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THE PDQ-5 AND PDQ-6 PROGRAMS FOR THE SOLUTION OF THE TWO-DIMENSIONAL NEUTRON DIFFUSION-DEPLETION PROBLEM

January 1965

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W. R. Cadwell
P. F. Buerger
C. J. Pfeifer

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THE PDQ-5 AND PDQ-6 PROGRAMS
FOR THE SOLUTION OF THE TWO-DIMENSIONAL
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PDQ-5 and PDQ-6 are FORTRAN programs which solve the two-dimensional neutron diffusion-depletion problem with up to five lethargy groups. The geometry is rectangular or cylindrical in PDQ-5 and hexagonal in PDQ-6. Both programs provide for variable mesh spacing. Problems in excess of 50,000 mesh points have been run successfully.

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I. INTRODUCTION

The PDQ-5 and PDQ-6 programs solve the two-dimensional neutron diffusion-depletion problem with up to five lethargy groups. The geometry is rectangular or cylindrical in PDQ-5 and hexagonal in PDQ-6. Zero flux, zero current, and rotational symmetry boundary conditions are available. Between 300 and 500 mesh points are permitted in each coordinate direction, and both programs provide for variable mesh spacing. PDQ-5 problems in excess of 50,000 points and PDQ-6 problems in excess of 30,000 points have been run successfully.

This report supersedes a previous report (Reference 1) which described the initial version of PDQ-5. The present report, however, includes only the information required for spatial calculations. The depletion capabilities of the programs, which include a flexible representation of time-dependent cross sections and the input specification of nuclide chains, are described in Reference 2.

The flux iterations of both programs utilize single-line successive overrelaxation, and the source iterations are accelerated by Chebyshev extrapolation. The PDQ-5 difference equation derivations are standard and the PDQ-6 derivation is given in Reference 3. The iteration strategy is fully described in Reference 4.

The programs are written in FORTRAN II language and have been compiled and run only on the Philco-212 computer. They operate on this computer under control of the BKS monitor system (Reference 5) and also make use of the Bettis FORTRAN subroutine package (Reference 6). Conversion to another computer would require translation of the subroutine package and, for efficient operation, a rather extensive modification of the programs.

II. GENERAL DESCRIPTION

Diffusion Equations

The neutron-diffusion equations solved by the programs are

$$\left\{ -\nabla \cdot [D_g(x) \nabla \varphi_g(x)] + [\Sigma_g^a(x) + \Sigma_g^r(x) + D_g(x) B_g^2(x)] \varphi_g(x) \right. \\ \left. = \frac{\chi_g}{\lambda} \psi(x) + \Sigma_{g-1}^r(x) \varphi_{g-1}(x) \right\}_{g=1}^G \quad (2.1)$$

Here (x) represents the spatial variables, either $x-y$ or $r-z$; 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

$$\psi(x) = \sum_{g=1}^G \nu \Sigma_g^f(x) \varphi_g(x) \quad (2.2)$$

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 by composition or may be calculated by the programs using spatially varying nuclide concentrations

and input cross section tables. The composition input of these parameters is covered in the present report, while the use of cross section tables is described in Reference 2.

Problem Types - Convergence

The programs may be used to solve three different types of problems-- eigenvalue, one-iteration, and fixed-source. Equations (2.1) and (2.2) are the governing equations in eigenvalue and one-iteration problems. In fixed-source problems Equation (2.2) is not used and the term $x_g(x)/\lambda$ in Equation (2.1) is replaced by the input source S_g .

In an eigenvalue problem the flux iterations (inner iterations) in each group are terminated when

$$\sum_{s,t} |\varphi_{s,t}^{(n)} - \varphi_{s,t}^{(n-1)}| \leq \delta \sum_{s,t} |\varphi_{s,t}^{(1)} - \varphi_{s,t}^{(0)}| , \quad (2.3)$$

where $\varphi_{s,t}^{(n)}$ is the flux calculated at point s,t during inner iteration n and the parameter δ is determined by the program. The source iterations (outer iterations) are terminated when

$$\frac{\lambda^{(m)} - \lambda^{(m)}}{2\lambda^{(m)}} \leq \varepsilon^2 , \quad (2.4)$$

where $\lambda^{(m)}$ is the eigenvalue calculated at the end of outer iteration m , $\lambda^{(m)}$ and $\lambda^{(m)}$ are the calculated bounds on the eigenvalue, and ε is an input parameter.

A single outer iteration is performed in a one-iteration problem and the inner iterations in each group are terminated when

$$\max_{s,t} \frac{|\varphi_{s,t}^{(n)} - \varphi_{s,t}^{(n-1)}|}{|\varphi_{s,t}^{(n)}|} \leq \varepsilon(2 - \omega) . \quad (2.5)$$

Here ε is the same input parameter as above and $1 \leq \omega < 2$, is an overrelaxation factor calculated by the program. Equation (2.5) is also used to terminate the iterations in each group of a fixed-source problem.

Eigenvalue problems are run to obtain the fission source distribution and criticality corresponding to a given reactor configuration, while fixed-source problems are run to obtain the flux distribution corresponding to a known neutron source. One-iteration problems are generally used as successive generations in neutron importance calculations. The method requires solving an eigenvalue problem in the first case of a job and one-iteration problems in all succeeding cases.

Adjoint Calculations

By changing one of the input control numbers, the adjoint solution for any problem may be obtained in place of the normal solution. There is no provision in the programs, however, for performing perturbation edits. The output flux of a normal and an adjoint calculation must be saved on a filetape and a separate program must be used to obtain these edits.

One-Dimensional Option

PDQ-5 may be used to run one-dimensional problems in rectangular or cylindrical geometry. No criticality search is provided. A one-dimensional problem is described in the input as a two-dimensional problem with only two rows, zero and one, along each of which a zero derivative boundary condition is applied. (A row boundary of one is not permitted in a true two-dimensional problem and hence this sets the one-dimensional option.) All of the two-dimensional features are available in one-dimensional problems, including depletion and the full use of filetapes.

III. GEOMETRY

PDQ-5

The PDQ-5 region of solution is a rectangle in the x-y or r-z plane. This rectangle is subdivided into a number of material compositions, with the interfaces between these compositions parallel to the outer boundaries of the rectangle. Within a composition the input macroscopic data (or initial nuclide concentrations) are required to be constant. A nonuniform grid of mesh lines is imposed on the region of solution. The mesh lines are parallel to the outer boundaries of the rectangle and each extends from one boundary to the opposite boundary. The mesh intervals must be chosen in such a way that the boundaries of the rectangle and the interfaces between compositions exactly coincide with mesh lines.

The axes of the coordinate system coincide with boundary lines of the rectangle. As shown in Figure 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 flux or the normal derivative of the flux may be set to zero along each boundary of the rectangle. In addition, a 180° 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. In contrast to previous versions of PDQ, each of the boundary conditions is applied along the boundary line itself. Hence, the number of solution points in a mesh depends both upon the number of mesh lines in each direction and upon the boundary conditions imposed.

The placement of material compositions in the mesh is described in the input by means of a composition overlay. This consists of a series of overlay sets, each of which superimposes a particular composition number throughout a specified rectangle of the mesh. The sets are processed sequentially and any set may overlay regions of the mesh specified in previous sets. Every mesh rectangle must be included within at least one of the overlay sets and for each mesh rectangle, the last overlay set which includes the rectangle determines its composition number. If several different regions of the mesh have the same material properties, they may all be assigned the same composition number. As an example, Figure 2 may be described by overlaying composition 1 on the entire

mesh; composition 3 between columns 1 and 3, rows 2 and 4; composition 2 between columns 2 and 4, rows 0 and 3; and composition 3 between columns 3 and 4, rows 0 and 1.

