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PDQ-7 REFERENCE MANUAL

JANUARY 1967

CONTRACT AT-11-1-GEN-14

BETTIS ATOMIC POWER LABORATORY, PITTSBURGH, PA.,
OPERATED FOR THE U. S. ATOMIC ENERGY COMMISSION
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PDQ-7 REFERENCE MANUAL

PRICES

W. R. Cadwell

H.C. \$ 3.00; MN .65

January 1967

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Copies of this program may be obtained by domestic
users from

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PDQ-7 REFERENCE MANUAL

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PDQ-7 REFERENCE MANUAL

W. R. Cadwell

ABSTRACT (1/67)

The PDQ-7 program solves the neutron diffusion-depletion problem in one, two, and three dimensions on the CDC-6600 computer. Up to five lethargy groups are permitted, with the thermal neutrons represented by a single group or a pair of overlapping groups. Adjoint and boundary value calculations may be performed and the depletion may be by point or block. The geometries available are rectangular, cylindrical, spherical, and hexagonal.

I.A. INTRODUCTION (1/67)

The PDQ-7 program solves the neutron diffusion-depletion problem in one, two, and three dimensions on the CDC-6600 computer. Up to five lethargy groups are permitted, with the thermal neutrons represented by a single group or a pair of overlapping groups. Adjoint and boundary value calculations may be performed and the depletion may be by point or block. The geometries available are rectangular, cylindrical, spherical, and hexagonal.

The macroscopic data and depletion calculations utilize the HARMONY system which is described in Reference 1. This system provides a flexible representation of time-dependent cross sections and a general format for the specification of nuclide chains. The reference contains a complete description of HARMONY input, including macroscopic and microscopic cross sections, chain descriptions, and initial nuclide concentrations, and these topics are not fully covered in the present manual.

The format of this manual has been chosen to facilitate additions and modifications. Three-hole paper is used, the pages are printed on only one side, each section begins on a new page, and the pages are numbered by section. In addition, the heading of each section contains the date of issue. Each distribution will include a table of contents which gives the most recent issue date for each section.

I.B. DIFFUSION EQUATIONS (5/66)

If there is a single thermal group, the diffusion equations solved by the program are

$$\begin{aligned} & \left\{ -\nabla \cdot [D_g(x) \nabla \varphi_g(x)] + [\Sigma_g^a(x) + \Sigma_g^r(x) + D_g(x) B_g^2(x)] \varphi_g(x) \right. \\ & \quad \left. = \frac{\chi_g}{\lambda} \psi(x) + \Sigma_{g-1}^r(x) \varphi_{g-1}(x) \right\}_{g=1}^G \end{aligned} \quad (\text{I.B./1})$$

Here (x) represents the spatial variable(s); g is the lethargy group index; and G , the index of the thermal group, may be one, two, three, four, or five. In addition,

$$\Sigma_0^r(x) \equiv 0$$

and

$$\psi(x) = \sum_{g=1}^G \nu \Sigma_g^f(x) \varphi_g(x) . \quad (\text{I.B./2})$$

The physical interpretations of these symbols are

- D = the diffusion coefficient,
- Σ^a = the macroscopic absorption cross section,
- Σ^r = the macroscopic removal cross section,
- B^2 = the geometric buckling,
- ν = the average number of neutrons produced per fission,
- Σ^f = the macroscopic fission cross section,
- χ = the fission source fraction,
- φ = the neutron flux,
- ψ = the fission source, and
- λ = the eigenvalue.

Diffusion coefficients and macroscopic cross sections may be input directly or may be calculated by the program using spatially varying nuclide concentrations and input microscopic cross section tables and/or interpolating tables.

In the case of a two-thermal-group problem, Equations (I.B./1) are unchanged for the fast groups but are replaced, for $g = G-1$ and G , by the equations

$$\begin{aligned}
 & - \nabla \cdot [D_{G-1}^1(x) \nabla \varphi_{G-1}(x)] + [\Sigma_{G-1}^1(x) + D_{G-1}^1(x) B_{G-1}^2(x)] \varphi_{G-1}(x) \\
 & = \frac{\chi_{G-1}}{\lambda} \psi(x) + R_{G-1}(x) \Sigma_{G-2}^r(x) \varphi_{G-2}(x) + \nabla \cdot [D_{G-1}^2(x) \nabla \varphi_G(x)] \\
 & - [\Sigma_{G-1}^2(x) + D_{G-1}^2(x) B_G^2(x)] \varphi_G(x) \quad (\text{I.B./3})
 \end{aligned}$$

and

$$\begin{aligned}
 & - \nabla \cdot [D_G^1(x) \nabla \varphi_G(x)] + [\Sigma_G^1(x) + D_G^1(x) B_G^2(x)] \varphi_G(x) \\
 & = \frac{\chi_G}{\lambda} \psi(x) + R_G(x) \Sigma_{G-2}^r(x) \varphi_{G-2}(x) + \nabla \cdot [D_G^2(x) \nabla \varphi_{G-1}(x)] \\
 & - [\Sigma_G^2(x) + D_G^2(x) B_{G-1}^2(x)] \varphi_{G-1}(x) \quad (\text{I.B./4})
 \end{aligned}$$

Although these appear to be general equations for the treatment of two thermal groups, the spatial calculation of the program actually ignores the two terms in Equation (I.B./3) involving φ_G . This is only acceptable if D_{G-1}^2 and Σ_{G-1}^2 are several orders of magnitude smaller than D_{G-1}^1 , Σ_{G-1}^1 , and R_{G-1} . One model which satisfies this restriction treats the thermal neutrons as two overlapping groups and is described in Reference 2. In this model φ_{G-1} and φ_G are the magnitudes of the thermal flux components corresponding respectively to a hardened and a Maxwellian thermal spectrum.

I.C. PROBLEM TYPES - CONVERGENCE (1/67)

The program may be used to solve four different types of problems - eigenvalue, boundary value, one iteration, and fixed source. Equations (I.B./1)-(I.B./4) are the governing equations in eigenvalue, boundary value, and one iteration problems. In fixed source problems Equation (I.B./2) is not used and the $\chi_g \psi(x)/\lambda$ term in the remaining equations is replaced by the input source $S_g(x)$. Zero flux, zero current, and rotational symmetry boundary conditions are permitted in all problems, with fixed flux boundaries also permitted in boundary value problems. In addition, an internal symmetry boundary condition may be obtained in any problem by setting all of the macroscopic data in a region to zero. The program then sets the flux to zero interior to the region and imposes a zero current condition on its boundary.

The convergence criterion used in the program is

$$\text{Max}_x \left| \frac{\phi_n(x)}{\phi_{n-1}(x)} - 1 \right| < \epsilon, \quad (\text{I.C./1})$$

where $\phi_n(x)$ is the flux at point x at the end of iteration n and ϵ is an input parameter. In eigenvalue and boundary value problems, source iterations are performed until this criterion is satisfied in all groups. A single source iteration is performed in one iteration problems and in both these and fixed source problems, flux iterations are performed in each group until the criterion is satisfied. In slowly convergent problems, Equation (I.C./1) is altered slightly to assure that the maximum relative error in the flux does not exceed $\sqrt{\epsilon}$.

I.D. MATHEMATICS (1/67)

The difference equation coefficients are described in terms of the contribution of a single mesh figure to the difference equations at its vertices. If P and Q are two vertices of a mesh figure, C_{PP} and C_{PQ} represent the contribution of this figure to the coefficients of ϕ_P and ϕ_Q in the equation for point P. Fission and removal coefficients are not given explicitly since these are calculated in the same manner as the absorption contribution.

The one-dimensional mesh figure is

and the coefficient contributions are

$$C_{PQ} = C_{QP} = - \frac{(r + h/2)^p}{h} D$$

$$C_{PP} = \frac{(r + h/2)^{p+1} - r^{p+1}}{p + 1} \Sigma^t - C_{PQ} \quad (\text{I.D./1})$$

$$C_{QQ} = \frac{(r + h)^{p+1} - (r + h/2)^{p+1}}{p + 1} \Sigma^t - C_{QP}$$

Here r is the distance from the origin to point P and p is 0, 1, and 2 for rectangular, cylindrical, and spherical geometry.

The two-dimensional mesh figure for rectangular and cylindrical geometry is

The rectangular contributions are

$$\begin{aligned}
 C_{PQ} &= C_{QP} = C_{RS} = C_{SR} = -\frac{h_2}{2h_1} D \\
 C_{PR} &= C_{RP} = C_{QS} = C_{SQ} = -\frac{h_1}{2h_2} D \\
 C_{PP} &= C_{QQ} = C_{RR} = C_{SS} = \frac{h_1 h_2}{4} \Sigma^t - C_{PQ} - C_{PR}
 \end{aligned} \tag{I.D./2}$$

and the cylindrical contributions are

$$\begin{aligned}
 C_{PQ} &= C_{QP} = C_{RS} = C_{SR} = -\frac{(r + h_1/2)h_2}{2h_1} D \\
 C_{PR} &= C_{RP} = -\frac{(r + h_1/4)h_1}{2h_2} D \\
 C_{QS} &= C_{SQ} = -\frac{(r + 3h_1/4)h_1}{2h_2} D \\
 C_{PP} &= C_{RR} = \frac{(r + h_1/4)h_1 h_2}{4} \Sigma^t - C_{PQ} - C_{PR} \\
 C_{QQ} &= C_{SS} = \frac{(r + 3h_1/4)h_1 h_2}{4} \Sigma^t - C_{QP} - C_{QS}
 \end{aligned} \tag{I.D./3}$$

where r is the distance from the origin to line PR . In the three-dimensional case, if rectangle $TUVW$ is a distance h_3 below rectangle $PQRS$, the contributions are

$$\begin{aligned}
 C_{PQ} &= C_{QP} = C_{RS} = C_{SR} = C_{TU} = C_{UT} = C_{VW} = C_{WV} \\
 &= -\frac{h_2 h_3}{4h_1} D \\
 C_{PR} &= C_{RP} = C_{QS} = C_{SQ} = C_{TV} = C_{VT} = C_{UW} = C_{WU} \\
 &= -\frac{h_1 h_3}{4h_2} D
 \end{aligned} \tag{I.D./4}$$

I.D.(2)

$$C_{PT} = C_{TP} = C_{QU} = C_{UQ} = C_{RV} = C_{VR} = C_{SW} = C_{WS}$$

$$= - \frac{h_1 h_2}{4h_3} D$$

$$C_{PP} = C_{QQ} = C_{RR} = C_{SS} = C_{TT} = C_{UU} = C_{VV} = C_{WW}$$

$$= \frac{h_1 h_2 h_3}{8} \Sigma^t - C_{PQ} - C_{PR} - C_{PT}$$

The two-dimensional mesh figure for hexagonal geometry is

and the coefficient contributions (Reference 3) are

$$C_{PQ} = C_{QP} = \frac{h_1 - 2h_2}{2\sqrt{3} h_1} D$$

$$C_{PR} = C_{RP} = \frac{h_2 - 2h_1}{2\sqrt{3} h_2} D$$

$$C_{QR} = C_{RQ} = - \frac{1}{2\sqrt{3}} D$$

$$C_{PP} = \frac{h_1^2 + h_2^2 - h_1 h_2}{\sqrt{3} h_1 h_2} D + \frac{h_1 h_2}{4\sqrt{3}} \Sigma^t$$

$$C_{QQ} = \frac{h_2}{\sqrt{3} h_1} D + \frac{h_1 h_2}{4\sqrt{3}} \Sigma^t$$

$$C_{RR} = \frac{h_1}{\sqrt{3} h_2} D + \frac{h_1 h_2}{4\sqrt{3}} \Sigma^t$$

(I.D./5)

I.D.(3)

In the three-dimensional case, if triangle STU is a distance h_3 below triangle PQR, the contributions are

$$\begin{aligned}
 C_{PQ} &= C_{QP} = C_{ST} = C_{TS} = \frac{(h_1 - 2h_2)h_3}{4\sqrt{3} h_1} D \\
 C_{PR} &= C_{RP} = C_{SU} = C_{US} = \frac{(h_2 - 2h_1)h_3}{4\sqrt{3} h_2} D \\
 C_{QR} &= C_{RQ} = C_{TU} = C_{UT} = -\frac{h_3}{4\sqrt{3}} D \\
 C_{PS} &= C_{SP} = C_{QT} = C_{TQ} = C_{RU} = C_{UR} = -\frac{h_1 h_2}{4\sqrt{3} h_3} D \quad (\text{I.D./6}) \\
 C_{PP} &= C_{SS} = \frac{(h_1^2 + h_2^2 - h_1 h_2)h_3}{2\sqrt{3} h_1 h_2} D + \frac{h_1 h_2 h_3}{8\sqrt{3}} \Sigma^t - C_{PS} \\
 C_{QQ} &= C_{TT} = \frac{h_2 h_3}{2\sqrt{3} h_1} D + \frac{h_1 h_2 h_3}{8\sqrt{3}} \Sigma^t - C_{QT} \\
 C_{RR} &= C_{UU} = \frac{h_1 h_3}{2\sqrt{3} h_2} D + \frac{h_1 h_2 h_3}{8\sqrt{3}} \Sigma^t - C_{RU}
 \end{aligned}$$

The one-dimensional group equations are solved by Gauss elimination and the two-dimensional equations are solved using a single-line cyclic Chebyshev semi-iterative technique (Reference 4). A block Gauss-Seidel procedure is used in three dimensions, each block consisting of a single plane, with the equations for a plane solved by the same technique as used in two dimensions. The outer iterations are accelerated by extrapolating the group fluxes using a procedure based on Chebyshev polynomials. This extrapolation and the inner-outer iteration strategy are described in Reference 5.

