change in k from initial interval of current pass through (I, I+1).
(DK/K)/DV	$\frac{\Delta k}{k} / \Delta V$	Fractional change in k over (I, I+1), divided by corresponding increment in volume.
TOTAL		Accumulated fractional change in k from initial interval of current pass through (I, I+1), divided by the corresponding accumulated increments in volume.
		GRAND TOTALS.
		(This section will include the results of previous passes in the quantities indicated under the option KLRT = 0.)

2. Punched Output

The following card types are produced in the punched output:

(A.1) Problem Title Card

The problem title card (80 columns of BCD information) is punched out. One card for each problem.

(A.2) Problem Data Card

Format: 18H, 3I3.

18H: (NUMBER OF PASSES).

I3: Number of passes for this problem.

I3: Number of regions specified for this problem.

I3: Number of energy groups specified for this problem.

One card for each problem.

(A.3) Central Flux Card

Format: 6E12.5 (three pairs of 2E12.5)

Each pairs contains { E12.5: central flux;
E12.5: adjoint.

One pair for each energy group.

(Number of energy groups + 2)/3 cards for each problem.

These Type A cards are punched once only, at the beginning of the punched output for a given problem.

The Type B cards appear for each pass.

(B.1) Perturbation Data Card

Format: 8I3, 3E12.5, 6I3.

I3, INTS: Same as input card.

I3, MATP: Same as input card.

I3, ISOP: Same as input card.

I3, NTR2: Same as input card.

I3, NPPASS: The number of passes that call
-punching.

I3, NPR1: Same as input card.

I3, NPU: Same as input card.

E12.5, MFRAC: Same as input card.

E12.5, IDENS: Same as input card.

E12.5, DB2: Same as input card.

6I3: Same as input card.

One card for each perturbation pass.

(B.2) Regional Data Card

Format: 2I3, E12.5, I3, 4E12.5.

I3: Region number.

I3: = 0 if this is not a core region;

= 1 if this is a core region.

E12.5: Outer radius of this region.

I3: Number of intervals in this region.

4E12.5 { H: See Section II.C.2.
DX: See Section II.C.2.
Y: See Section II.C.2.
DY: See Section II.C.2.

(Number of regions) cards for each pass.

(B.3) Isotope Data Card

Format: A6, 15X, 23H, I3, 6X, 13H, E12.5.

A6, 15X: Alphanumeric name of perturbed isotope.

23H: (LIBRARY ISOTOPE NUMBER).

I3, 6X: Library number of the perturbed isotope.

13H: (ATOM DENSITY).

E12.5: Atom density of perturbed isotope.

One card for each pass.

The Type C cards may appear for each region, in every pass. Four possible data types may appear for each region in every pass. Each regional data type contains a data title card and associated data block.

C.8 Energy-group-dependent Perturbation Data Type

(C.8.a) Energy-dependent Perturbation Card

Format: I3, 35H, I3, 10H, I4, 7H, E14.6.

I3: Numerical data type name (8).

35H: (ENERGY DEP. PERTURBATIONS -
REGION).

I3: Region number.
 10H: (INTERVAL).
 I4: Interval number.
 7H: (RADIUS).
 E14.6: Outer radius of this interval.
 If this data type is called, one of these cards appears for each interval called.

(C.8.b) Energy-dependent Perturbation Data Block

Format: 8E10.3.

Fields are as follows:

PHI, PHI*, DPHI, DPHI*, NSF, C + F, DIFF, SCAT.

Number of energy-group C.8.b cards for every C.8.a card.

C.1 (DK/K)/CC Interval-dependent Perturbation Data Type

(C.1.a) (DK/K)CC Data Title Card

Format: I3, 35H, I3, 10H, I4, 3H, I4.

I3: Numerical data type name (1).

35H: ((DK/K)/CC REGION).

I3: Region number.

10H: (INTERVALS).

I4: First perturbation interval in this region.

3H: (T $\emptyset$).