The composition overlay describes the geometry of the problem to be solved. This overlay is also used for integration editing purposes unless an optional edit region overlay is provided. The two overlays have the same general format but it is not required that their interfaces coincide. An edit region overlay is normally used if editing is to be done for subregions of a composition or for regions containing segments of several compositions.

PDQ-6

The PDQ-6 region of solution is a 120° chevron in the x-y plane. The chevron is oriented as in Figure 3, 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. A zero flux or zero normal derivative condition may be applied along each boundary, and a 120° rotational symmetry condition may be applied along the top boundary. In the latter case the chevron must be symmetric, with an equal number of intervals on each side of the diagonal column.

The geometry of the chevron is described by overlaying it with basic figures, which are 60° parallelograms oriented as in Figure 4. Each basic figure is described as a separate mesh, by specifying its row and column boundaries, composition overlay, and mesh intervals. The basic figures are overlaid on the chevron by giving the row and column of the chevron at which the origin is to be placed and the multiple of 60° through which the basic figure is to be clockwise rotated. The basic figure also may be reflected, which implies an interchange of rows and columns. The six rotational orientations of a basic figure are shown in Figure 5 and the reflections of these figures are shown in Figure 6. In both cases the origins are all at the center of the star. Note that both composition and edit region basic figures may be described and overlaid on the chevron. Since each edit region basic figure must have the same mesh as some composition basic figure, mesh intervals are given only for the composition figures.

As in a composition overlay, the basic figure overlay is sequential and may overlay regions of the chevron that have been specified previously. Any portion of a basic figure which extends outside the chevron boundaries is ignored, and no region of the chevron may remain unspecified when the overlay is complete. The fundamental restriction on the final overlay is that the mesh in the basic figures must be so chosen that mesh lines in adjoining basic figures meet at common boundary points. It is important to note that the rows and columns of Figure 3 are not necessarily mesh lines, since the network of mesh lines is determined entirely by the placement of basic figures. The rows and columns of the chevron are used only to locate basic figure origins and may actually be extended to locate origins outside the chevron. The top row is always a mesh line, however, and if there is rotational symmetry, the mesh intervals in this row must be symmetric about the diagonal column.

In addition to the chevron, four types of figures must be carefully distinguished. A basic figure is as described above, a 60° parallelogram for which mesh intervals and a composition overlay are specified. Basic figures are numbered sequentially from 01 to 99. An auxiliary figure is obtained by modifying the composition overlay of a basic figure. If two or more 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 may range from 010 to 999 and it is initial figures, rather than basic figures, which are actually overlaid on the chevron. A final figure number is associated with each initial figure overlay of the chevron. 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.

Figure 7 represents one-third of an hexagonal array. Mesh points have been added in Figure 8, and the dotted lines are present to aid in the overlay. Note that all mesh lines in adjoining figures meet at common boundary points. As a result, some of the figures contain more mesh lines than are

required to describe their interfaces. All of the initial figures required for the overlay are shown in Figure 9, with (b), (c), and (d) representing the same geometry but different meshes. In order to locate the initial figure origins, it is convenient to construct Figure 10, 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 8 because of the variable mesh. The right half of Figure 8 may be described by positioning Figure 9(a) with its origin at row 0, column 10; Figure 9(b) with its origin at row 0, column 12, rotated through 120° ; Figure 9(c) with its origin at row 0, column 12, rotated through 60° ; Figure 9(d) with its origin at row -3, column 15, rotated through 60° ; Figure 9(d) with its origin at row 0, column 15, rotated through 60° ; and Figure 9(e) with its origin at row 3, column 12, rotated through 60° and reflected. The left half of Figure 8 is described in a similar manner.