I.E. PROGRAMMING (1/67)

PDQ-7 is written almost entirely in FORTRAN IV. The program includes six ASCENT subroutines but less efficient FORTRAN versions are provided for five of these. OPTION, the exclusively ASCENT routine, provides shift and extract capability required by the geometry picture edits. MOVE is a storage move routine, FINDIT and FINDER are identical routines in different overlays which search a table of edit specifications, and WNVERT and INVERT are the line inversion routines for the omega and iteration overlays.

The hardware and software environment assumed by the program is described in Reference 6. In particular, the SCOPE 2.0 operating system must be used, there must be four non-system disks, each on its own channel, and the central memory size must be at least 64K. Most of the routines of the FCHIP package are required, INPF is used for input conversion and processing, IFM is used for the storage and retrieval of permanent files, and FTB-3 is used for storage allocation and scratch input-output.

The sense switch options available through FCHIP are effective in PDQ-7. In particular, sense switch 2 causes the current outer iteration to be the last performed, sense switch 3 causes the current case to be the last executed, and sense switch 4 causes monitor information to be displayed at the console and entered in the dayfile. This information includes the time at which each overlay is loaded and the time, the current eigenvalue, and the expected final iteration number at the end of each outer iteration. Independent of sense switch 4, the case number is displayed at the beginning of each case and is set negative if this is the last case of the job.

The program contains a main overlay, twelve primary overlays, and four secondary overlays. Overall program control is vested in the main overlay, and the other overlays are loaded and executed through use of the NEXT routine. With the exception of trivial arrays, all storage allocation is performed in blank common under the control of FTB. Blank common is declared only in the main overlay and is given a length of one. When this overlay is loaded, the actual length of blank common is obtained from common block SIZE and passed to FTB. All primary overlays are loaded at blank common origin, and an FTB file (ID = 1) is reserved to hold these overlays. A special version

of the ORIGIN routine is used to adjust the length of this file after each overlay has been loaded.

The PDQ-7 routines in each overlay are listed below. The numbers in parentheses are the primary and secondary overlay levels. DMY0 is not executed but is used to force FCHIP and FTB routines into the main overlay, as DMY1 forces INP into the (1,0) overlay. DMY1, DMY2, DMY3, DMY51, DMY52, DMY101, and DMY102 are do-nothing routines which force loading of a primary or secondary overlay before storage is allocated in a higher level overlay.

(0,0)

PDQ07	ORIGIN	MOVE	DMYO
-------	--------	------	------

(1,0)

CNTINP	IFILES	CASENN	DMY1
--------	--------	--------	------

(2,0)

GEOCNT	GEOMIN	RECMSH	RECOVR	HEXMSH
HEXOVR	RECPIC	HEXPIC	PCUNPC	OPTION
EDTINP	DMY2			

(3,0)

DPLIN1	CHANE	FILER	PRID	INPID
NUCHN	CHLIST	INDEX1	PACK1	STOVFL
NUCON	UNFIT	UNPK1	OVLAY	PRERC1
OVERC	NC1C2	ITYPEC	NPACK2	TABCTL
CDTABS	MORDER	NPK2A	BUCKIN	REQTAB
MSKSCH	UNPK2	PROVER	INDEX2	DPLIN2
ARATIO	EXPCON	EXPFLX	DMY3	

(4,0)

SIGMA	TABLES	STORE1	STORE2	INTERP
STORE4	DECOD2	DECOD1	INTRP	STORE3
ENCOD1	ENCOD2	REGCMP	GEOMWD	LCHECK

(5,0)

COEF	SORT	NORM
------	------	------

(5,1)

COFROW	DELINT	SIGINT	DMY51
--------	--------	--------	-------

(5,2)

HEXROW	HEXDEL	HEXSIG	DMY52
--------	--------	--------	-------

(6,0)

OMEGA	WNNERS	WNVERT	WLLOC1	WLLOC2
WLLOC3	WLLOC4	WLLOC5	WCANDO	WNIT3D
WNDSTK	WAST3D	WUDGER	WCRI BR	WNPRNT
STRATG				

(7,0)

ITERAT	INITSC	GRPSRC	INNERS	OUTERS
EXTRAP	INVERT	TOTRUE	ALLOC1	ALLOC2
ALLOC3	ALLOC4	ALLOC5	INVT1D	PREDCT
INIT3D	ENDSTK	LAST3D	FUDGER	SCRIBR
INPRNT	DELCPL	MONFOR		

(8,0)

INTEDT	JCHECK	FINDRG	SIGEDT	RECINT
PLNSET	EDFLUX	EDKSF	EDSIGA	KINFIN
KEFFEC	INDBUC	DEPBUC	AVERAG	EDFLWT
EDITAL	FINDER	SPACIT	FLUXAV	INTEG

(9,0)

DEPLET	PACKER	STORE5	INTVAL	DOINTR
DECOD4	DECOD3	INTPRT	ENCOD3	ENCOD4
RATES1	DEPLT1	DEPLT2	EDITRT	EDITNS
DOEDTN	DOEDTR	SETPLN	FINDIT	WDGEOM
KCHECK	CMPREG	SPACER		

(10,0)

EDITCON	NUMPIC	FINDB	PTPART	FIXFOR
---------	--------	-------	--------	--------

(10,1)

POWER1	POWER2	EDIT1D	POWER3	POWER4
RMAX2	DMY101			

(10,2)

POWER5	POWER6	RMAX3	DMY102	
--------	--------	-------	--------	--

(11,0)

OFFILES

(15,0)

CONCEDT

EDT1ID

DSPLPG

BLKDAT

II.A.1. REGIONS OF SOLUTION (5/66)

The available geometries are rectangular, cylindrical, and spherical in one dimension; rectangular, cylindrical, and hexagonal in two dimensions; and rectangular and hexagonal in three dimensions. The two-dimensional regions of solution will be described first, and the one-dimensional and three-dimensional will be derived from these.

For rectangular and cylindrical geometry, the region of solution is a rectangle of the x-y or r-z plane. The axes of the coordinate system coincide with boundary lines of the rectangle. As shown in Figure (II.A.1./1), the origin is placed in the upper left corner, column numbers increase to the right along the x axis (r axis), and row numbers increase downward along the y axis (z axis).

The hexagonal region of solution is a 120° chevron in the x-y plane. The chevron is oriented as in Figure (II.A.1./2), with column numbers increasing to the right and row numbers increasing downward. The rows bend through a 60° angle at the diagonal column of the chevron. The first and last rows are considered the top and bottom boundaries, and the first and last columns are the left and right boundaries.

Zero flux, zero current, and fixed flux conditions may be applied along each boundary of both regions of solution. In addition, a rotational symmetry condition may be applied along the top boundary. The program imposes this condition by forcing the flux values on this boundary to be symmetric about the midpoint and the current values to be symmetric in magnitude but opposite in sign. The rotational symmetry condition is 180° in rectangular geometry and 120° in hexagonal geometry, and in the latter case the chevron must be symmetric, with an equal number of intervals on each side of the diagonal column.

For geometry purposes, one-dimensional problems are treated as two-dimensional problems with only two rows, zero and one. Three-dimensional problems are oriented with plane numbers increasing downward along the z axis. The top plane is plane zero, the bottom plane is the plane boundary, and each may have a zero flux, zero current, or fixed flux boundary condition.

(II.A.1./1)

(II.A.1./2)

II.A.1.(2)

II.A.2. MESH DESCRIPTION (5/66)

The row and column intersections in Figures (II.A.1./1) and (II.A.1./2) are the mesh points at which the flux solution is obtained. Figure (II.A.1./1) also determines an array of mesh rectangles and Figure (II.A.1./2) an array of mesh parallelograms, the latter cut along the short diagonal to form mesh triangles. The purpose of the mesh description is to specify the location of all mesh points and also the location of all internal boundaries, or interfaces. Note that interfaces are composed of line segments which are the boundaries of mesh rectangles or mesh triangles.

The fundamental entities of a mesh description are basic figures. Basic figures are rectangles in rectangular geometry and 60° parallelograms in hexagonal geometry, oriented as in Figures (II.A.2./1) and (II.A.2./2). (Cylindrical and spherical geometries are not considered here since their mesh descriptions are identical to rectangular geometry.) Note that each basic figure has its origin at row 0, column 0 and has its own row and column boundaries.

A basic figure is described by giving a planar region overlay together with sequences of mesh intervals along both row 0 and column 0. The planar region overlay consists of a series of overlay sets, each of which superimposes a particular planar region number throughout a specified rectangle (parallelogram) of the mesh. The sets are processed sequentially and any set may overlay areas of the mesh specified in previous sets. Every mesh figure (rectangle or parallelogram) must be included within at least one of the overlay sets and for each mesh figure, the last overlay set which includes the figure determines its planar region number. As an example, Figures (II.A.2./1) and (II.A.2./2) may both be described by overlaying region 1 on the entire mesh; region 3 between columns 1 and 3, rows 2 and 4; region 2 between columns 2 and 4, rows 0 and 3; and region 3 between columns 3 and 4, rows 0 and 1.

Basic figures are numbered sequentially from 01 to 99. An auxiliary figure is obtained by modifying the planar region overlay of a basic figure. If two or more rectangles (parallelograms) have the same mesh but different overlays, the use of auxiliary figures makes it unnecessary to repeat the mesh interval specification. The auxiliary figures for a particular basic figure are numbered sequentially from 1 to 9, and the basic figure itself is assigned auxiliary figure

number 0. A basic figure number followed by an auxiliary figure number identifies an initial figure. Initial figure numbers thus range from 010 to 999.

The region of solution (rectangle or chevron) is described by means of a final figure overlay. This consists of a series of overlay sets, each of which superimposes a particular initial figure on the solution region. The initial figure is positioned by giving the row and column of the solution region at which the initial figure origin is to be placed and the angle through which the initial figure is to be clockwise rotated. The angle must be a multiple of 90° in rectangular geometry and a multiple of 60° in hexagonal geometry. The initial figure also may be reflected, which implies an interchange of rows and columns. The rotational orientations of two initial figures are shown in Figures (II.A.2./3) and (II.A.2./5), and the reflections of these figures are shown in Figures (II.A.2./4) and (II.A.2./6). In all cases the origins are at the center.