I4: Last perturbation interval in this region.

One card for every region from which these perturbations are called.

(C.1.b) (DK/K)/CC Data Block

Format: 8E10.3.

Fields are as follows:

RADIUS, NSF, C + F, RLEAK, BLEAK, SCAT,

(DK/K)/CC, TLEAK.

(Number of intervals spanned in C.1.a card plus one).

C.1.b cards appear for every C.1.a card.

C.2 DK/K Interval-dependent Perturbation Data Type

(C.2.a) Format: I3, 35H, I3, 10H, I4, 3H, I4.

I3: Numerical data type name (2).

35H: (DK/K REGION).

I3, 10H, I4, 3H, I4: Same as C.1.a.

One card for every region from which these perturbations are called.

(C.2.b) DK/K Data Block

Format: 8E10.3.

Fields are as follows:

RADIUS, NSF, C + F, RLEAK, TLEAK, BLEAK, SCAT, DK/K.

(Number of intervals spanned in C.2.a card).
C.2.b cards appear for every C.2.a card.

C.4 (DK/K)/DV Interval Dependent Perturbation Data Type

(C.4.a) (DK/K)DV Data Title Card

Format: I3, 35H, I3, 10H, I4, 3H, I4.

I3: Numerical data type name (4).

35H: ((DK/K)/DV - REGION).

I3, 10H, I4, 3H, I4: Same as in C.1.a.

One card for every region from which these perturbations are called.

(C.4.b) (DK/K)/DV Data Block

Format: 8E10.3.

Fields are as follows:

VOLUME, NSF, C + F, RLEAK, TLEAK, BLEAK,
SCAT, (DK/K)/DV.

(Number of intervals spanned in C.4.a card).

C.4.b cards appear for every C.4.a card.

The four possible types of data are punched, by region, in the order mentioned, namely:

Type C.8 Cards: For as many intervals, in that region requested.

Type C.1 Cards: One data block per region, if any requested.

Type C.2 Cards: One data block per region, if any requested.

Type C.4 Cards: One data block per region, if any requested.

In any given pass, the above C data are repeated for each region from which perturbation data are called. Types B and C data are then repeated for each pass, up to the number of passes to be punched by the problem. After all the C data are punched for a pass, an "End of Pass" (Card Type D) is punched.

(D) End of Pass Card

Format: 3X, 12H.

3X, 12H: (END OF PASS).

One card for each pass.

Note: All fields are right-justified.

D. BAILIFF and INHOUR

The BAILIFF printout begins with a section titled MACH1 BAILIFF INPUT DATA, which is an edit of the pertinent input data, including a list of BETA SETS. Each BETA SET consists of three lists to be read from left to right. The first list presents decay constants for six delayed families, or groups. The second list presents the fraction of the fission neutrons emitted, which appear in each of the same six delayed families, followed by the total fraction (the sum of the first six items). The third list presents the energy-group distribution of the delayed-fission neutrons. The remaining sections are described below and follow the general heading MACH1 BAILIFF RESULTS.

<u>FORTTRAN</u> <u>Symbol</u>	<u>Definition of Symbol or Section Title</u>
	POINTWISE SUMMATIONS (Printed when NBEF > 1.)
I	Radial-point index.
R	Radial distance from midplane.
$\phi\phi^*/V$	Radial distribution of $\sum_j \phi_j \phi_j^*/v_j$.
$X\phi^*$	Radial distribution of $\sum_j \chi_{n,j} \phi_j^*$.
ISO	Identification number of fissile or fertile nuclide.
NUSIGF ϕ	Radial and nuclide distribution of $\sum_j (\nu\Sigma_f)_j \phi_j$.
BETD ϕ	Radial and nuclide distribution of $\sum_j \beta_{d,j} \phi_j^*$.
	REGIONAL INTEGRALS
N	Regional index number.
BDRY	Outer boundary of region.
GEOF1	Geometric integration constant for terms involving one flux.
GEOF2	Geometric integration constant for terms involving the product of two fluxes.
$\phi\phi^*/V$	Regional integral of $\sum_j \phi_j \phi_j^*/v_j$.