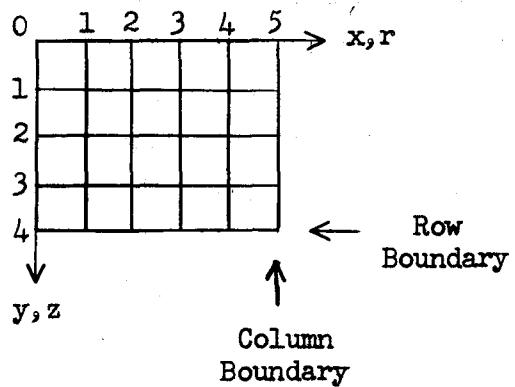


FIGURE 1

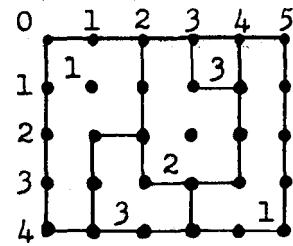


FIGURE 2

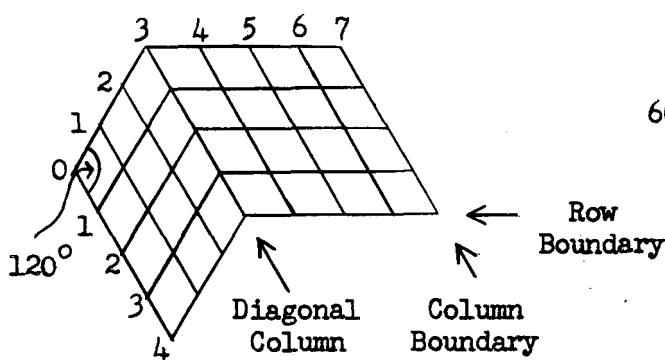


FIGURE 3

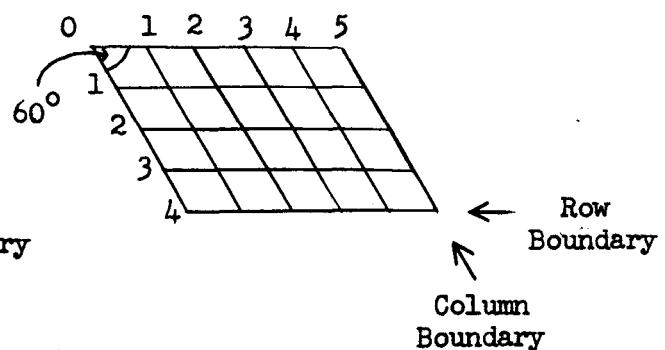


FIGURE 4

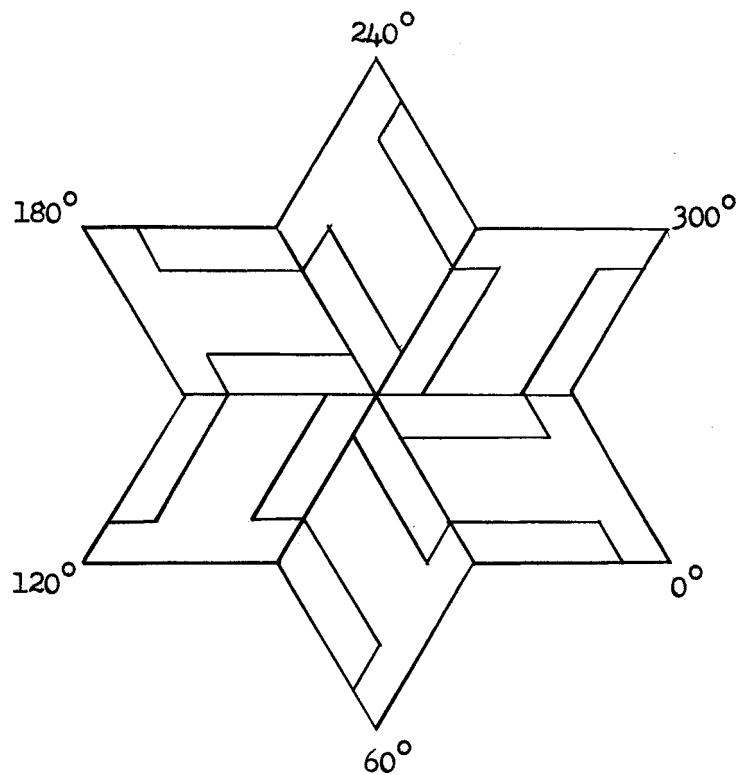


FIGURE 5

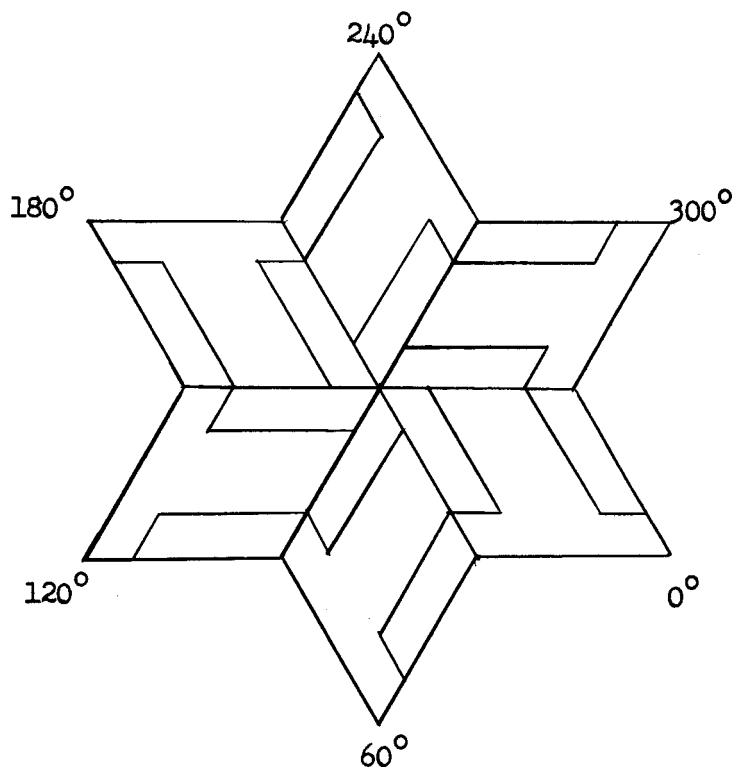


FIGURE 6

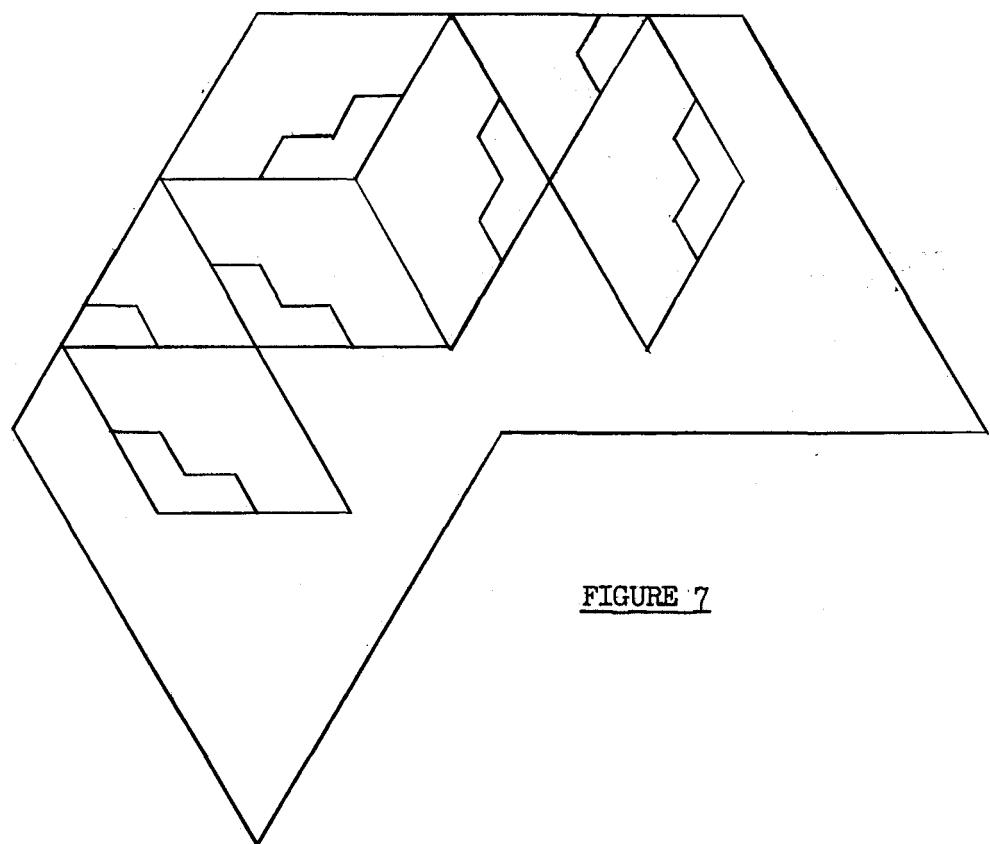


FIGURE 7

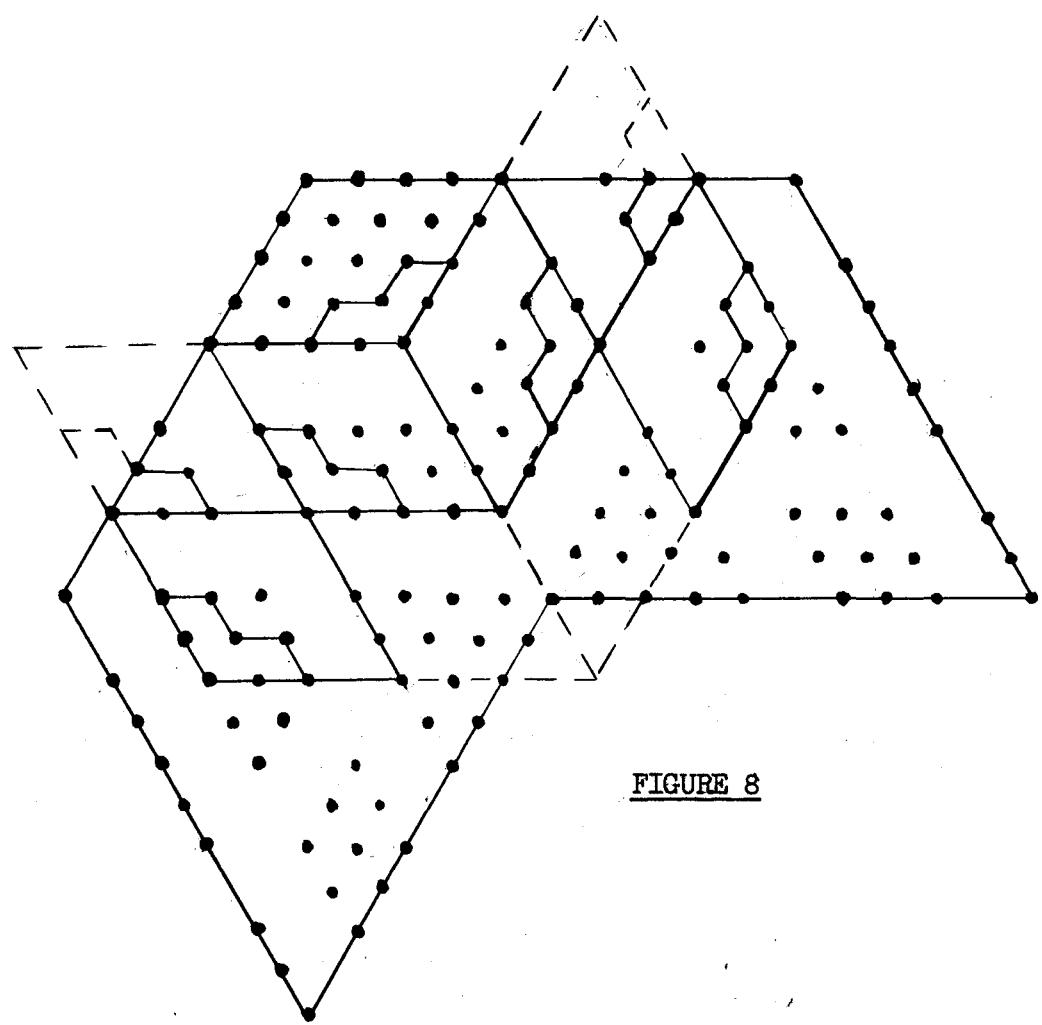


FIGURE 8

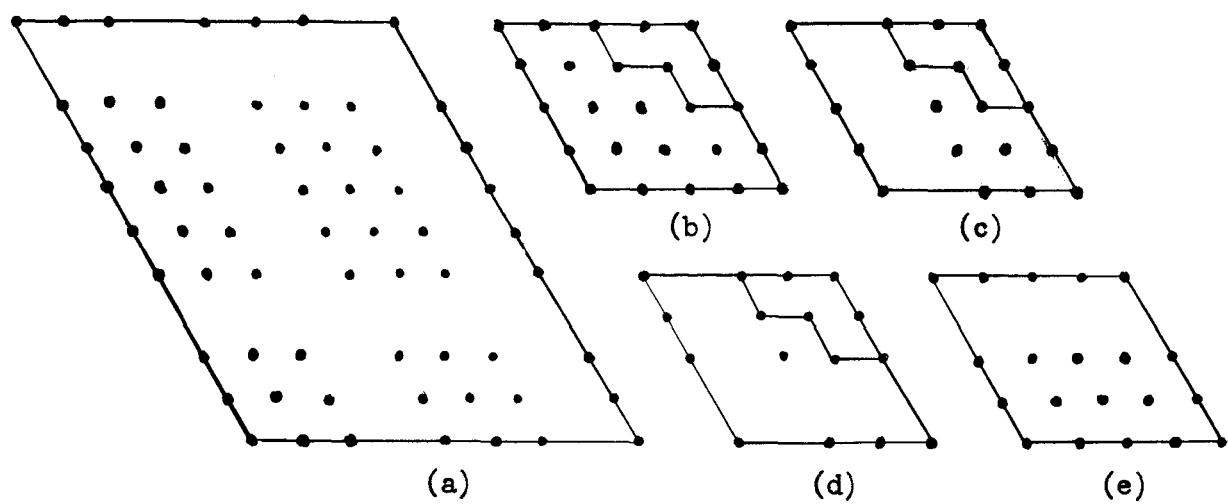


FIGURE 9

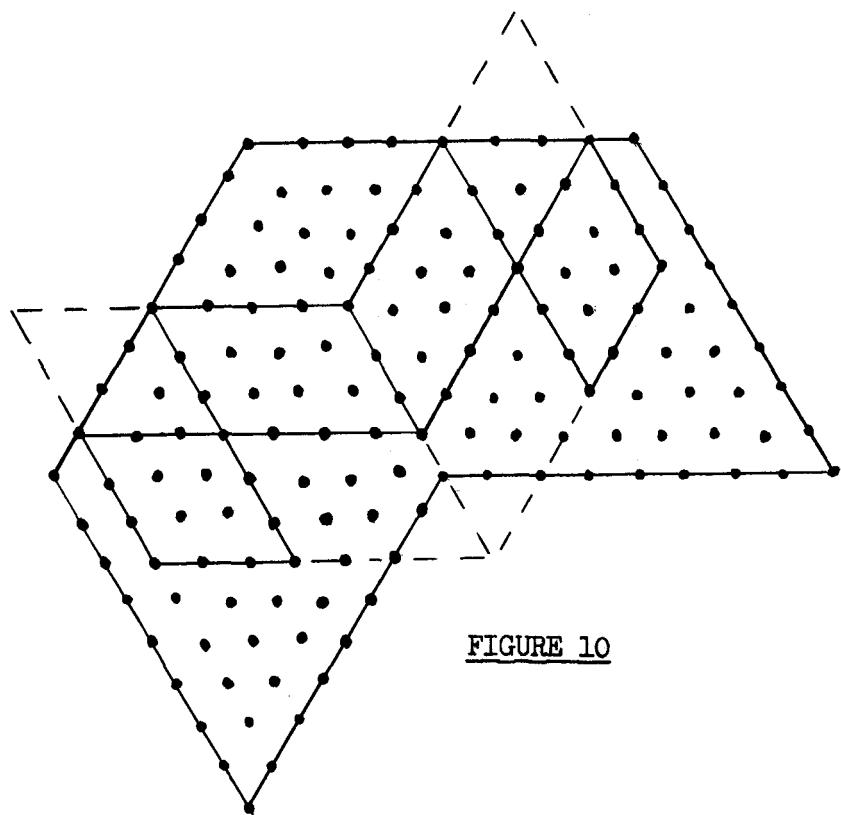


FIGURE 10

IV. EDITING

Integration Edits

The integration editing includes flux integrals, power fractions, absorption rates, fission rates, average nuclide concentrations, group-dependent and group-independent bucklings, k^∞ and k^{eff} , and flux-weighted average macroscopic parameters. As mentioned in Section III, this editing is done using the composition overlay unless an edit region overlay is provided, in which case this overlay is used instead. The following description is in terms of compositions but edit regions are implied if this overlay is present.

Each of the integral quantities is edited only for those individual compositions and sets of compositions specified in the input. In PDQ-6, however, a set of composition numbers alone may not define the integrals required, since a single initial figure may appear several places in the mesh. For this reason, a set of final figure numbers is specified with each set of composition numbers. The programs assign a unique EDIT number to each set of compositions (PDQ-5) or to each figure-composition set (PDQ-6), and all integral quantities are then listed by EDIT. Note that, in PDQ-6, a mesh element is included in a particular EDIT only if it is within one of the specified final figures and also a part of one of the specified compositions.