As in the planar region overlay, the final figure overlay is sequential and may overlay areas of the solution region which have been specified previously. Any portion of an initial figure which extends outside the solution boundaries is ignored, and initial figure origins may actually be located outside these boundaries. No part of the solution region may remain unspecified when the overlay is complete. If there is rotational symmetry, the mesh intervals along row 0 must be symmetric about the midpoint in rectangular geometry, symmetric about the diagonal column in hexagonal geometry.

A final figure number is associated with each initial figure overlay of the solution region. This permits the various overlays by a particular initial figure to be distinguished for editing purposes. Final figure numbers may range from 01 to 99 but need not be sequential or distinct. Note that the final figure overlay actually assigns two numbers to each mesh rectangle or mesh triangle - a final figure number and a planar region number.

The fundamental restriction on the final figure overlay is that the mesh in the initial figures must be so chosen that rows and columns in adjoining initial figures meet at common boundary points. (This need not be true at every stage of the overlay but only when the overlay is complete.) It is important to note a significant difference between rectangular and hexagonal geometry. In rectangular geometry the final figure overlay determines the spacing of the rows and columns in Figure (II.A.1./1) but does not change their orientation. In

addition, all interfaces coincide with these rows and columns. In hexagonal geometry, on the other hand, the final figure overlay may cause the rows and columns of Figure (II.A.1./2) to bend at various mesh points. Furthermore, interfaces may coincide with the parrallelogram diagonals. The examples in Section II.A.3. make these distinctions between the two geometries more evident.

In a three-dimensional problem, all planar interfaces are projected onto a single plane which is then described as specified above. The only other mesh information required is the sequence of mesh intervals along the z axis.

(II.A.2./1)

(II.A.2./2)

II.A.2.(4)

(II.A.2./3)

(II.A.2./4)

II.A.2.(5)

(II, A. 2. /5)

(II, A. 2. /6)

II.A.3. GEOMETRY EXAMPLES (5/66)

Figure (II.A.3./1) represents one-fourth of a rectangular array and Figure (II.A.3./4) represents one-third of an hexagonal array. Mesh points have been added in Figures (II.A.3./2) and (II.A.3./5), and the dotted lines are present to aid in the overlay. Note that the rows and columns in adjoining figures all meet at common boundary points. As a result, some of the figures contain more rows and columns than are required to describe their interfaces.

All of the initial figures required for the rectangular overlay are shown in Figure (II.A.3./3). Note that (b) and (d) are auxiliary figures of the same basic figure. The overlay may be accomplished in the following steps.

<u>Initial Figure</u>	<u>Origin (Column, Row)</u>	<u>Rotation</u>
a	0,0	0°
a	4,4	90°
a	4,4	270°
b	4,8	90°
b	8,4	270° Reflected
a	8,8	180°
d	8,8	90°
d	8,4	0°
c	8,8	0°
e	0,11	0° Reflected
e	11,0	0°

The initial figures required for the hexagonal overlay are shown in Figure (II.A.3./6). Here, (c) and (e) are auxiliary figures of the same basic figure. In order to locate the initial figure origins, it is convenient to construct a unitized mesh, Figure (II.A.3./7), in which all mesh intervals have been set to unity. This figure clearly displays the rows and columns of the chevron, which are obscured in Figure (II.A.3./5) because of the variable mesh. The overlay may be performed as follows.

<u>Initial Figure</u>	<u>Origin (Column, Row)</u>	<u>Rotation</u>
a	6,0	60° Reflected
a	10,0	0°
b	12,0	120°
d	4,3	180°
d	15,-3	60°
c	4,0	0° Reflected
c	12,0	60°
d	4,6	180°
d	15,0	60°
e	4,3	0° Reflected
e	12,3	60°

(II.A.3./1)

(II.A.3./2)

II.A.3.(3)

(a)

(b)

(c)

(d)

(e)

(II.A.3./3)

(II.A.3./4)

(II.A.3./5)

(II.A.3./6)

(II.A.3./7)

II.A.4. DEPLETION BLOCKS - COMPOSITIONS (5/66)

The depletion block is the basic planar mesh unit for depletion and editing purposes. Nuclide concentrations are carried by depletion block and all integration editing is performed over sets of depletion blocks. In the case of point depletion, every mesh rectangle (mesh triangle) is a separate depletion block. In the case of block depletion, each unique final figure - planar region pair is a separate depletion block. Note that a nondepletable problem is treated as a block depletion problem for editing purposes. Note also, in the case of block depletion, that there is no requirement that a depletion block be connected.

The depletion plane is the basic axial mesh unit for depletion and editing purposes. Every depletion plane has an identical array of depletion blocks and integration editing is performed over sets of depletion planes. In the case of point depletion, every mesh plane is a separate depletion plane. In the case of block depletion, the axial points which determine the depletion plane boundaries must be specified. Note that every mesh figure is included in some depletion block and every mesh plane in some depletion plane; the terms "depletion block" and "depletion plane" do not imply that each of these is actually depleted.

A composition number identifies a specific combination of chain list, table set, and initial nuclide concentrations which is to be used in a particular region of the mesh. The placement of compositions is described by assigning a composition number to each final figure or to each planar region. Thus, every depletion block is a single composition. A planar region correspondence is normally used; the final figure correspondence is useful only when each final figure is a single homogenized composition. In a three-dimensional problem the composition correspondence may be different in each depletion plane.

II.A.5. MESH LIMITATIONS (1/67)

The following table gives the column boundary limit for various types of problems.

<u>Number of Dimensions</u>	<u>Number of Thermal Groups</u>	<u>Hexagonal Geometry</u>	<u>Column Bdry. Limit</u>
1	1	No	492
1	2	No	393
2	1	No	492
2	1	Yes	327
2	2	No	138
2	2	Yes	107
3	1	No	327
3	1	Yes	244

No specific limitations are imposed on the row and plane boundaries. However, the inner iteration procedure used in three-dimensional problems may fail to converge if the planes are closely spaced and hence tightly coupled.

Core and disk storage are allocated dynamically during program execution. This increases the range of problems which may be handled, but the restrictions on total problem size become rather complex. In two-dimensional problems, core storage imposes no restriction in the case of point depletion but limits the number of depletion blocks to about 3000 in the case of block depletion. In three-dimensional point depletion problems, the limitation is about 3500 points per plane in rectangular geometry and half this value in hexagonal geometry. In three-dimensional block depletion problems, the sum of the number of points per plane (twice this number in hexagonal geometry) and eight times the number of depletion blocks per plane cannot exceed about 16,000. With 1000 depletion blocks, the limitation is thus about 8000 points per plane in rectangular geometry and half this value in hexagonal geometry.

The restrictions imposed by disk storage are independent of dimensionality. In block depletion problems, the product of groups and total points is limited to about 600,000. In point depletion problems, this limit is

reduced to 300,000 for rectangular geometry and 200,000 for hexagonal geometry. Point depletion also restricts the product of nuclides and total points to about 1,500,000 in rectangular geometry and to half this value in hexagonal geometry.

II.B.1. INTEGRATION EDITS (5/66)

The integration editing includes flux integrals, power fractions, absorption rates, fission rates, group-dependent and group-independent bucklings, K^∞ and K^{eff} , average and flux-weighted average macroscopic parameters, and average nuclide concentrations.

An edit set is a collection of final figure numbers together with a collection of planar region numbers. Each edit set defines a region of the mesh, not necessarily connected, which is to be treated as a unit for integration editing purposes. A particular mesh figure (rectangle or triangle) belongs to each edit set whose definition includes both the final figure number and the planar region number of the mesh figure. Every integral quantity is calculated for each edit set in each depletion plane. Note that the edit sets are the same in every depletion plane since they depend only upon final figures and planar regions.

A plane grouping is a collection of depletion planes, not necessarily connected, which is to be treated as an axial editing unit. Note that a particular depletion plane may belong to any number of plane groupings. All edit sets are summed over the planes comprising a plane grouping before being printed. Thus, to identify the region of integration for a single printed quantity requires a list of final figures, a list of planar regions, and a list of depletion planes. The program solves this identification problem by numbering both the edit sets and the plane groupings. The definition of each of these is printed once, and integral quantities are then identified by edit set number and plane grouping number.

II.B.2. INTEGRAL APPROXIMATIONS (1/67)

The integral of any quantity over a region of the mesh is calculated by summing the integrals for the individual mesh figures comprising the region. Further, since all macroscopic parameters are constant within a mesh figure, the mesh figure integral of $\Sigma\phi$ is simply $\Sigma\int\phi$.

In rectangular and hexagonal geometry, the flux integral for a mesh figure is approximated by the numerical average of the flux values at the vertices multiplied by the length, area, or volume of the figure. In cylindrical geometry, the one-dimensional integral is approximated by

$$\begin{aligned} \int_{r_1}^{r_2=r_1+h} \phi(r) dV &\doteq 2\pi \left\{ \frac{h}{2} [r_1\phi(r_1) + r_2\phi(r_2)] \right. \\ &\quad \left. + \frac{h^2}{6} [\phi(r_1) - \phi(r_2)] \right\} \end{aligned} \quad (\text{II.B.2./1})$$

and the two-dimensional integral is obtained by averaging the integrals along the top and bottom of a mesh rectangle and multiplying by its height. Finally, the spherical geometry integral is approximated by

$$\begin{aligned} \int_{r_1}^{r_2=r_1+h} \phi(r) dV &\doteq 4\pi \left\{ \frac{h}{2} [r_1^2\phi(r_1) + r_2^2\phi(r_2)] \right. \\ &\quad \left. + \frac{h^2}{3} [r_1\phi(r_1) - r_2\phi(r_2)] + \frac{h^3}{12} [\phi(r_1) + \phi(r_2)] \right\}. \end{aligned} \quad (\text{II.B.2./2})$$

For depletion purposes, the average flux in a depletion block is $\int\phi dV/\int dV$, where the integrals are evaluated as indicated above.

II.B.3. POINTWISE EDITS (1/67)

All pointwise editing is done over three regions of the mesh, the first for flux, the second for power, and the third for concentrations. Editing of each pointwise quantity is optional, including the flux in each group, the total thermal flux in a two-thermal-group problem, the partition power, the point power, and the initial and final concentrations for each nuclide. Partition power consists of a value for each mesh figure at each point and is printed only for those points at which any two nonzero values differ by more than 5%. There are two partition values per point in one dimension, four or six values per point in two dimensions, and eight or twelve values per point in three dimensions. Point power may be edited either as the average of the nonzero partition values at a point or as the largest of these values. In either case a relative maximum edit may also be obtained which identifies each point at which the power exceeds the value at any of its neighbors.

II.C.1. INPUT AND OUTPUT FILES (1/67)

Permanent files are stored and retrieved through the IFM File Manager system (Reference 6). Briefly, this system permits a program to process files in terms of their logical structure, with no knowledge of the physical format of the files required. File processing is also independent of the physical device used, which may be either a magnetic tape or a collection of disk tracks reserved for IFM use.

Three levels of identification are associated with each file: the seven-character job ID of the job creating the file, a file ID of up to ten characters supplied as input by the user, and a file type number supplied by the program. Thus, files created in different jobs are distinguished by job ID, files created in different cases of the same job are distinguished by file ID, and files created in the same case are distinguished by type number.

PDQ-7 will accept flux, concentration, geometry, and HARMONY table-set files as input and will store flux, concentration, power, integral, and geometry files for subsequent use. Input files are retrieved near the beginning of a case, and a comment is added to the printed output after each file has been successfully read. Because of the inefficiencies involved in searching tape, input files are required to be on disk. An auxiliary program incorporating IFM may be used to move such files from tape to disk.

An input flux file must be compatible with the current problem in number of groups, column boundary, row boundary, and plane boundary. Boundary value problems may only be run by creating a file containing the proper boundary values in an auxiliary program. If an input flux file is not used, the flux is set to zero at all zero flux boundary points and to one everywhere else.

An input concentration file must be compatible in number of nuclides, number of depletion blocks, and number of depletion planes. In addition, the order in which the nuclides are listed in the input and the location and size of the depletion blocks must not be changed. In the case of block depletion, since the user has no control over the ordering of depletion blocks, the problem generating a concentration file and the problem using this file must have identical geometry descriptions.