<u>FORTRAN Symbol</u>	<u>Definition of Symbol or Section Title</u>
ISO	Identification number of fissile or fertile nuclide.
NUSIGF ϕ	Regional integral of $\sum_j (\nu \Sigma_f)_j \phi_j$.
NUSIGF ϕ B ϕ^*	Regional integral of $\sum_j (\nu \Sigma_f)_j \phi_j \sum_j \beta_j \phi_j^*$.
NUSIGF ϕ X ϕ^*	Regional integral of $\sum_j (\nu \Sigma_f)_j \phi_j \sum_j \chi_{n,j} \phi_j^*$.
WORTHS OF DELAYED AND PROMPT FISSION NEUTRONS IN REGION N	
N	As above.
ISO	
DWRTH	Relative worth of a delayed fission neutron emitted by ISO.
PWRTH	Relative worth of a prompt fission neutron emitted by ISO.
EFFECTIVE DELAYED FISSION NEUTRONS	
ISO	As above.
BEFK(M,L)	Nuclide distribution of the effective delayed fission neutron fraction for delayed family L.
BEFM(M)	Total effective delayed fission neutron fraction for ISO (sum of first six items).
SUMS	Total effective delayed fission neutron fraction for family L (sum of the column items). The last item in this list is also the sum of the column items above it and represents the total effective delayed fission neutron fraction.
Note: The remaining items printed in this section are self-explanatory. The prompt neutron lifetime is given, along with the numerator and denominator of Eq. (I.E.2).	
INHOURL EQUATION RESULTS (Available when N21 = 1.)	
PERIOD	Asymptotic reactor period.
RHO	Reactivity, $(k - 1)/k$.
KEX	Excess reactivity, $k - 1$.
RHO/BETA	Dollars one.
KEX/BETA	Dollars two.
INHOURS	Reactivity in inhours.

E. Group Collapsing

The punched deck for each problem is preceded by the problem title card. The formats of the punched deck depend on which output option has been used (Section II.C.4). If option 1 is operative, a complete deck of macroscopic collapsed cross sections for each region will be punched, ready for input to the standard Argonne cross-section processing code, XLIBIT. On option 2, the same cross sections will be punched in MACH1 format, preceded by the appropriate cards for direct input to MACH1 under the problem type option NTP (Section II.B.3.i).

Option 3 is DDF-2 format, in a form slightly modified from the Los Alamos format. The cards for each group are punched in the following order:

$$\Sigma_{c+f}, \nu\Sigma_f, \Sigma_{tr}, \Sigma_{j,j}, \Sigma_{j-1,j}, \Sigma_{j-2,j}, \dots$$

Each group starts a new card.

The collapsed cross sections are also printed on the standard output tape.

F. Reaction Rates and Ratios

The output of this section is completely titled as to which nuclides and reactions are being considered, as well as the groups over which the reactions are summed.

Punched Output

The following card types are produced in the punched output:

(A.1) Problem Title Card

The problem title card is punched out (80 columns of BCD information), one card for each problem.

(A.2) Problem Data Card

Format 2I6

I6: Gives RATRACE input card number (reference to input or print-out to identify rate nuclide for a given card).

I6: Reaction type of punched card set immediately following, whether for reaction rate or ratio information. Only the rate nuclide reaction type is indicated.

(A.3) Rate/Ratio Data Cards

Format 8E10.4

The first, third, fifth, and seventh fields give point-by-point radii for rate/ratio data given in the second, fourth, sixth, and eighth fields, respectively. For a given rate nuclide, punched cards are obtained for all three reaction types, even though some rates may all be zeros, followed by a card set for each ratio specified for that rate nuclide, if any. Blank spaces may appear in the last rate-ratio data card for each region. The outer radius for a region is repeated on the following card as the first point of the subsequent region.