Pointwise Edits

All pointwise editing is done over a single region of the mesh. This region is specified in the input by giving left-hand and right-hand column numbers and top and bottom row numbers. The region is thus a rectangle in PDQ-5 and a parallelogram or a chevron in PDQ-6.

Editing of each pointwise quantity is optional, including the flux in each group, the point power, the quadrant power, and the initial and final concentrations for each nuclide. Point power may be edited either as the average of the nonzero quadrant values at a point or as the largest of these values. Quadrant power values are edited only for those points at which any two nonzero values differ by more than 5%. The quadrant values are actually triangle values in PDQ-6 and there are six at each point. Concentrations are edited by mesh rectangle in PDQ-5 and by mesh triangle in PDQ-6.

Re-Editing

If the output flux of a problem has been saved on a filetape, additional edits may be obtained by rerunning the problem under the re-edit option. The spatial and depletion calculations are automatically bypassed and all edits requested in the input are performed, with the exception of average and point-wise final nuclide concentrations.

The only input quantities that may not be changed between the original run and the re-edit are the number of groups and the number of mesh points in each direction. In particular, the changes may include altering the placement of compositions or edit regions in the mesh and altering the specification of composition or region sets for integration editing. Note that the group-dependent and group-independent buckling calculations are in error on a re-edit unless the input eigenvalue is replaced by the converged value.