An input geometry file must be compatible in geometry type, column boundary, row boundary, plane boundary, diagonal column, row 0 boundary condition (if rotational symmetry), largest final figure and planar region numbers, and point/block depletion indicator. When this option is used, picture edit requests are ignored and any geometry cards present (including region areas) are deleted from the input deck. However, if the composition correspondence is not one-to-one, the cards defining this correspondence must be present.

Output files are saved at the very end of a case and each may be stored on tape or disk or both. Positioning of the tape over all previously written files is done during the running of the case and causes no inefficiency. A comment is added to the output after each file has been successfully written on either device. Thus, if there is a failure during filing, the comments indicate which files had been saved before the error occurred. In the case of a tape failure, an attempt should not be made to write on the tape in any subsequent job. After all filing has been done, the total length which has been used on the reel of tape is included in the output. If this exceeds 2000 feet^{*}, no further additions should be made to the tape. Note that there is no provision in the program for using more than one reel of tape in a single job. If the total tape output of all cases of a job will exceed 2000 feet, the cases must be separated into two or more distinct jobs.

In general, disk may be used only for short-term communication of files and tape must be used for their long-term retention. If this strategy is not carefully followed, the disks quickly become saturated and lose their effectiveness. In an attempt to promote this strategy, the program examines disk usage at the end of each case after all filing has been successfully done. If a flux, concentration, or geometry file has been saved on disk in this case and if the same type of file was input from disk, the input file is automatically deleted. In addition, card input to the program permits the user to request such file deletion in the case that output files are not saved on disk.

*The length calculation assumes that tape is written at a density of 800 bits per inch. If the actual density is 556, the printed length must be increased by 45%

II.C.2. PROGRAMMING AUXILIARY ROUTINES (10/66)

It is occasionally necessary for a user to program an auxiliary routine which processes the files generated by PDQ-7. To facilitate this, Sections II.C.3.-II.C.7. contain detailed descriptions of the flux, concentration, power, integral, and geometry file formats. The present section defines the symbols used in describing these formats and contains general information required for the processing of any file.

IFM files are subdivided into sets of data, and the set structure of a file is fundamental to its processing. Three different set structures are provided by IFM and each is used for one or more PDQ-7 files. In the first structure, the set size is constant and the total number of sets is known in advance. The set size and number of sets are then given to IFM before the file is written and are returned by IFM before the file is read. In the second structure, the set size is constant but the number of sets is not known in advance. In this case the number of sets given to IFM and returned by IFM is zero. The writing program must indicate when it has written the last set and the reading program must recognize when the last set has been read. In the third structure, the set size is variable in which case it is assumed that the number of sets is not known. Here, the size of each set must be given to IFM as the set is written and is returned by IFM as the set is read.

The data filed by PDQ-7 is compressed by two different techniques, called pack and sqoz. Pack refers to the storing of several integer items in a single computer word, each item occupying a fixed set of bit positions. Sqoz refers to the storing of two floating-point quantities in a single word by decreasing the number of significant digits and the exponent range of each. A set of FORTRAN-CALLable subroutines is available to pack and sqoz and perform the inverse operations. The statements

```
CALL PACK (WORD, NOITMS, NOBITS, ITEMS)
CALL UNPACK (WORD, NOITMS, NOBITS, ITEMS)
```

may be used to pack (unpack) items into (from) a single computer word. Here WORD is the packed word, NOITMS is the number of items to pack (unpack), NOBITS is an array giving the number of bits for each item, and ITEMS is an

array containing (to be filled with) data items. Similarly, the statements

```
CALL SQOZ (SQZWDS, FPTWDS, NWORDS)
```

```
CALL UNSQOZ (SQZWDS, FPTWDS, NWORDS)
```

may be used to compress (expand) an array of floating-point words into (from) an array of sqoz words. Here SQZWDS is the array of sqoz words, FPTWDS the array of floating-point words, and NWORDS the number of floating-point words.

The table below defines the various symbols used in the file descriptions.

<u>Symbol</u>	<u>Definition</u>
ABSNUC	Number of nuclides for absorption rate edit
BDCOND	Array of six words containing boundary conditions along column 0, column COLBDY, row 0, row ROWBDY, plane 0, and plane PLNBDY (-1 = rotational symmetry, 0 = zero flux, +1 = zero current, +2 = fixed flux)
COLBDY	Column boundary
COLS	Total number of columns (COLBDY + 1)
CONCES	Last edit set for which average nuclide concentrations edited
CONNUC	Number of nuclides for average concentration edit
CORRES	Composition correspondence (1 = composition to figure, 2 = composition to region)
DIAG	Diagonal column (0 if not hexagonal geometry)
DPLBLK	Number of depletion blocks in each depletion plane (total number of mesh rectangles or mesh triangles per plane if point depletion)
DPLPLN	Number of depletion planes (1 if 1-D or 2-D)
EDTSTS	Total number of edit sets
EDTWDS	Number of words required to describe the edit sets
FISNUC	Number of nuclides for fission rate edit
FLUXES	Last edit set for which flux integrals and flux-weighted macroscopic data edited

<u>Symbol</u>	<u>Definition</u>
FNORM	Flux normalization factor
GEOM	Geometry (1 = rectangular, 2 = cylindrical, 3 = spherical, 4 = hexagonal)
GROUPS	Total number of groups
MAXCMP	Largest input composition number
MAXFIG	Largest input final figure number
MAXREG	Largest input planar region number
NUCLDS	Number of nuclides
PLANES	Total number of planes (1 if 1-D or 2-D, PLNBDY + 1 if 3-D)
PLNBDY	Plane boundary (1 if 1-D or 2-D)
PNORM	Power normalization factor
PNTBLK	Point/block depletion (1 = point, 2 = block)
PNTFIG	Number of mesh figures at a point (2 if 1-D, 4 if 2-D non-hexagonal, 6 if 2-D hexagonal, 8 if 3-D rectangular, 12 if 3-D hexagonal)
POWINT	Power integral (denominator of FNORM and PNORM)
POWNUC	Number of nuclides for power fraction edit
RATEES	Last edit set for which nuclide power fractions, absorption rates, and fission rates edited
ROWBDY	Row boundary (1 if 1-D)
ROWS	Total number of rows (1 if 1-D, ROWBDY + 1 if 2-D or 3-D)
THGRPS	Number of thermal groups (1 or 2)

II.C.3. FLUX FILE (10/66)

Type number = 220

Set size = $\max[5, (\text{COLS} + 1)/2]$

Number of sets = $1 + \text{ROWS} \star \text{PLANES} \star \text{GROUPS}$

The first set of this file contains the following information.

<u>Word</u>	<u>Value</u>
1	COLS
2	ROWS
3	PLANES
4	GROUPS
5	FNORM

Each of the remaining sets contains the flux values for a single row of the mesh. The sets are ordered by row, then by plane, and finally by group. Within a set there are COLS values in sqoz format, requiring $[(\text{COLS} + 1)/2]$ compressed words. The flux values are not normalized.

II.C.4. CONCENTRATION FILE (10/66)

Type number = 221

Set size = $\max[5, (\text{NUCLDS} + 1)/2 + 1]$

Number of sets = 0

The first set of this file contains the following information.

<u>Word</u>	<u>Value</u>
1	NUCLDS
2	PNTBLK
3	DPLBLK
4	DPLPLN
5	POWINT

The second and third sets contain the numeric nuclide ID's and the fourth and fifth sets contain the alphanumeric ID's. More specifically, if the third (fifth) set is appended to the second (fourth), the first NUCLDS values in the resulting array are the nuclide ID's. These ID's are in the same order as specified in the input and this is the order in which the concentrations are carried in subsequent sets.

Each of the remaining sets contains the concentration values for a single depletion block together with a skip indicator. The sets are ordered by depletion block, then by depletion plane. Not all depletion blocks are carried in the file, however. The first block is always carried but each of the remaining blocks is carried only if one or more of its concentration values is nonzero. The skip indicator in each set gives the number (≥ 0) of depletion blocks following the current block which have been omitted from the file. Zero concentrations must be supplied for these blocks as the file is read. Within each set there are NUCLDS concentration values in sqoz format, requiring $[(\text{NUCLDS} + 1)/2]$ compressed words, followed by an integer word containing the skip indicator.

II.C.5. PARTITION POWER FILE (10/66)

Type number = 222

Set size = $\max[4, (\text{PNTFIG}/2) \star \text{COLS}]$

Number of sets = $1 + \text{ROWS} \star \text{PLANES}$

The first set of this file contains the following information.

<u>Word</u>	<u>Value</u>
1	PNTFIG
2	COLS
3	ROWS
4	PLANES

Each of the remaining sets contains the partition power values for a single row of the mesh. The sets are ordered by row, then by plane. Within a set there are PNTFIG values in sqoz format at each of COLS points, requiring $[(\text{PNTFIG}/2) \star \text{COLS}]$ compressed words. The power values are normalized by PNORM.

In a one-dimensional problem the order of the values at a point is left followed by right. In a two-dimensional problem it is upper left, upper right, lower left, and lower right except for hexagonal geometry, where the order is as indicated in Figure (II.C.5./1). Finally, in a three-dimensional problem, the four or six values above the plane are ordered as in a two-dimensional problem and are followed by the corresponding values below the plane.

(II.C.5./1)

II.C.5.(2)

II.C.6. INTEGRAL FILE (1/67)

Type number = 224

Variable set size

The size of the first set is 13 words and it contains the following information.

<u>Word</u>	<u>Value</u>
1	DPLPLN
2	GROUPS
3	THGRPS
4	EDTSTS
5	EDTWDS
6	FLUXES
7	RATEES
8	CONCES
9	POWNUC
10	ABSNUC
11	FISNUC
12	CONNUC
13	FNORM

The edit set descriptions appear next in the file. The total of EDTWDS words is arranged in 1980-word sets, with the last set reduced in size to the number of words remaining. The description for each edit set consists of a sequence of final figure numbers and a zero followed by a sequence of planar region numbers and a zero. Each sequence is in order of increasing absolute value, with a negative number indicating the previous value through the negative value.

The remainder of the file consists primarily of three collections of integral data. Within each collection the data is ordered by edit set, then by depletion plane. Since the data for each set is in sqoz format, the set size is obtained by adding 1 to the number of values in a set and then dividing by 2.

There are (FLUXES * DPLPLN) sets in the first collection, each containing the volume, flux integrals, and macro-flux integrals for a single edit set. The data for a set consists of

$$\int dV, \int \phi_1 dV, \int \phi_2 dV, \dots, \int \phi_G dV$$

followed by

$$\int D_g \phi_g dV, \int \Sigma_g^a \phi_g dV, \int \Sigma_g^r \phi_g dV, \int \Sigma_g^f \phi_g dV, \int \kappa \Sigma_g^f \phi_g dV, \int \Sigma_g^t \phi_g dV$$

for each group g . If THGRPS = 2, the above quantities are replaced, in groups $G-1$ and G , by

$$\int D_{G-1}^1 \phi_{G-1} dV, \int D_{G-1}^2 \phi_G dV, \int \Sigma_{G-1}^1 \phi_{G-1} dV, \int \Sigma_{G-1}^2 \phi_G dV, \int \Sigma_{G-1}^f \phi_{G-1} dV, \\ \int \kappa \Sigma_{G-1}^f \phi_{G-1} dV, \int (\Sigma_{G-1}^{t1} \phi_{G-1} + \Sigma_{G-1}^{t2} \phi_G) dV, \int R_{G-1} \Sigma_{G-2}^r \phi_{G-2} dV$$

and

$$\int D_G^1 \phi_G dV, \int D_G^2 \phi_{G-1} dV, \int \Sigma_G^1 \phi_G dV, \int \Sigma_G^2 \phi_{G-1} dV, \int \Sigma_G^f \phi_G dV, \\ \int \kappa \Sigma_G^f \phi_G dV, \int (\Sigma_G^{t1} \phi_G + \Sigma_G^{t2} \phi_{G-1}) dV, \int R_G \Sigma_{G-2}^r \phi_{G-2} dV, \\ \int \Sigma_{G-1}^{t2} \phi_G dV, \int \Sigma_G^{t2} \phi_{G-1} dV$$

The total number of values per set is $[1 + \text{GROUPS} + 6 * (\text{GROUPS} + \text{THGRPS} - 1)]$. Note that the fluxes used in these integrations are not normalized. Note also that $\int \Sigma_g^f \phi_g dV$ is replaced by $\int S_g \phi_g dV$ in a fixed source problem.