Microscopic or macroscopic rate and ratio data, directly comparable with print-out, are obtained on the punched cards subject to input specifications for a given card.

APPENDIX A

MACHLIB

This appendix describes the MACHLIB cross-section library preparation code and the card formats required for direct cross-section input and external-source energy distribution.

The MACHLIB program can be used to prepare a binary library tape from MACH1, MC², or Standard Argonne format cards, or a mixture of these three. The cards may be input at run time or put onto a BCD tape prior to run time (see card a). The BCD tape may also be obtained from the translation code RXMACH (see Appendix B). The block of data that precedes the actual cross sections is the same in all cases, with the exception of card a.

1. Initial Data Block

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
a	I6	The logical unit number from which the cross sections are to be read. If the cards are input directly, this number must be 60; otherwise, it must be 9. (Note: Omit this card in the case of direct cross-section set input under the NTP option. See Section II.B.3.)
b	I6	NOSET: Cross-section set number.
	I6	NOMAT: The number of nuclides in the set.
	I6	NOG: The number of energy groups.
	I6	NDS: The number of downscatter groups.
	I6	NBET: The number of delayed group sets to be input. $0 \leq \text{NBET} \leq 6$.
c	2413	Nuclide cross-section format identification (NOMAT numbers). (Note: Omit this card for NTP input.) 0: MC ² format. 1: MACH1 format. 2: Standard Argonne format.
d	I0A8	Alphanumeric description of the cross-section set.
e	6E12.5	Prompt fission spectrum. NOG numbers.
f	6E12.5	Average neutron velocity in each energy group.

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
g	6E12.5	Upper lethargy limit of each group. The base energy must be 10 MeV.

The following card set is required if NBET > 0. There must be NBET sets of cards present. The beta sets will be numbered in the order of their appearance.

h(1)	6E12.5	The decay constants for the delayed families.
h(2)	6E12.5	The delayed neutron fractions for each member of the family in the same order as on the previous card.
h(3)	6E12.5	The delayed fission spectrum of this beta set. NOG numbers.

2. MACH1 Card Formats (Direct-input cross sections must be in this format.)

These formats apply both to the MACHLIB program and to direct-input cross sections, as described in Section II.B.3.

a. Nuclide Identification Card

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
a	I3	Nuclide number. Ignored by MACHLIB. In direct input, this number is stored in place of the negative number in the nuclide list.
	I3	The beta-set number of the set to be used for this nuclide.
	E12.5	Atomic weight of this nuclide.
	A4	Alphanumeric nuclide type identification. The options are: FISS: This nuclide will be treated as fissile by the reaction summary. FERT: The reaction summary will treat this nuclide as fertile. SPEC: This nuclide will not be included in the conversion or breeding ratios, but fission and source reaction rates will be calculated. HYDR: This nuclide will be considered to be hydrogen, and its downscattering will be treated as described in Section I.B.1. If the cross-section cards are in MACH1 format, cards appropriate to hydrogen must follow the identification card (see the next card set).
	7A8	Alphanumeric identification of this nuclide.

b. Cross-section Deck; Nonhydrogen Nuclides

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
a	I6	Group number.
	E12.5	Capture plus fission cross section.
	E12.5	Transport cross section.
	E12.5	Nu sigma fission (source cross section).
	E12.5	Number of neutrons per fission.
b	6E12.5	Downscatter matrix. The first element is the scatter into the group from the highest energy group that can scatter into this group (i.e., either group 1 or group j - NDS). The elements are in order of decreasing energy, so that the last element is the scatter to group j from group j - 1. Zeros are inserted following this last element to make up NDS numbers for each group. (Note that there will be NDS zeros in group 1.)

Card sets a and b are repeated to the number of energy groups.

c. Cross-section Deck; Hydrogen Nuclides

a	I6	Group number.
	E12.5	Capture plus fission cross section.
	E12.5	Transport cross section.
	E12.5	Scattering-removal cross section. The scatter to individual groups will be calculated by the method of Section I.B.1 using the lethargy limits given above for the lower energy bound of each group.