V. FILETAPES

The input for a complete job may be preceded by cards giving the reel numbers of one or two input filetapes. These tapes, designated filetape 12 and filetape 13, are mounted at the beginning of the job and are not removed until the job is finished. The filetapes are actually merge tapes, and selected quantities from any problem (case) may be added to either tape. An option permits a blank to be mounted as filetape 13 and the output of some problem to be placed on this tape as the beginning of a new merge. The quantities that may be saved include pointwise flux, quadrant power, nuclide concentrations, cross-section tables, and integrals. An identification number provided in the input is placed on the filetape with the output quantities; this number should be different from all other identifications on the tape. Note that each problem on a filetape is completely independent of every other problem. Spatial and depletion problems for both PDQ-5 and PDQ-6 may be intermingled on a single filetape in any manner.

The first case of any job may specify filetape input for the flux, concentrations, and tables. These may be taken from any problem or set of problems on either or both filetapes. The flux must be compatible with the current problem in number of groups, column boundary, and row boundary, and the concentrations must be compatible in number of time-varying nuclides and number of depleting mesh elements. Beyond the first case of a job, the input flux and concentrations must be obtained either from cards or from the output of the previous case. Filetape tables used in the first case, however, are automatically retained by the programs and used as input to all subsequent cases.

A comment is included in the output after each quantity is read from or added to a filetape. The current number of data blocks is also indicated at the end of each problem which adds to a tape. If this number exceeds 15,000, no further additions may be made.

Care must be exercised if there is a failure during a problem which adds to a filetape. The faulty problem must generally be rerun before any other data can be added to the tape. The input deck need not be altered for a rerun, but the operator must be informed that it is a rerun and of which case. The operator must also know whether the flux was added to a filetape

before the failure occurred, since the spatial calculation can be bypassed in this case. If the faulty problem is not to be rerun, its output identification number must be repeated in the next problem which adds to the filetape, and the operator must be told that the new problem is a rerun.

A detailed description of the merge filetape is given below for use in programming auxiliary calculations which require this data. Assuming all possible data is saved, files (2) through (20) are present for each problem in the order listed. File (1) precedes the first problem on the tape and file (21) follows the last problem. The quantities N3, N4, N5, and N6 are as defined in the FTB program description (Reference 6).

Filetape Sentinel

(1) N3 = -1111
 N4 = 122
 N5 = 1
 N6 = 128

<u>Word</u>	<u>Data</u>
1	Reel number

Problem Sentinel

(2) N3 = -2222
 N4 = 122
 N5 = 1
 N6 = 128

<u>Word</u>	<u>Data</u>
1	Output ID
2	Number of blocks of data on tape through this block
3	Problem type (1 = fixed-source, 2 = eigenvalue, 3 = one-iteration)
4	Adjoint (0 = no, 1 = yes)
5	Geometry (1 = xy, 2 = rz, 4 = hexagonal)
6	Total number of groups
7	Number of thermal groups

<u>Word</u>	<u>Data</u>
8	Column boundary
9	Row boundary
10	Top boundary condition (0, ± 1)
11	Left boundary condition (0, 1)
12	Bottom boundary condition (0, 1)
13	Right boundary condition (0, 1)
14	$N_4 \left. \right\}$
15	$N_5 \left. \right\}$ for nuclide concentration file (12), if present
16	$N_6 \left. \right\}$
101	1 if flux saved, 0 otherwise
102	1 if quadrant power saved, 0 otherwise
103	1 if concentrations saved, 0 otherwise
104	1 if tables saved, 0 otherwise
105	1 if integrals saved, 0 otherwise

Table Data Files

(3)

$N_3 = -6661$

$N_4 = 122$

$N_5 = 1$

$N_6 = 128$

Words 1 through 4 of this file are N_3 through N_6 for file (4). The constant values are $N_3 = -6662$, $N_4 = 1$, and $N_6 = 256$.

(4)

$N_3 - N_6$ are given in file (3). This file contains the index for each table set as follows:

<u>Word</u>	<u>Data</u>
1	Numeric ID
2 - 5	Alphanumeric ID (4A6 format)
6 - 7	T, u for Σ_0 table
8	Number of $\sigma(i,g)$ tables
9	Number of interpolating tables
10	Four words for each $\sigma(i,g)$ table (if any) giving T, u, g, i . Followed by six words for each interpolating table giving T, u, g, i, t, θ .
:	

In the above, T = table number

$u = 0$ if no fission in Σ_0 or $\sigma(i,g)$, $u = 1$ if fission cross sections

$u = 0$ in interpolating tables for Σ_0 and σ , $u = 1$ for G

g = group

i = nuclide ID, except i = t for interpolating $\Sigma_0(t,g)$

t = type for interpolating $\sigma(i,g,t)$ or $G(i,g,t)$

t = 8 for $\Sigma_0(t,g)$ with t given as i

θ = order of interpolation

(5) $N_3 = -6663$

$N_4 = 122$

$N_5 = 1$

$N_6 = 128$

Words 1 through 4 of this file are N_3 through N_6 for file (6). The constant values are $N_3 = -6664$, $N_4 = 1$, and $N_6 = 256$.

(6) $N_3 - N_6$ are given in file (5). This file contains tables, which may be Σ_0 , $\sigma(i,g)$, mask, or function tables. For each table:

<u>Word</u>	<u>Data</u>
1	Number of words in table <u>following</u> word 3
2	Table number
3	ID of table set in which table is defined for Σ_0 , $\sigma(i,g)$, and function tables; zero for mask tables

For Σ_0 tables words 4, ... contain D_g , Σ_g^a , Σ_g^r , $\nu\Sigma_g^f$, and $\kappa\Sigma_g^f$ for $g = 1, \dots$, number of groups. Values of $\nu\Sigma_g^f$ and $\kappa\Sigma_g^f$ may be missing.

For $\sigma(i,g)$ tables words 4, ... contain σ^{tr} , σ^a , σ^r , σ^f , ν , and κ for group g; the final three numbers may be omitted.

For function tables word 4 is the mask table number, word 5 is 0 or 1 for normal or inverse interpolation, words 6 and on contain diagonal function values followed by off-diagonal values ordered according to the mask.

For mask tables words 4, 5, and 6 are the nuclide ID's of variables N_1 , N_2 , and N_3 which are negative to signal that $N(t)/N(0)$ is to be used.

$ID_2 = ID_3 = 0$ for one-dimensional tables; $ID_3 = 0$ for two-dimensional tables.

Following are blank words for each negative ID (if any). Following the blanks (if any) are words containing dimension, number of diagonals, and number of off-diagonals. Next are values of N_1 (or $N/N(0)$) for each diagonal, then values of N_2 , and finally N_3 (if any). Following the diagonal values are off-diagonal values of N_1 , then N_2 , and finally N_3 .

(7)

N3 = -6660
 N4 = 122
 N5 = 1
 N6 = 128

<u>Word</u>	<u>Data</u>
1	Output ID

Flux Files

(8)

N3 = -3330 - g, where $g = 1, 2, \dots$, number of groups
 N4 = column boundary + 1
 N5 = row boundary + 1
 N6 = 768

These files contain the flux for each group by column within each row, including zero values on zero flux boundaries. The flux values are not normalized.

(9)

N3 = -3330
 N4 = 122
 N5 = 1
 N6 = 128

<u>Word</u>	<u>Data</u>
1	Output ID
2	Converged eigenvalue

Quadrant Power File

(10)

PDQ-5	N3 = -4444 $\{$ N4 = 4 * (column boundary + 1) N5 = row boundary + 1 N6 = 3072 $\}$ N4 = 6 PDQ-6 $\{$ N5 = (column boundary + 1) * (row boundary + 1) N6 = 256 $\}$
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This file contains quadrant (PDQ-5) or triangle (PDQ-6) power values by point for each row. In PDQ-5 the four values at each point represent the upper left, upper right, lower left, and lower right quadrants. In PDQ-6 the six values at each point represent the upper left, upper, upper right, lower left, lower, and lower right triangles. The power values are not normalized.