The second collection is present only if at least one of POWNUC, ABSNUC, and FISNUC is nonzero. If present, it is preceded by a set of length $(\text{POWNUC} + \text{ABSNUC} + \text{FISNUC})$ which contains the numeric nuclide ID's for the power fraction, absorption rate, and fission rate edits. The ID's are in the same order as specified in the input and this is the order in which the nuclide integrals are carried.

There are $(\text{RATEES} * \text{DPLPLN})$ sets in the second collection, each containing the power, absorption rate, and fission rate values for a single edit set. The data for a set consists of

$$\int \kappa_i^g \sigma_i^f, \epsilon_{G_i}^f, \epsilon_{N_i}^f \phi_g dV$$

for all groups g , then all power fraction nuclides i , followed by

$$\int \sigma_i^a, \epsilon_{G_i}^a, \epsilon_{N_i}^a \phi_g dV$$

for all groups g , then all absorption rate nuclides i , followed by

$$\int \sigma_i^f, \epsilon_{G_i}^f, \epsilon_{N_i}^f \phi_g dV$$

for all groups g , then all fission rate nuclides i . The total number of values per set is $[\text{GROUPS} * (\text{POWNUC} + \text{ABSNUC} + \text{FISNUC})]$, and the fluxes used in these integrations are normalized by $(\text{FNORM}/10^{24})$.

The third collection is present only if CONNUC is nonzero. If present, it is preceded by a set of length CONNUC which contains the numeric nuclide ID's for the average concentration edit. The ID's are in the same order as specified in the input and this is the order in which the concentration integrals are carried.

There are $(\text{CONCES} * \text{DPLPLN})$ sets in the third collection, each containing the volume and the concentration integrals for a single edit set. The data for a set consists of

$$\int dV$$

followed by

$$\int N_i dV$$

for each average concentration nuclide i . The total number of values per set is $(1 + \text{CONNUC})$.

II.C.7. GEOMETRY FILE (10/66)

Type number = 225

Variable set size

The size of the first set is 18 words and it contains the following information.

<u>Word</u>	<u>Value</u>
1	GEOM
2	COLBDY
3	ROWBDY
4	PLNBDY
5	DIAG
6-11	BDCOND
12	MAXCMP
13	MAXFIG
14	MAXREG
15	CORRES
16	PNTBLK
17	DPLBLK
18	DPLPLN

The second set is of length (COLBDY + ROWBDY + PLNBDY) and contains the column mesh intervals followed by the row intervals followed by the plane intervals (all in centimeters). A single row interval of unity is carried in 1-D problems and a single plane interval of unity is carried in both 1-D and 2-D problems. In hexagonal geometry there actually are no column and row intervals. The distance between two adjacent columns, for example, may change from row to row. As a result, the first (COLBDY + ROWBDY) locations in this set are used to store all the distinct triangle side lengths. Any of these locations not required for this purpose are set to zero. The particular side lengths to be associated with each triangle are then specified in the mesh figure descriptions beginning in set five.

The third set contains the composition correspondence by depletion plane. The correspondence gives the composition number of each final figure if CORRES = 1 and of each planar region if CORRES = 2. Thus, there are either MAXFIG or MAXREG composition numbers for each plane. These numbers are carried in pack format, with six numbers per computer word and seven bits per number. Each depletion plane begins a new packed word, giving a total set size of $\{[(N+5)/6] * DPLPLN\}$, where N is MAXFIG or MAXREG.

The fourth set is of length DPLPLN and contains the depletion plane boundaries. The plane numbers are in increasing order and the last number is PLNBDY. A single value of 1 is carried in both 1-D and 2-D problems.

Each of the next ROWBDY sets contains the mesh figure descriptions for a single row of figures. There are (2 * COLBDY) mesh triangles per row in hexagonal geometry and COLBDY mesh rectangles per row in all other geometries. Since a single packed word is carried for each mesh figure, the set size is the number of figures in a row. The packed word consists of six items, as follows.

<u>Item</u>	<u>Value</u>	<u>No. of Bits</u>
1	Final figure number	7
2	Planar region number	7
3	Vertex number	2
4	Left side length index	10
5	Right side length index	10
6	Depletion block number	24

Items 3-5 are zero in all but hexagonal problems and item 6 is zero unless PNTBLK = 2. Item 3 specifies the location of the 60° vertex in each triangle, where the vertices are numbered as follows.

If the triangle is equilateral, any one of the three may be designated the 60° vertex. Note that the first and last triangles in every row are upward pointing and that the two types alternate across the row except at the diagonal column. Items 4 and 5 are the indices of two side length values in the mesh interval array (set 2). These values are the lengths of the sides which form the 60° angle. Item 4 indexes the left value and item 5 the right value, where left and right are determined by looking from the vertex toward the center of the triangle.

The remaining sets contain the depletion block descriptions and are present only if PNTBLK = 2. A pair of words is carried for each of depletion blocks 1,2,...,DPLBLK. The first word of each pair contains the final figure and planar region numbers packed as in the mesh figure descriptions, and the second word is the planar area of the depletion block. The total of $(2 \star \text{DPLBLK})$ words is arranged in 1980-word sets, with the last set reduced in size to the number of words remaining.

III.A.1. SYSTEM CONTROL CARDS (1/67)

All system control cards are punched beginning in column 1. The first card of every input deck is a job card whose format is as follows.

<u>Fields 1-8</u>	<u>No. of Columns</u>
Job ID	7
Priority	1
Run Time Limit	5
Field Length (154000)	6
Program Name (PDQ07)	5
User Name	5
Classification (U/C)	1
Charge Classification	1

The fields are separated by commas, except that there is a period between the field length and program name. There is also a period following the charge classification which brings the total number of columns to 39.

The first four columns of the job ID identify the user for accounting purposes, and the last three columns are the job sequence number for this user. It is advisable that every job have a unique ID. The following table gives the octal conversions (rounded) for typical running times.

<u>Minutes</u>	<u>Hours</u>
1 - 00100	1.0 - 07000
2 - 00200	1.5 - 12400
5 - 00500	2.0 - 16000
10 - 01200	2.5 - 21400
15 - 01600	3.0 - 25000
20 - 02300	4.0 - 34000
30 - 03400	5.0 - 43000
45 - 05200	

If a filetype is required, a request card must immediately follow the job card. An assigned filetype is requested via

REQUEST FILE1.Rxxxx.

and a blank is requested via

REQUEST FILE1.BLANK.

Note that there must be a blank column following the word REQUEST but that there may be no other blank columns until after the second period.

A task card of the form

TASK (PDQ07)

or

TASK (PDQ07,1)

must follow the job card (or the request card if one is present). This card is automatically supplied by the Computing Center and is normally of no concern to the user. If a special version of the program is required, however, the user must supply a task card with the digit 1 replaced by the special version number.

III.A.2. INPUT CARDS (1/67)

All input cards are listed in the printer output as they are processed. Columns 1-8 of these cards are ignored and may be used for identification purposes. Additional comment information may follow the data on any card if a dollar sign is punched between the last data item and the comment. An asterisk in column 9 denotes a card containing only comments. The first card of an input deck should be a title card, denoted by an equal sign in column 9. The information on this card is used to title each page of printer output. If more than one title card is present, the last such card is used. Blank cards in the input deck are ignored.

Columns 9-14 of data cards must contain a six-digit card number, followed by a comma in column 15. The card number consists of a series number (one or two digits), a subseries number (zero to three digits), and a sequence number (remaining digits). The series and subseries numbers identify the type of data on the card; the sequence number begins at 1 for each subseries.

Data cards are divided into fields of arbitrary length, with the fields separated by commas and the comma following the last field optional. Each field contains an integer number, a floating-point number, or an alphanumeric identifier. Leading and trailing blanks are ignored in all fields, and imbedded blanks are ignored in numeric fields.

The integer format is

$\pm xx \dots xx$

and the floating-point format is

$\pm xx \dots xx \pm yy$,

where the leading sign may be dropped if it is plus and where each x and y is a decimal digit or a blank. In the floating-point format the decimal point is assumed to precede the fractional part and the signed one- or two-digit exponent must be present. An alphanumeric field must contain at least one non-numeric character or must be enclosed in parentheses. Note that all input

described in this manual is integer unless floating-point or alphanumeric is explicitly indicated.

Several different types of input are specified in expansion format. This format consists of sets of data, each set containing one or more floating-point numbers followed by an integer. The floating-point numbers are the parameters to be expanded and the integer is the termination point for the expansion. The expansion begins at the termination point of the previous set and continues to the termination point of the current set. These termination points are generally composition numbers or mesh point numbers and always form a strictly increasing sequence. Source values, for example, are specified in the form

$$S_1, c_1, S_2, c_2, \dots,$$

indicating that S_1 is to be associated with compositions 1 through c_1 , S_2 with compositions c_1+1 through c_2 , and so forth. Similarly, mesh intervals are specified in the form

$$M_1, p_1, M_2, p_2, \dots$$

Here M_1 is associated with each of the intervals between points 0 and p_1 and M_2 with each of the intervals between points p_1 and p_2 .

The number of data fields may vary from card to card in any series or subseries. If the data consists of sets of numbers, however, each card must contain an integral number of sets. In general, the input data cards may appear in any order. If two or more cards have the same card number, however, only the last of these cards is retained. If this last card contains no data, it also is not retained, and the comma following the card number on such a card is optional. Note that every input restriction stated in this manual is checked by the program. A problem which violates one or more restrictions will be rejected with suitable error comments.

III.A.3. MULTIPLE CASES - DECK ARRANGEMENT (1/67)

A single job may consist of several related cases. An end-case card is required between case decks and an end-input card is required following the last case deck. The end-case card is designated by a slash in column 9 and the end-input card by a period in column 9. Note that the end-input card replaces the end-case card for the last case and that both may not be present.

The input deck for the first case must be complete and self-contained, but the cards for each succeeding case represent changes to be made in the input of the previous case. The first such card should be a title card to alter the output page title. If a change card duplicates a card number in the previous case, the new card replaces the old. If the new card contains no data, it also is deleted. If a change card contains a new card number, it is added to the previous case input. Such a card must continue the sequence numbering of the subseries to which it is appended.

Note that the resulting input for a particular case is exactly equivalent to that obtained by removing all preceding end-case cards and running as the first case of a job. Note also that the cases of a job are related only through the above processing of the input deck. In particular, quantities such as flux and concentrations which are calculated in one case are not automatically available to the next case. This can only be accomplished by including control input which causes these files to be stored in one case and to be retrieved in the next.

The job deck submitted by a user normally consists of a job card followed by a request card (if needed) followed by the input data. The Computing Center will precede the input data with a task card and an end-of-record card (7-8-9 punches in column 1) and will follow the input data with an end-of-file card (6-7-8-9 punches in column 1).

III.A.4. INPUT CHECK LIST (1/67)

This check list does not include the control data described in Section III.B. but does include selected HARMONY input described in Reference 1.

010101 - 010109

Replacement composition numbers in any order.

0101x1 - 0101x9

Nuclide ID's for HARMONY edits (optional)

x = 1: power fraction x = 4: average concentration

x = 2: absorption rate x = 5: pointwise initial concentration

x = 3: fission rate x = 6: pointwise final concentration

011001 - 014999

Edit set data $f_1, {}^+f_2, \dots, 0, r_1, {}^+r_2, \dots$ with at least one subseries required.