Card set a is repeated to the number of energy groups. No card set b is required.

3. MC² Card Formats

a. Nuclide Identification Card

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
a	I3	Nuclide number. Ignored by the code.
	I3	The beta-set number of the set to be used for this nuclide.

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
	I6	ELMOE correction cue 0: no ELMOE-corrected $3\sigma_{tr}$ and σ_{el} in this nuclide. 1: ELMOE-corrected $3\sigma_{tr}$ and σ_{el} are present (see below).
	A4	Alphanumeric nuclide type identification. See options on p. 58.
	7A8,2XA6	Alphanumeric identification of this nuclide.
b	E12.5	Atomic weight of this nuclide.
b.	<u>Cross-section Deck</u>	
a	5E12.5	σ_c , σ_f , σ_{tr} , σ_{el} , ν .

Card a is repeated for each group up to NOG.

- b 3(2E12.5) $3\sigma_{tr}$, σ_{el} (ELMOE-corrected). If $3\sigma_{tr}$ is zero for any group, the σ_{tr} and σ_{el} given in card set a for that group will be used.

NOG pairs of numbers are required. This card set is present only if the ELMOE correction cue on the identification card is nonzero.

- c 4(E12.5,2I3) Inelastic-scattering matrix, arranged in the order $\sigma_{j \rightarrow j}$, $\sigma_{j \rightarrow j+1}$, ..., $\sigma_{j \rightarrow \text{NOG}}$. Each element is followed by the initial group number and the final group number.

Card c is repeated for each group up to NOG - 1.

4. Standard Argonne Card Formats

a. Nuclide Identification Card

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
a	I3	Nuclide number. Ignored by the code.
	I3	The beta set number of the set to be used for this nuclide.
	E12.5	Atomic weight of this nuclide.
	A4	Alphanumeric nuclide type identification. See options on p. 58.

b. Cross-section Deck

See Reference 13 for Standard Argonne formats. The type plus card is required in this case. The alphanumeric material identification in columns 26 to 75 of the plus card will be stored on the MACH cross-section tape, followed by the six-character "material name" from the Standard Argonne cards.

5. External-source Energy Distributions (Direct Input Only)

To conserve storage, the external source spectra are input as pseudo nuclides. These spectra may not be added to a cross-section library tape.

Up to 15 different source spectra may be specified; additional information input at this time is the identification of which spectrum is to be used for each region of the problem. An external source "nuclide" is identified by the letters SRCE in the A4 field of the nuclide identification card.

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
a	Nuclide identification card.	
	I3	Nuclide number.
	I3	The number of source spectra to be input.
	E12.5	Blank.
	A4	The letters SRCE.
	7A8	Alphanumeric identifier.
b	20I3	The number of the source spectrum to be used in each region of the problem. Set equal to zero if there is no external source in a particular region. Any one spectrum may be used in any number of regions.
	6E12.5	The external source energy spectrum NOG numbers must be entered.

Card set c is repeated up to the number of different source spectra specified on the nuclide identification card.

APPENDIX B

RXMACH

This appendix describes the procedure for producing a BCD cross-section tape from the RE122 (see Reference 8) binary library tape on the IBM-704. The program RXMACH is set up for the IBM-704 OOPS monitor system. It requires two extra tapes, namely, the RE122 library tape on logical unit 9, and a blank tape on logical unit 5. Unit 5 tape will contain BCD records of the cross-section tape in MACH1 format at the end of the job.

Input Data

<u>Card</u>	<u>Format</u>	<u>Data Description</u>
a	E12.5	Floating-point cross-section set number.
	I6	The number of delayed group sets to be input.
b	6E12.5	Mean neutron velocities for each energy group of the set.
c	6E12.5	Upper lethargy limits for each group of the set.