(11) N3 = -4440
 N4 = 122
 N5 = 1
 N6 = 128

<u>Word</u>	<u>Data</u>
1	Output ID

Nuclide Concentration File

(12) N3 = -5555
 N4 = number of nuclides
 N5 = number of depletable mesh elements (in right address)
 N6 = 2 * (least multiple of 128 which is \geq (N4 + 6))

This file contains nuclide concentrations for each depletable mesh element by column, then by row.

(13) N3 = -5550
 N4 = 122
 N5 = 1
 N6 = 128

<u>Word</u>	<u>Data</u>
1	Output ID

Integral Files

(14) N3 = -7771
 N4 = 122
 N5 = 1
 N6 = 128

<u>Word</u>	<u>Data</u>
1	$K_1 = (\text{total number of EDITS}) * (7 * (\text{number of groups}) + 1)$
2	Flux normalization factor, β , if problem is <u>not</u> depletable, or fast flux normalization factor, β_1 , if problem <u>is</u> depletable, where

$$\beta = \frac{\int_{\text{fuel}} dV}{\sum_g \int \kappa \sum_g^f \varphi_g dV}$$

and

$$\beta_1 = \frac{\text{input power (in watts)} * \text{power fraction}}{\sum_g \int \kappa \sum_g^f \varphi_g dV}$$

and $\beta = \beta_1 = 1.0$ if the denominator is zero.

- 3 β
- 4 Total number of groups
- 5 Number of thermal groups
- 6 Total number of EDITS
- 7 Number of EDITS actually performed

(15) $N_3 = -7772$

$N_4 = 1$

$N_5 = K_1$ (file (14), word 1)

$N_6 = 256$

For each EDIT, this file contains

$$\int dV, \int \varphi_1 dV, \int \varphi_2 dV, \dots, \int \varphi_G dV$$

followed by

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

for each group g . The symbol φ_g refers to un-normalized flux. If the number of EDITS was reduced due to storage limitations (as noted in the output), the

number of words in this file does not reflect this; however, the amount of useful data does.

(16) $N_3 = -7773$

$N_4 = 122$

$N_5 = 1$

$N_6 = 128$

<u>Word</u>	<u>Data</u>
1	$K_2 = (\text{total number of EDITs}) * (\text{number of groups}) * (\text{number of power fraction + absorption rate + fission rate edit requests})$
2	Elapsed time (in hours) at beginning of depletion calculation (T_0)
3	Elapsed time (in hours) at end of depletion calculation (T_1)
4	Input power (in watts) * power fraction
5	Fast flux normalization factor
6	Thermal flux normalization factor (for <u>last</u> interval)
7	Number of thermal flux <u>re</u> -normalizations + 1
8	Number of power fraction edit requests
9	Number of absorption rate edit requests
10	Number of fission rate edit requests
11	Total number of EDITs
12	Number of EDITs actually performed
13	Total number of groups
14	Number of thermal groups

If the problem is not depletable, words 1 through 14 are zero.

(17) $N_3 = -7774$

$N_4 = 1$

$N_5 = K_2$ (file (16), word 1)

$N_6 = 256$

This file is present only if $K_2 \neq 0$. It contains, for each EDIT, the power for all groups g , then all nuclides i in the order requested,

$$\int \kappa_i \sigma_i^f, g_{G_i}^f, g_{N_i} \varphi_g dV ,$$

followed by the absorption rate for all groups g, then all nuclides i in the order requested,

$$\int \sigma_i^a, g_{G_i}^a, g_{N_i} \varphi_g dV ,$$

followed by the fission rate for all groups g, then all nuclides i in the order requested,

$$\int \sigma_i^f, g_{G_i}^f, g_{N_i} \varphi_g dV .$$

The flux φ_g in the above integrals has been normalized by $\beta_1/10^{24}$. The same comments as in file (15) with respect to the number of EDITS performed are true here also.

(18) $N_3 = -7775$

$N_4 = 122$

$N_5 = 1$

$N_6 = 128$

<u>Word</u>	<u>Data</u>
1	$K_3 = (\text{total number of EDITS}) * (\text{number of average nuclide concentration edit requests} + 1)$
2	Elapsed time (in hours) at beginning of depletion calculation (T_0)
3	Elapsed time (in hours) at end of depletion calculation (T_1)
4	Input power (in watts) * power fraction
5	Fast flux normalization factor
6	Thermal flux normalization factor (for <u>last</u> interval)
7	Number of thermal flux <u>re</u> -normalizations + 1
8	Number of average nuclide concentration edit requests
9	Total number of EDITS
10	Number of EDITS actually performed

If the problem is not depletable, words 1 through 10 are zero.

(19) $N_3 = -7776$

$N_4 = 1$

$N_5 = K_3$ (file (18), word 1)

$N_6 = 256$

This file is present only if $K_3 \neq 0$. It contains, for each EDIT, $\int dV$ followed by $\int N_i dV$ for each nuclide i in the order requested. The same comments as in file (15) with respect to the number of EDITS performed are true here also.

(20) $N_3 = -7770$

$N_4 = 122$

$N_5 = 1$

$N_6 = 128$

<u>Word</u>	<u>Data</u>
1	Output ID

End-of-Tape Sentinel

(21) $N_3 = -2222$

$N_4 = 122$

$N_5 = 1$

$N_6 = 128$

This file is identical to the last file (2) on the tape except that word 1 is zero and the block count in word 2 is updated.

VI. INPUT PREPARATION

This section describes all of the input required for spatial problems in which macroscopic cross sections are input by composition. Cross section tables and the additional input required for depletion calculations are described in Reference 2.

Familiarity with the definitions and concepts developed in Reference 7 is assumed in what follows. In particular the reader must be familiar with the makeup of an input deck, the representation of fixed- and floating-point numbers on input forms, sequential expansions, and the use of job decks consisting of multiple cases. All of the input forms required are attached to this report. The phrase "complete set of values" as used below means that the final termination point must equal the total number of such items (compositions, edit regions) as specified in the control data. Note that every input restriction is checked by the programs; a problem that violates one or more restrictions will be rejected with suitable error comments. Note also that a PDQ-5 input deck may not contain more than 13,000 numbers, card numbers included; the PDQ-6 limitation is 14,500 numbers.

Control Data

All of the control data is specified on PDQ-5/6 Input Forms I and II.

(1) FILETAPE Cards

These cards precede the input for the first case of a job. Filetapes are generally identified by an "R" followed by the reel number. If a new merge is being started, the filetape 13 reel is identified as a blank by using the problem number followed by a "Z".

(2) Title Card

The information on this card is used to title each page of problem output. There should be a different title card for each case of a job.

(3) Card 010001

The three problem types are described in Section II. The present version of PDQ-6 is restricted to eigenvalue problems.

Table input of cross sections may be used in all except fixed-source problems and must be used in depletion problems.

The adjoint solution may only be requested in eigenvalue or one-iteration problems with at least one nonthermal group.

The geometry option is omitted in PDQ-6.

Input areas, if present, must be in the same units as the mesh intervals and the input editing is done in these units. If the mesh intervals are in inches, however, they are converted to centimeters for all calculations, including the integration edits.

The total number of groups must be ≥ 1 and ≤ 5 and may not change between cases of a job.

In the present versions the number of thermal groups is restricted to 1.

(4) Card 010002

The number of compositions (which is actually the largest composition number present in the input) must be ≥ 1 and ≤ 100 (PDQ-5) or ≤ 99 (PDQ-6). It is not necessary that every composition appear in the mesh.

The number of edit regions (largest edit region number present in the input) must be ≥ 0 and ≤ 500 (PDQ-5) or ≤ 99 (PDQ-6). If 0, integration editing is done by composition rather than by edit region. It is not necessary that every edit region appear in the mesh.