100 - 199: each subseries an edit set

200 - 299: each figure an edit set

300 - 399: each region an edit set

400 - 499: each figure-region pair an edit set

015001 - 015999

Plane grouping data $p_1, -p_2, p_3, -p_4, \dots$ with at least one subseries required in 3-D.

020001 - 020099

Area ratios by composition in expansion format.

030001 - 030009

Triples of form n_i, c_j, n_k which assign composition c_j to regions (or figures) $n_i - n_k$.

03ppp1 - 03ppp9

Modifications at plane ppp to composition correspondence of previous plane.

04g001 - 04g099

Source values by composition for group g in expansion format (fixed source only).

05xx01 - 05xx99

Planar mesh intervals in expansion format, where xx may be any of

01 - 99.

III.A.4.(1)

060001 - 060999

Depletion plane boundaries in increasing order, with last value equal to plane boundary (3-D block depletion only).

070001 - 070999

Axial mesh intervals in expansion format (3-D only).

08g001 - 08g099

Buckling values by composition for group g in expansion format (optional).
Subseries 0: values for all groups for which there are no group-dependent values (also optional).

10cc01 - 10ccc9

Initial nuclide concentration data $ID_1, N_1, ID_2, N_2, \dots$ for composition ccc.

110001 - 110099

Table set assignment by composition in expansion format.

170001 - 170999

Final figure overlay sets (final figure number, initial figure number, origin column, origin row, rotation number, reflection indicator).

180001 - 180099

Planar region areas in expansion format (optional).

300001 - 300499

Numeric nuclide ID's.

300501 - 300999

Alphanumeric nuclide ID's.

4tt000 - 4tt001

Numeric table set ID on card 0 and (optional) alphanumeric ID on card 1.
The values of tt must be sequential from 01.

4ttg00

Values of D or Σ^{tr} , Σ^a , Σ^r , $v\Sigma^f$, $\kappa\Sigma^f$ for group g. D is used in non-depleting compositions and Σ^{tr} is used in depleting compositions.

4ttg01 - 4ttg99

Values of σ^{tr} , σ^a , σ^r , σ^f , ν , κ for a particular nuclide (whose ID precedes σ^{tr}) in group g.

8bb000

Control card for basic figure bb containing column boundary, row boundary, column interval subseries numbers, zero, row interval subseries numbers. Basic figures must be numbered sequentially from 01.

8bba01 - 8bba99

Planar region overlay sets (planar region number, left column, right column, top row, bottom row) for auxiliary figure a of basic figure bb (initial figure bba). Basic figure has auxiliary figure number 0 and auxiliary figures must be numbered sequentially from 1.

III.B. CONTROL DATA (1/67)

The following optional cards are deleted from the input at the end of each case. Hence, if they are required, these cards must be supplied with the input for every case.

010005	Flux edit control
010006	Power edit control
010007	Concentration edit control
010009	Miscellaneous edit control
010021	Output file control
01015n	} Concentration edit control
01016n	

Card 010001

- (1) Problem type (1 = fixed source, 2 = eigenvalue, 3 = one iteration, 4 = boundary value).
- (2) Adjoint solution (0 = no, 1 = yes). If an adjoint solution is requested, the number of thermal groups must be 1 and the total number of groups must exceed 1.
- (3) Total number of groups (≥ 1 , ≤ 5).
- (4) Number of thermal groups (1 or 2). There may not be two thermal groups in a 3-D problem.
- (5) Point (1) or block (2) depletion. The running time of non-depletable problem is decreased by using the block depletion option.
- (6) Geometry (1 = rectangular, 2 = cylindrical, 3 = spherical, 4 = hexagonal). Spherical geometry is available only in 1-D, cylindrical geometry only in 1-D and 2-D, and hexagonal geometry only in 2-D and 3-D.
- (7) Largest final figure number used (≥ 1 , ≤ 99).
- (8) Largest planar region number used (≥ 1 , ≤ 99).
- (9) Largest composition number used (≥ 1 , ≤ 99).

- (10) Composition correspondence (1 = figure, 2 = region, -1 = figure one-to-one, -2 = region one-to-one). The correspondence may only be one-to-one if the largest composition and final figure (or planar region) numbers are equal.
- (11) Column boundary (≥ 2 , $\leq$ limit in Section II.A.5). The number of solution columns must be at least 3.
- (12) Row boundary (1 if 1-D, > 1 otherwise). The number of solution rows must be at least 2 in 2-D and 3-D.
- (13) Plane boundary (1 if 1-D or 2-D, > 1 otherwise). The number of solution planes must be at least 2 in 3-D.
- (14) Diagonal column (≥ 2 , $\leq$ column boundary - 2, 0 if not hexagonal geometry). In hexagonal geometry, if the row 0 boundary condition is rotational symmetry, the diagonal column must be exactly half the column boundary.
- (15) Mesh intervals in inches (0 = no, 1 = yes).

Card 010002

Boundary conditions on column 0 and the column boundary, row 0 and the row boundary, plane 0 and the plane boundary (-1 = rotational symmetry (row 0 only), 0 = zero flux, +1 = zero current, +2 = fixed flux). Six values may be provided in any problem, but only the first two are required in 1-D and only the first four are required in 2-D. The column 0 boundary condition must be zero current in cylindrical and spherical geometry, and the rotational symmetry condition may not be used in cylindrical geometry. The boundary conditions on column 0 and the column boundary must be the same in the case of rotational symmetry.

Card 010003

Input eigenvalue followed by convergence parameter (both floating-point). Up to three additional floating-point numbers may be supplied for special options, and these are ignored if zero.

Card 010004

A value of X (floating-point) for each group. This card must not be present in fixed source problems and is required in all other problems.

Card 010005 (optional)

This card is used to request pointwise flux edits. The first six numbers describe the flux edit region (left and right columns, top and bottom rows, upper and lower planes) and the remaining numbers are the edit indicators for each group (0 = no edit, 1 = edit). An edit indicator may be included at the end of the card for the total thermal flux in a two-thermal-group problem.

Card 010006 (optional)

This card is used to request pointwise and partition power edits. The first six numbers describe the power edit region (left and right columns, top and bottom rows, upper and lower planes), the seventh number is the pointwise power indicator (0 = no edit, 1 = average power, 2 = peak power, 3 = average and relative maximum, 4 = peak and relative maximum), and the eighth number is the partition power indicator (0 = no edit, 1 = edit in floating-point format, 2 = edit in fixed-point format). In the case of pointwise power, options 1 and 2 provide a floating-point format and options 3 and 4 a fixed-point format.

Card 010007 (optional)

This card is used to specify the pointwise concentration edit region. The six numbers on this card (left and right columns, top and bottom rows, upper and lower planes) are used in conjunction with the concentration edit requests on cards 01015n and 01016n. Note that these edit requests are effective only in point depletion problems.

Card 010008 (optional)

The presence of this card determines that a problem is depletable (nuclide concentrations are being used).

- (1) T_0 (≥ 0 , floating-point). This is the time (in hours) at the beginning of the depletion calculation.
- (2) T_1 ($\geq T_0$, floating-point). This is the time (in hours) at the end of the depletion calculation. If $T_1 = T_0$, the depletion calculation is by-passed but depletion editing (if any) is performed.

- (3) $\Delta T_{\max}$ (≥ 0 , > 0 if $T_1 > T_0$, floating-point). This is the maximum time interval (in hours) for a thermal flux renormalization.
- (4) Power level (≥ 0 , floating-point). This is the power (in watts) extracted from that portion of the core represented by the problem.
- (5) Flux reversal (0 = no, 1 = yes). This refers to reversal of the flux in each row between the thermal flux renormalizations in the depletion calculation. The option is initialized to zero and this value need not be supplied on the card.

Card 010009 (optional)

- (1) HARMONY table usage edit (0 = no, 1 = yes).
- (2) Final figure picture edit (0 = no, 1 = yes).
- (3) Planar region picture edit (0 = no, 1 = yes).
- (4) Macroscopic data edit (0 = no, 1 = yes).

If this card contains fewer than four numbers (or is missing) zeros are automatically supplied.

Cards 010011 - 010014 (optional)

These cards refer respectively to input tableset, flux, concentration, and geometry files. Each card is present only if the corresponding data is to be obtained from an IFM file stored on disk. The card contains the job ID followed by the file ID (both alphanumeric) under which the file was created. On all but card 010011, there may be an optional third field containing the letters REMOVE which causes the corresponding file to be deleted from the disk at the end of the case. Note that an input flux, concentration, or geometry file is automatically deleted if the same type of file is saved on disk at the end of the case.

Cards 010021 - 010022 (optional)

These cards must both be present if files are to be saved and must both be missing otherwise. Since card 010021 is automatically deleted after every case, the next case must either supply a new card 010021 or delete card 010022 (by providing a card containing the card number only).

Card 010021 contains the file ID (alphanumeric, 1-10 characters) to be associated with the output files. Card 010022 contains from two to five numbers referring respectively to flux, concentrations, partition power, integrals, and geometry. Each number is 0 if the file is not to be saved, 1 if it is to be saved on tape only, 2 if it is to be saved on disk only, and 3 if it is to be saved on both. If the card contains fewer than five numbers, zeros are automatically supplied.

III.C.1. MESH INTERVAL DATA (5/66)

Mesh interval data is specified in expansion format, each set consisting of a floating-point interval value followed by a point number.

For planar mesh intervals, the series number is 05 and any of subseries 01 - 99 may be used. Each such subseries specifies a sequence of intervals extending from point 0 to an arbitrary final termination point. The data might consist of the following cards, for example.

```
050301, 1+1, 2
051701, 2+1, 2, 3+1, 3
052601, 4+1, 1
```

The use of this data is illustrated in Section III.C.2.

Axial mesh intervals are required in three-dimensional problems. The series number is 07, there is no subseries number, and the final termination point must be the plane boundary.

III.C.2. OVERLAY DATA (5/66)

A control card is required for each basic figure containing the column boundary, the row boundary, a set of column interval subseries numbers, a zero, and a set of row interval subseries numbers. The series number for the control card is 8, the subseries number is the two-digit basic figure number, and the sequence number is 0. The control card for basic figure 07 might be

807000, 4, 7, -17, 26, 0, 03, 17, 03

where the interval subseries numbers refer to the example in Section III.C.1. This basic figure has a column boundary of 4 and a row boundary of 7, the column intervals consist of subseries 17 (reversed because of the minus sign) followed by subseries 26, and the row intervals consist of subseries 03 followed by subseries 17 followed by subseries 03. Thus, the column intervals are equivalent to a single subseries of the form

$3+1, 1, 2+1, 3, 4+1, 4$

and the row intervals to a single subseries of the form

$1+1, 2, 2+1, 4, 3+1, 5, 1+1, 7$.

The advantage of multiple subseries is that repeating sequences of intervals need be specified only once. Note that the final termination points of the column subseries must exactly add to the column boundary, and similarly for the row subseries. Note also that the column and row boundaries may be as small as 1 and as large as desired.

Planar region overlay data consists of five-word sets: planar region number, left column, right column, top row, and bottom row. The column and row numbers must define a nondegenerate rectangle which does not extend outside the basic figure boundaries. The series number for this data is 8 and the subseries number is the initial figure number, consisting of a two-digit basic figure number followed by a one-digit auxiliary figure number. A complete overlay is given using auxiliary figure number 0 and then modifications to this overlay are given for each auxiliary figure. The complete set of card numbers for basic figure 16 might be

816000
816001
816002
816101
816201
816202

The first card is the basic figure control card, the next two cards contain the basic figure overlay sets, the fourth card contains overlay sets which modify the basic figure to form auxiliary figure 1, and the last two cards modify the basic figure to form auxiliary figure 2. Note that the basic figures must be numbered sequentially from 01 and for each basic figure, the auxiliary figures must also be numbered sequentially from 1. It is not necessary, however, that every basic figure and auxiliary figure actually be used in the final figure overlay.