The following three card sets are required only if the number of beta sets on the first card is greater than zero.

d	6E12.5	Decay constants for this delayed-group set.
e	6E12.5	Delayed neutron fractions corresponding to the decay constants given above.
f	6E12.5	Delayed fission spectrum. One number for each group.

Cards d, e, and f are repeated to the number of beta sets.

g	I3	Nuclide number.
	I3	Number of the beta set to be used with this nuclide.
	E12.5	Atomic mass of this nuclide.
	A4	Alphanumeric nuclide type identification. The options are the same as on p. 58.
	14A4	Alphanumeric nuclide identification.
h	6E12.5	Required only if the nuclide type identifier is FISS, FERT, or SPEC. These are the number of neutrons per fission for each energy group.

Card sets g and h are repeated to the number of nuclides in the set.

A maximum of 20 min should be adequate to convert any existing REX library tape.

APPENDIX C

GROUP-DEPENDENT BUCKLINGS

Considering cylindrical geometry with symmetry in the θ direction, and assuming that the (r, z) variables are separable, the flux may be written as

$$\phi(r, z) = \phi(r)\psi(z), \quad \text{with } \psi(0) = 1.$$

The diffusion equation for one energy group can then be written

$$\begin{aligned} D_j \nabla_{r,j}^2 \phi_j + \phi_j D_j \left(\frac{\nabla_{z,j}^2 \psi_j}{\psi_j} \right) - \Sigma_a \phi_j + \sum_{k < j} \Sigma_{k \rightarrow j} \phi_k \frac{\psi_k}{\psi_j} \\ + \chi_{f,j} \sum_k (\nu \Sigma_f)_k \phi_k \frac{\psi_k}{\psi_j} + \chi_{e,j} S_e \frac{\psi_e}{\psi_j} = 0. \end{aligned}$$

The usual approach, and the one used in MACH1, is to set

$$\frac{\nabla_{z,j}^2 \psi_j}{\psi_j} = -B_j^2$$

and to assume that all $\psi_k/\psi_j = 1.0$. This condition is met only over the asymptotic range of the z direction fluxes, and can only be true if all B_j^2 are equal. Alternatively, one could normalize ψ_k to 1.0 at some point z_1 and calculate B_j^2 over the range $z_1 \pm \Delta z$, Δz being chosen small enough so that ψ_k/ψ_j does not vary appreciably over the range. This is roughly equivalent to performing the radial calculation at z_1 .

APPENDIX D

SAMPLE PROBLEMS

Five sample problems are listed in this appendix; they are all part of a single series.

The first problem is a two-region sphere with two materials, on which a composition search is to be run with nuclide 55 as the fuel and nuclide 1 as the diluent. The reaction summary is to be normalized to a total power of 1 W.

The second problem is modified by addition of a nuclide to the core. The reaction summary is to be done for group 16 alone, then for all groups. Three perturbation passes are to be run, and beta effective and the prompt neutron lifetime are to be calculated.

The third problem is a repeat of the second with one DEL pass, the addition of group collapsing to a four-group structure, and punching in XLIBIT format.

The fourth problem is a three-region parallelepiped slab with two materials. Two DEL passes, as well as beta effective, lifetime, and an inhour curve, are to be run. Note that H and Y must be entered for DEL and/or BAILIFF.

The fifth problem is a three-region cylinder with a fuel-loading search option. Four reaction rate cards are included.

In all problems, the options that are not reset explicitly will remain as set in previous cases.

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ACKNOWLEDGMENTS

Contributions to this work have been many and varied. Several individuals, notably Ken Phillips and Dwight Kucera, have suffered through the "production-run debugging" of MAIM-6. John Ohde of AMD has offered many helpful suggestions on the use of the CDC-3600 system. Dorothy Bingaman of AMD provided the AIM-6 program deck. Dwight Kucera wrote the subroutine MINX, which punches XLIBIT format cards, and the point-by-point reaction rate and ratio routine.

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