The row and column boundaries may not change between cases of a job.

The number of solution columns is given by (column boundary + left boundary condition + right boundary condition - 1) and the number of solution rows by (row boundary + |top boundary condition| + bottom boundary condition - 1), where the boundary conditions are -1, 0 and +1 for rotation, zero flux, and zero derivative, respectively.

In PDQ-5 the number of solution columns must be ≥ 3 and ≤ 376 . The number of solution rows must be exactly 2 in one-dimensional problems and must be ≥ 3 and ≤ 501 in all other problems.

In PDQ-6 the column boundary must be ≤ 299 and the row boundary must be ≥ 3 and ≤ 499 . The column boundary must be divisible by 2 if the top boundary condition is rotation.

The diagonal column is omitted in PDQ-5. In PDQ-6 it must be ≥ 2 and \leq (column boundary - 2). The diagonal column must equal half the column boundary if the top boundary condition is rotation.

In r-z geometry the top boundary condition may not be rotation and the left boundary condition must be zero derivative.

The left and right boundary conditions must be the same if the top boundary condition is rotation.

The top and bottom boundary conditions must be zero derivative in one-dimensional problems.

(5) Card 010003

λ_0 is actually used only in the first case of a job. In all succeeding cases the output eigenvalue of the previous case is used automatically.

ϵ_1 is used as indicated in Equations (2.4) and (2.5).

ϵ_2 is not used in the present versions and should be zero.

If table input is used, the macroscopic edit calculates average macroscopic parameters for each edit region (or set of regions) specified in the edit control data. Otherwise, this edit lists the input macroscopic parameters by composition.

The absorption rate edit calculates, for each edit region (or set of regions) specified in the edit control data, the fraction of the total absorption contributed by the region together with the fraction of the total absorption and the fraction of the region absorption contributed by each group.

An edit region picture may not be requested if edit regions are not used in the problem.

If certain errors are found in the geometry description or in the input areas, the corresponding picture edit is performed even if not requested.

(6) Card 010004

The number of X values specified must exactly equal the total number of groups. This card must be present in eigenvalue and one-iteration problems and may not be present in fixed-source problems.

(7) Card 010005

The boundaries for pointwise editing must satisfy the inequalities ($0 \leq$ left boundary $<$ right boundary \leq column boundary) and ($0 \leq$ top boundary $<$ bottom boundary \leq row boundary).

The number of flux options specified must exactly equal the total number of groups, and the special thermal flux option may not be used in the present versions.

The quadrant power edit lists the four quadrant values (PDQ-5) or six triangle values (PDQ-6) at each point in the pointwise edit region at which any two nonzero values differ by more than 5%.

The pointwise average power is the arithmetic average of the nonzero quadrant (triangle) values at a point; the pointwise peak power is the largest of these values.

(8) Card 010006

This card must appear in the input deck for each case of a job.

A source of input concentrations must be specified in depletion problems, and the concentrations must be specified as not used in all other problems. Similarly, a source of input tables must be specified if table input has been indicated, and the tables must be specified as not used otherwise.

Filetape data may be used as input only in the first case of a job, and previous case output may be used as input only beyond the first case. Card input may be used in any case. If input tables are from both cards and filetape, the filetape source is indicated.

The input tables specification is ignored beyond case one and may be zero. If the case one tables are from a filetape, this data is automatically retained and used as input to all subsequent cases. Otherwise, card input is used in every case.

The ID's must be nonzero if the corresponding input is from a filetape; they are ignored and may be zero otherwise.

(9) Card 010007

This card must appear in the input deck for each case of a job.

A new merge may not be specified in some case if filetape 13 has been used for input or output in a previous case. On the other hand, if a new merge has been started in some case, a subsequent case may use the filetape 13 option to add to the new merge.

The output ID must be nonzero if output is saved; it is ignored and may be zero otherwise. The ID should never exceed 32767 in absolute value.

Concentrations may be saved only in depletion problems and tables may be saved only if table input is indicated.

The output save option and quantities to be saved must be compatible. Either an output tape is not specified and nothing is saved or an output tape is specified and at least one quantity is saved.

(10) Card 010008

A depletion problem is one for which this card is present in the input deck.

The initial and final times are the total elapsed times (in hours) at the beginning and end of the depletion calculation. The initial time must be nonnegative and may not exceed the final time. If the two times are equal, the depletion calculation is bypassed but depletion editing is performed.

ΔT_{max} is the maximum elapsed time (in hours) for a flux renormalization. It may be zero if the initial and final times are equal but must be strictly positive otherwise.

The power (in watts) and power fraction must both be nonnegative.

The maximum xenon option is used to bypass the flux calculation and use the input flux in the depletion calculation. In this case the input may not specify that the output flux is to be saved on a filetape.

The replacement option refers to the replacement of spatially-varying concentrations in specified compositions with homogeneous concentrations in the input deck. When this option is used, the input concentrations option must specify a filetape or the output of the previous case.

(11) Card 010009

This card may be used to re-edit a problem which has been successfully completed. It may only be used in a single-case job. The input flux option

must specify a filetape, the output ID used when the problem was originally run must be made the input flux ID, and the output eigenvalue should be provided in place of λ_0 . The programs bypass the flux calculation, set the final time equal to the initial time to bypass the depletion calculation (except for editing), ignore the output save option, and delete any requests for average concentration edits and pointwise final concentration edits.

(12) Card 010010

This card may be used to check an input deck without running the problem. The standard input check processes all of the cases in a job, even if errors are found. FILETAPE cards should be omitted from the deck, but cards 010006 and 010007 need not be changed since all filetape usage is automatically bypassed. All input editing is done except for the macroscopic edit when there is table input.

To obtain this edit, the macro input check must be used. This is available only in the first case of a job and only this case is processed. Output filetape usage is automatically bypassed but FILETAPE cards must be present for any input filetapes. Note that the macroscopic edit is actually performed only if no input errors are detected.

Integration Sets

Those individual edit regions and sets of edit regions for which integrals are required are specified on PDQ-5/6 Input Form III. The subseries numbers range from 100 to 999 for PDQ-5 and from 100 to 499 for PDQ-6. There must always be at least one subseries present. If an edit region overlay is not used, composition numbers are specified in place of edit region numbers.

(1) PDQ-5

The data for each subseries is of the general form

$$r_1, \pm r_2, \pm r_3, \dots, \pm r_n .$$

A negative number indicates all regions from the previous region number through the negative region number. The region 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 2, 5, -7, 9, 14 specifies regions 2, 5, 6, 7, 9, and 14.

Subseries 100 specifies individual edit regions and each of subseries 101 - 999 specifies a single set of edit regions. Subseries 100 may be omitted but then subseries 101 must be present. The first missing subseries (other than 100) terminates the data.

(2) PDQ-6

The data for each subseries is of the general 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 set of final figure numbers from a set of edit region numbers. A negative figure number indicates all figures from the previous figure number through the negative figure number, and similarly for a negative region number. For each set, 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 figure-region set. In each of subseries 200 - 299, the figure numbers are expanded to remove negative signs and a figure-region set of the form

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

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

$$f_i, 0, r_j$$

is constructed for each figure-region pair.

Macroscopic Data

Values of D , Σ^a , Σ^r , $\nu\Sigma^f$, and $\kappa\Sigma^f$ are specified by group and composition on PDQ-5/6 Input Form IV. The series number is 02 and the subseries number is the group number. There must be subseries for each group and a complete set of values for each subseries. If every value of $\kappa\Sigma^f$ in the entire series is zero, $\kappa\Sigma^f$ is set equal to $\nu\Sigma^f$.