Final figure overlay data is specified using series number 17. This data consists of six-word sets as follows:

final figure number
initial figure number
origin column
origin row
rotation number
reflection indicator

The final figure number may be any number between 01 and 99. The initial figure number must be between 010 and 999 and designates the particular basic figure or auxiliary figure being overlaid on the region of solution. There is no limitation whatever on the origin column and row numbers. The rotation number is the multiple of 90° (60° in hexagonal geometry) through which the initial figure is to be clockwise rotated and must lie between 0 and 3 (0 and 5 in hexagonal geometry). The reflection indicator is 1 for reflection and 0 for no reflection.

III.C.3. MISCELLANEOUS GEOMETRY DATA (5/66)

The use of input planar region areas is optional. They are specified in expansion format using series number 18. Each set consists of a floating-point area value followed by a planar region number, and the last such number must equal the largest planar region number as specified in the control input. If this data is present, it is compared with the areas calculated using the mesh interval and overlay data. If the input and calculated areas for any planar region differ by more than 1%, all of the calculated values are printed and the problem is rejected. Note that the calculated areas may be obtained during an input check by inputting zero areas.

Depletion plane boundaries are required in three-dimensional block depletion problems. The series number is 06 and the plane numbers must be specified in increasing order, with the last value equal to the plane boundary. The top boundary at plane 0 is understood and must not be included.

If the composition correspondence is not one-to-one, it must be specified using series number 03. The data consists of triples of the form n_i, c_j, n_k which assign composition c_j to planar regions (or final figures) $n_i - n_k$. The triples are processed sequentially and any triple may change an assignment established by a previous triple. For example, the set of triples

2, 1, 5
1, 3, 1
3, 2, 4

assigns composition 2 to regions 3 and 4, composition 3 to region 1, and composition 1 to regions 2 and 5. Note that every planar region (or final figure) must be assigned a composition number by this process.

Subseries 000 is used for the composition correspondence in two-dimensional problems and for the first plane of three-dimensional problems. An additional subseries is required for each plane at which the correspondence changes. The three-digit subseries number is the plane number at which the change occurs, and the triples in such a subseries are used to modify the correspondence of the previous plane. The correspondence may be changed at any plane in the case of point depletion, but in the case of block depletion it may be changed only at the depletion plane boundaries specified in the 06 series.

III.D.1. EDIT CONTROL DATA (1/67)

Edit control data is specified using series number 01. Subseries 100 - 499 are used for edit sets and subseries 500 - 599 are used for plane groupings.

The data for each edit set subseries is of the form

$$f_1, \pm f_2, \pm f_3, \dots, \pm f_m, 0, r_1, \pm r_2, \pm r_3, \dots, \pm r_n$$

where the zero is used to separate a collection of planar region numbers from a collection of final figure numbers. A negative figure number designates all figures from the previous figure number through the negative figure number, and similarly for a negative region number. For both the figures and the regions, the numbers must be strictly increasing in absolute value, there may not be two consecutive negative numbers, and the first number must be positive. As an example, the sequence 3, 5, -7, 0, 2, -4, 9 specifies figure numbers 3, 5, 6, and 7 and region numbers 2, 3, 4, and 9.

The subseries are separated into four ranges: 100 - 199, 200 - 299, 300 - 399, and 400 - 499. Any (but not all) of the ranges may be omitted and the first missing subseries in each range terminates the range. Each of subseries 100 - 199 specifies a single edit set. In each of subseries 200 - 299, the figure numbers are expanded to remove negative signs and an edit set of the form

$$f_1, 0, r_1, \pm r_2, \pm r_3, \dots, \pm r_n$$

is constructed for each figure number. Similarly, in each of subseries 300 - 399, the region numbers are expanded and an edit set of the form

$$f_1, \pm f_2, \pm f_3, \dots, \pm f_m, 0, r_j$$

is constructed for each region number. Finally, in each of subseries 400 - 499, both the figure and region numbers are expanded and an edit set of the form

$$f_1, 0, r_j$$

is constructed for each figure-region pair.

At least one plane grouping subseries is required in three-dimensional problems and the subseries numbers present must be sequential. The data for each subseries specifies a single plane grouping and is of the form

$$P_1, -P_2, P_3, -P_4, \dots, P_{n-1}, -P_n \cdot$$

The plane numbers in a subseries must be strictly increasing in absolute value and occur in plus-minus pairs, each pair designating the axial region between the two planes. The sequence 0, -3, 5, -8, for example, specifies a plane grouping consisting of planes 0 - 3 together with planes 5 - 8. Any plane numbers may be used in the case of point depletion, but in the case of block depletion only zero and the depletion plane boundaries specified in the 06 series are permitted.

An option is available which permits a significant reduction in the volume of integral output, particularly in three-dimensional problems. This is accomplished by including in the input a card 011000 containing exactly eight numbers. The first pair of numbers refers to the volume-weighted macroscopic data edits, the second pair refers to the integration edits (flux integrals and flux-weighted macroscopic data), the third pair refers to the nuclide rate edits (power fractions, absorption rates, and fission rates), and the fourth pair refers to the average nuclide concentration edits. Each pair consists of the last edit set and the last plane grouping for which the corresponding integrals are to be printed. Either number (or both numbers) in a pair may be input as zero to request that printing be done for all edit sets or all plane groupings.

III.D.2. SOURCE VALUES (5/66)

Source values are required only in fixed source problems. They are specified in expansion format using series number 04. The one-digit subseries number is the group number and there must be a subseries for each group. Each set of data consists of a floating-point source value followed by a composition number, and the last such number must equal the largest composition number as specified in the control data.

III.D.3. HARMONY DATA (1/67)

The following description includes only that portion of the HARMONY data required for non-depletable problems. Changes made in the HARMONY system since Reference 1 was issued are also indicated.

Macroscopic data is input by table set, and a table set is then assigned to each composition. The input for a table set consists of a numeric ID, an optional alphanumeric ID, and a set of floating-point macroscopic parameters for each group. Card numbers have the form 4ttxxx, where tt=01,02,... sequences the table set input (not necessarily the table set ID) and xxx differentiates the types of data. The subseries numbers tt must be sequential from 01. Card 4tt000 contains the numeric ID of the table set and optional card 4tt001 contains an alphanumeric ID of up to 40 characters. There must be a card 4ttg00 for each group g containing D_g , Σ_g^a , Σ_g^r , $\nu\Sigma_g^f$, and $\kappa\Sigma_g^f$. If g is one of a pair of thermal groups, the card instead contains D_g^1 , D_g^2 , Σ_g^1 , Σ_g^2 , $\nu\Sigma_g^f$, $\kappa\Sigma_g^f$, and R_g . If $\nu\Sigma_g^f = \kappa\Sigma_g^f = 0$ for all g , these values may be omitted from the cards, but they must be omitted from all of the cards in a table set or from none of them.

The assignment of a table set to each composition is specified in expansion format using series number 11. Each set of data consists of a numeric table set ID followed by a composition number, and the last such number must equal the largest composition number as specified in the control input.

Buckling values are optional in all problems. They are specified in expansion format using series number 08. The one-digit subseries number is the group number but there need not be a subseries for each group. Each set of data consists of a floating-point buckling value followed by a composition number, and the last such number must equal the largest composition number as specified in the control input. Subseries 0 may be used to specify values for all groups in which group-dependent values are not provided.

The primary change made in the HARMONY system is that dummy input to define a single nuclide, chain, and chain list is no longer required (or permitted) in non-depletable problems. In addition, alphanumeric nuclide ID's

may now contain up to 10 characters and alphanumeric table set ID's up to 40 characters, these need not begin with an alphabetic character, and the last ID on a card need not be followed by a comma.

IV.A. MACROSCOPIC DATA OUTPUT (1/67)

Under input option, volume-weighted average macroscopic data may be obtained for each group. For any macroscopic parameter Σ , the average value is calculated via

$$\bar{\Sigma} = \frac{\int \Sigma dV}{\int dV} . \quad (\text{IV.A./1})$$

The parameters edited are D , Σ^a , Σ^r , $\nu\Sigma^f$, $\kappa\Sigma^f$, and B^2 . In each of a pair of thermal groups, these are replaced by D^1 , D^2 , Σ^1 , Σ^2 , $\nu\Sigma^f$, $\kappa\Sigma^f$, $R\Sigma_{G-2}^r$ and B^2 . Note that B^2 is calculated from a total cross section and hence may not match exactly the input value. Note also that $\nu\Sigma^f$ is replaced by the input source S in a fixed source problem.

IV.B. ITERATION OUTPUT (1/67)

The omega calculation edits the quantities RHO, OMEGA, SIGMA, and DELTA for each group. In a two-dimensional problem this editing is done for each pass through a group, and in a three-dimensional problem it is done for the last pass in each plane. The number of passes performed depends upon the rate of convergence of the calculation. RHO is an estimate of the largest eigenvalue of the iteration matrix, OMEGA is an overrelaxation parameter calculated from RHO, and the quantity in parentheses following OMEGA is the current iteration count. SIGMA is an estimate of the second largest eigenvalue divided by RHO, DELTA is the factor by which the initial residual should be reduced each outer iteration, and the quantity in parentheses following DELTA is an estimate of the number of inner iterations required to achieve this residual reduction.

A summary of the inner iteration results in each group is given for each outer iteration. In a two-dimensional problem this includes the total number of iterations performed, values of R(1) and DELTA, and the number of passes required (if greater than 1), where R(1) is the initial residual and DELTA is some factor times the error reduction achieved. In a three-dimensional problem the summary includes the number of passes performed and values of RATE and DELTA, where RATE is a measure of the rate of error reduction and DELTA is the actual reduction achieved.

The outer iteration results edited are SIG/I, SIG/O, MAX, MIN, GAMMA, PT/AV, RATIO, EPS, and LAMBDA^{*}. SIG/I and SIG/O are estimates of the convergence rate as measured by the inner and the outer iterations. MAX and MIN are the largest and smallest pointwise flux ratios between the current and previous iterations, each multiplied by LAMBDA. GAMMA is a normalizing factor (which approaches unity), and PT/AV is the largest point flux error divided by the average error. RATIO is the convergence rate obtained during a Chebyshev extrapolation cycle divided by the predicted rate, and the quantity in parentheses following RATIO is the degree of the Chebyshev polynomial. EPS is the largest (in absolute value) deviation of the pointwise flux ratio from unity, and the quantity in parentheses following EPS is the

^{*}These quantities are discussed in detail in Reference 5.

outer iteration number (which is negative if there is a negative flux in the fueled region of the mesh). LAMBDA is the length of the current fission source vector divided by the length of the initial vector, where length is calculated as the sum of the absolute values of the components.

Multiple outer iterations are performed in fixed source and one iteration problems, but the input or fission source is not altered between iterations. LAMBDA is set to unity in fixed source problems and approaches unity in boundary value problems. The percentage reactivity, defined as $100(\lambda - 1)/\lambda$, is edited following the last iteration. In slowly convergent problems, the message INPUT EPS. CRITERION CHANGED is included in the output to signal that equation (I.C./1) has been altered to assure adequate convergence. Under operator control the current outer iteration number, the value of LAMBDA, and the estimated final iteration number (E.T.A.) may be monitored at the display console.

IV.C. INTEGRATION OUTPUT (1/67)

The first section of the integration edits the volume and the integrated and averaged flux for each group. The integrated and averaged total thermal flux, $\phi_{G-1} + \phi_G$, is also edited in a two-thermal-group problem. These values are preceded by the flux and power normalization factors, FNORM and PNORM. The normalization factors are defined by

$$\text{FNORM} = \frac{\text{Input Power}}{\sum_{g=1}^G \int \kappa \Sigma_g^f \phi_g dV} \quad (\text{IV.C./1})$$

and

$$\text{PNORM} = \frac{\int dV}{\sum_{g=1}^G \int \kappa \Sigma_g^f \phi_g dV}, \quad (\text{IV.C./2})$$

where the integrals are taken over the fueled regions of the mesh. If a power level is not provided in the input, FNORM is set equal to PNORM. All flux integrals and averages are multiplied by FNORM before being edited.

The second section edits the fraction of the total power contributed by the region being integrated together with the relative power density, which is the fraction of the total power contributed by the region divided by the fraction of the total fuel area present in the region. The fraction of the region power contributed by each group is also edited, as is the total thermal fraction in a two-thermal-group problem.

The third section edits the fraction of the total absorption contributed by the region being integrated together with the fraction of the total absorption and the fraction of the region absorption contributed by each group. In a two-thermal-group problem these fractions are also edited for the total thermal absorption, $\sum_{G-1}^2 \phi_{G-1} + \sum_G^1 \phi_G$.

The fourth section edits the group-independent buckling, K^∞ by group and the sum over groups, and K^{eff} by group and the sum over groups. The group-independent buckling is obtained by eliminating the flux and solving

for B^2 in the set of equations

$$\left\{ (B^2 \overline{D}_g + \overline{\Sigma}_g^t) \phi_g = \frac{\chi_g}{\lambda} \sum_{j=1}^G \overline{v\Sigma}_j^f \phi_j + \overline{\Sigma}_{g-1}^r \phi_{g-1} \right\}_{g=1}^G \quad (\text{IV.C./3})$$

Here $\Sigma_g^t = \Sigma_g^a + \Sigma_g^r + D_g B_g^2$, where B_g^2 is the input buckling, and

$$\overline{\Sigma} = \frac{\int \Sigma \phi dv}{\int \phi dv} \quad (\text{IV.C./4})$$

is the flux-weighted average value for any macroscopic parameter Σ . If there are two thermal groups, the last two of Equations (IV.C./3) are replaced by the equations

$$\begin{aligned} (B^2 \overline{D}_{G-1}^1 + \overline{\Sigma}_{G-1}^{t1}) \phi_{G-1} &= \frac{\chi_{G-1}}{\lambda} \sum_{j=1}^G \overline{v\Sigma}_j^f \phi_j + \overline{R}_{G-1} \overline{\Sigma}_{G-2}^r \phi_{G-2} \\ &\quad - (B^2 \overline{D}_{G-1}^2 + \overline{\Sigma}_{G-1}^{t2}) \phi_G \end{aligned} \quad (\text{IV.C./5})$$

and

$$(\overline{B^2 D}_G^1 + \overline{\Sigma}_G^{t1}) \phi_G = \frac{\chi_G}{\lambda} \sum_{j=1}^G \overline{v\Sigma}_j^f \phi_j + \overline{R}_G \overline{\Sigma}_{G-2}^r \phi_{G-2} - (\overline{B^2 D}_G^2 + \overline{\Sigma}_G^{t2}) \phi_{G-1}, \quad (\text{IV.C./6})$$

where

$$\Sigma_{G-1}^{t1} = \Sigma_{G-1}^1 + D_{G-1}^1 B_{G-1}^2, \quad \Sigma_{G-1}^{t2} = \Sigma_{G-1}^2 + D_{G-1}^2 B_G^2, \quad \Sigma_G^{t1} = \Sigma_G^1 + D_G^1 B_G^2,$$

and

$$\Sigma_G^{t2} = \Sigma_G^2 + D_G^2 B_{G-1}^2.$$

K_g^{eff} is the contribution of group g to the total criticality, calculated by

$$K_g^{\text{eff}} = \left(\frac{\overline{\Sigma_{g-1}^r} K_{g-1}^{\text{eff}}}{\overline{\nu \Sigma_{g-1}^f}} + \chi_g \right) \frac{\overline{\nu \Sigma_g^f}}{\overline{\Sigma_g^t} + \overline{D_g} \overline{B_g^2}}, \quad (\text{IV.C./7})$$

where

$$K_1^{\text{eff}} = \frac{\chi_1 \overline{\nu \Sigma_1^f}}{\overline{\Sigma_1^t} + \overline{D_1} \overline{B_1^2}}. \quad (\text{IV.C./8})$$

K_g^{∞} is calculated in the same manner but with leakage ignored, that is, with $\overline{\Sigma_g^t} + \overline{D_g} \overline{B_g^2}$ replaced by $\overline{\Sigma_g^a} + \overline{\Sigma_g^r}$. In a two-thermal-group problem a single thermal K^{eff} is calculated via

$$K_{\text{th}}^{\text{eff}} = \frac{K_{G-2}^{\text{eff}}}{\overline{\nu \Sigma_{G-2}^f}} \left\{ \left[\overline{R_{G-2} \Sigma_{G-2}^r} (\overline{\Sigma_{G-1}^{t1}} + \overline{D_{G-1}^1} \overline{B_{G-1}^2}) - \overline{R_{G-1} \Sigma_{G-2}^r} (\overline{\Sigma_G^{t2}} + \overline{D_G^2} \overline{B_{G-1}^2}) \right] \overline{\nu \Sigma_G^f} \right. \\ \left. + \left[\overline{R_{G-1} \Sigma_{G-2}^r} (\overline{\Sigma_G^{t1}} + \overline{D_G^1} \overline{B_G^2}) - \overline{R_{G-2} \Sigma_{G-2}^r} (\overline{\Sigma_{G-1}^{t2}} + \overline{D_{G-1}^2} \overline{B_G^2}) \right] \overline{\nu \Sigma_{G-1}^f} \right\} / \quad (\text{IV.C./9}) \\ \left[(\overline{\Sigma_{G-1}^{t1}} + \overline{D_{G-1}^1} \overline{B_{G-1}^2}) (\overline{\Sigma_G^{t1}} + \overline{D_G^1} \overline{B_G^2}) - (\overline{\Sigma_{G-1}^{t2}} + \overline{D_{G-1}^2} \overline{B_G^2}) (\overline{\Sigma_G^{t2}} + \overline{D_G^2} \overline{B_{G-1}^2}) \right],$$

and similarly for K_{th}^{∞} .

The fifth and final section edits flux-weighted average macroscopic parameters. In all but a pair of thermal groups the quantities edited are $\overline{D_g}$, $\overline{\Sigma_g^a}$, $\overline{\Sigma_g^r}$, $\overline{\nu \Sigma_g^f}$, and

$$\overline{B}_g^2 = \frac{1}{\overline{D}_g} \left(\frac{\chi_g}{\lambda} \sum_{j=1}^G \overline{\nu \Sigma}_j^f \tilde{\phi}_j + \overline{\Sigma}_{g-1}^r \tilde{\phi}_{g-1} - \overline{\Sigma}_g^t \tilde{\phi}_g \right), \quad (\text{IV.C./10})$$

where $\tilde{\phi}$ designates the integral of the flux. In a fixed source problem, the edit of $\overline{\nu \Sigma}_g^f$ is replaced by

$$\overline{S}_g = \frac{\int S_g \phi_g dV}{\int \phi_g dV}. \quad (\text{IV.C./11})$$

The quantities edited in the first group of a thermal pair are $\overline{D}_{G-1}^1$, $\overline{D}_{G-1}^2$, $\overline{\Sigma}_{G-1}^1$, $\overline{\Sigma}_{G-1}^2$, $\overline{\nu \Sigma}_{G-1}^f$, $\overline{R_{G-1} \Sigma_{G-2}^r}$, and $\overline{B}_{G-1}^2$, and in the second group are $\overline{D}_G^1$, $\overline{D}_G^2$, $\overline{\Sigma}_G^1$, $\overline{\Sigma}_G^2$, $\overline{\nu \Sigma}_G^f$, $\overline{R_G \Sigma_{G-2}^r}$, and $\overline{B}_G^2$, where each macroscopic parameter is weighted by the group flux with which it is associated in Equations (I.B./3) and (I.B./4). $\overline{B}_{G-1}^2$ and $\overline{B}_G^2$ are obtained by solving simultaneously the pair of equations

$$\begin{aligned} (\overline{B}_{G-1}^2 \overline{D}_{G-1}^1 + \overline{\Sigma}_{G-1}^{t1}) \tilde{\phi}_{G-1} &= \frac{\chi_{G-1}}{\lambda} \sum_{j=1}^G \overline{\nu \Sigma}_j^f \tilde{\phi}_j + \overline{R_{G-1} \Sigma_{G-2}^r} \tilde{\phi}_{G-2} \\ &\quad - (\overline{B}_G^2 \overline{D}_{G-1}^2 + \overline{\Sigma}_{G-1}^{t2}) \tilde{\phi}_G \end{aligned} \quad (\text{IV.C./12})$$

and

$$\begin{aligned} (\overline{B}_G^2 \overline{D}_G^1 + \overline{\Sigma}_G^{t1}) \tilde{\phi}_G &= \frac{\chi_G}{\lambda} \sum_{j=1}^G \overline{\nu \Sigma}_j^f \tilde{\phi}_j + \overline{R_G \Sigma_{G-2}^r} \tilde{\phi}_{G-2} \\ &\quad - (\overline{B}_{G-1}^2 \overline{D}_G^2 + \overline{\Sigma}_G^{t2}) \tilde{\phi}_{G-1}. \end{aligned} \quad (\text{IV.C./13})$$

The calculations of K^{∞} and K^{eff} and of the group-dependent and group-independent buckling all require knowledge of the source integral. Since the integral of the input source is not available in fixed-source problems, these calculations are bypassed in such problems. Except for the group-dependent buckling, these calculations are also bypassed in any region in which the source integral is zero.

IV.D. DEPLETION OUTPUT (1/67)

Depletion editing is preceded by a description of the depletion performed. This includes the time at the beginning and end of the depletion, the power level, the thermal flux renormalization interval, and the number of such intervals. In addition, the subinterval length for cross section re-evaluation and the number of subintervals is given for each composition.

Power fractions, absorption rates, and fission rates are edited at the beginning of the depletion interval. Values are edited by group and summed over groups for each nuclide requested. The power fraction in group g for nuclide i is given by

$$P_i^g = \frac{\int \kappa_i^g \sigma_i^f, g_{G_i}^f, g_{N_i}^f \phi_g dV}{\sum_{g=1}^G \sum_j \kappa_j^g \sigma_j^f, g_{G_j}^f, g_{N_j}^f \phi_g dV} , \quad (\text{IV.D./1})$$

where $\sum_j$ represents a sum over only those nuclides j for which a power fraction edit was requested. Similarly, the absorption and fission rates are given by

$$A_i^g = \int \sigma_i^a, g_{G_i}^a, g_{N_i}^a \phi_g dV \quad (\text{IV.D./2})$$

and

$$F_i^g = \int \sigma_i^f, g_{G_i}^f, g_{N_i}^f \phi_g dV , \quad (\text{IV.D./3})$$

where the flux used in these integrals is normalized by FNORM (Equation (IV.C./1)). In a two-thermal-group problem, $\sigma^{a,G-1} = \sigma_{21}^a$ and $\sigma^{a,G} = \sigma_{11}^a$.

Average nuclide concentrations are edited at the end of the depletion interval for each nuclide requested. The average concentration for nuclide i is given by

(IV.D./4)

IV.E. POINTWISE OUTPUT (1/67)

Before editing, pointwise flux values are normalized by FNORM (Equation IV.C./1) and pointwise and partition power values are normalized by PNORM (Equation IV.C./2). Concentration values can be edited only in point depletion problems and the editing is by mesh figure rather than by mesh point.

A partition power value is calculated for each mesh figure at a point using the $\kappa \sum_g^f$ values in the mesh figure and the group flux values at the point. Partition power is edited only for those points at which any two nonzero values differ by more than 5%. In hexagonal geometry the order of the values at a point is as indicated in Figure (II.C.5./1). Pointwise average power is calculated as the numerical average of the nonzero partition values at a point and pointwise peak power is the largest of these values.

A relative maximum edit may be obtained in conjunction with either pointwise average or pointwise peak power. A point is considered a relative maximum if its power value exceeds the values at all its neighbors, where neighbors are determined in the difference equation sense (Section I.D.). The edit is performed by printing the pointwise values a second time, with the power set to zero at each point which is not a relative maximum.

Flux and concentration values are printed in floating-point format with a six-digit fraction. Power values are also printed in this format unless a relative maximum edit is requested. In this case all power editing is done using the fixed-point format x.xx which provides a higher density of information on each output page. In addition, the zero values at non-fuel points are suppressed to outline the fueled regions of the mesh.

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