An internal symmetry boundary condition may be obtained by setting all the cross sections in a composition to zero. The flux is then not defined interior to the composition and the flux derivative is set to zero on its boundary. It is extremely important that the input flux be zero for such a composition since the programs do not check this and a nonzero value may cause failure after several iterations.

Buckling Values

Buckling values are optional in all problems. They are specified by group and composition on PDQ-5/6 Input Form V. The series number is 08 and the subseries number is the group number. There need not be a subseries for each group but there must be a complete set of values for each subseries present. Subseries 0 may be used to specify values for all groups in which group-dependent values are not provided.

Source Values

Source values are present only in fixed-source problems. They are specified by group and composition on PDQ-5/6 Input Form V. The series number is 04 and the subseries number is the group number. There must be a subseries for each group and a complete set of values for each subseries.

Areas

Composition and edit region areas are optional. They are specified on PDQ-5/6 Input Form V using series number 18. The subseries number is 1 for composition areas and 2 for edit region areas, and there must be a complete set of values for each subseries present. The true composition and edit region areas are calculated, and if any input value is incorrect by more than 1%, the calculated values are printed and the problem is rejected. Note that the true areas may be obtained during an input check by inputting zero areas.

Input Flux

If the input flux is from cards, flux values are specified by group and composition on PDQ-5/6 Input Form V. The series number is 21 and the subseries number is the group number. There must be a subseries for each group and a complete set of values for each subseries. If this series is present but not required, the cards are processed and checked for errors but the data is not used.

Geometry

(1) PDQ-5 Mesh Intervals

Mesh intervals for each coordinate direction are specified on PDQ-5/6 Input Form V. The series number for the column intervals is 05 and for the row intervals is 06, the subseries number is 0, and the final termination points are the column boundary and row boundary. If the two sets of mesh intervals are identical, the 06 series may be omitted. If there is 180° rotational symmetry, the column intervals must be symmetric about the midpoint. In a one-dimensional problem, if the row interval is not unity, it is set to unity by the program.

(2) PDQ-5 Composition and Edit Region Overlay

The placement of compositions and edit regions in the mesh is specified on PDQ-5/6 Input Form VI. The series number is 17 and the subseries number is 1 for the composition overlay and 2 for the edit region overlay. The total number of overlay sets in either subseries may not exceed 1000. Note that no portion of the mesh may remain unspecified after either overlay is complete. Note also that the edit region overlay is present only if edit regions are being used.

(3) PDQ-6 Mesh Intervals

Mesh intervals are specified for each composition basic figure on PDQ-5/6 Input Form V. The series number is 05 for the column intervals and 06 for the row intervals, the subseries number is the composition basic figure number, and the final termination points are the basic figure column and row boundaries. If the two sets of mesh intervals are identical for some basic figure, the 06 subseries may be omitted.

(4) PDQ-6 Composition and Edit Region Overlay

The overlays for the composition and edit region basic figures are specified on PDQ-5/6 Input Form VI. The series number is 8 for the composition overlays and 9 for the edit region overlays. The subseries number is the initial figure number, which consists of a two-digit basic figure number followed by a one-digit auxiliary figure number.

Each basic figure is described using auxiliary figure number 0. The description consists of a control card (sequence number 00) giving the column and row boundaries of the basic figure, followed by a complete overlay beginning with sequence number 01. Composition and edit region basic figures are each numbered consecutively beginning at 01, but the basic figures of each type may be numbered in any order.

If there are several figures with the same mesh but with different overlays, one of these may be described as a basic figure and the rest may be described as auxiliary figures. In this way only one set of mesh intervals is required. The auxiliary figures of a basic figure are numbered consecutively beginning at 1. An overlay is provided for each auxiliary figure, beginning with sequence number 01. The auxiliary figure overlay need not be complete, however, since it is appended to the basic figure overlay and thus represents a modification in this overlay.

(5) PDQ-6 Initial Figure Overlay

The initial figure overlay is specified on PDQ-5/6 Input Form VI. The series number is 17 and the subseries number is 0. Each overlay set includes a final figure number ($\geq 1, \leq 99$), the composition initial figure number, the edit region initial figure number, the column and row at which the origins are to be placed, the multiple ($\geq 0, \leq 5$) of 60° through which the figures are to

be clockwise rotated, and the reflection indicator (0 = no, 1 = yes). The composition and edit region initial figures must have the same column and row boundaries, and the mesh intervals associated with the composition figure are also used for the edit region figure. If there are no edit regions, the edit region initial figure number is ignored and may be zero. The final figure numbers are arbitrary and need not be distinct; they are used only for integration editing.

VII. OUTPUT

This section describes all of the output that may be obtained from a spatial problem. The additional output available from a depletion problem is described in Reference 2.

Input Edit

The input edit includes a listing of each control parameter that cannot be deduced from the remainder of the output. It also includes the set of edit regions (compositions) corresponding to each EDIT, the sequence of mesh intervals in each coordinate direction, the distance from column 0 to each succeeding column and from row 0 to each succeeding row, and, optionally, macroscopic parameters and pictures of the placement of compositions and edit regions in the mesh. In addition, the reel number and identification number are given for each input quantity taken from a filetape. There is also an indication when the output of the previous case is used as input.

Iteration Edit

Values of $\bar{\omega}$, ω , and $\underline{\omega}$ are edited for each group, together with the number of omega iterations performed. For each outer iteration the initial residual (Equation (2.3)), ratio of final to initial residual, and number of iterations performed are edited for each group. In fixed-source and one-iteration problems the final maximum percentage change (Equation (2.5)) is edited in place of the residuals. Values of λ , $\bar{\lambda}$, $\underline{\lambda}$, and the convergence ratio (Equation (2.4)) are also edited, together with the parameters used to accelerate the outer iterations. A complete description of the iteration output is given in Reference 4.

Integration Edit

As described in Section IV, integrals are calculated only for those individual edit regions (compositions) and sets of edit regions specified in the input. The first integration section edits the area and the integrated and averaged flux for each group. All of the flux integrals and averages are multiplied by the normalization factor

$$N = \frac{\int dA}{\int \sum_{g=1}^G \kappa \sum_f \varphi_g dA} , \quad (7.1)$$

the integrals in this equation being taken over those segments of the mesh in which the power is nonzero.

The second integration section edits the fraction of the total power contributed by the region being integrated and the fraction of the region power contributed by each group.

The third integration section is the only one which is optional. It 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.

The fourth integration section edits the group-independent buckling, K^∞ by group and the sum over groups, and K_g^{eff} by group and the sum over groups. The group-independent buckling is obtained by eliminating the flux and solving for B_g^2 in the set of equations

$$\left\{ (B_g^2 D_g + \bar{\Sigma}_g^t) \varphi_g = \frac{\chi_g}{\lambda} \sum_{j=1}^G \bar{\Sigma}_j^f \varphi_j + \bar{\Sigma}_{g-1}^r \varphi_{g-1} \right\}_{g=1}^G \quad (7.2)$$

Here $\bar{\Sigma}_g^t = \bar{\Sigma}_g^a + \bar{\Sigma}_g^r + D_g B_g^2$, where B_g^2 is the input buckling, and

$$\bar{\Sigma} = \frac{\int \Sigma \varphi dA}{\int \varphi dA} \quad (7.3)$$

is the flux-weighted average value for any macroscopic parameter Σ . K_g^{eff} is the contribution of group g to the total criticality, calculated by

$$K_g^{\text{eff}} = \left(\frac{\bar{\Sigma}_{g-1}^r K_{g-1}^{\text{eff}}}{\bar{\Sigma}_{g-1}^f} + \chi_g \right) \frac{\bar{\Sigma}_g^f}{\bar{\Sigma}_g^t + D_g B_g^2} , \quad (7.4)$$

where

$$K_1^{\text{eff}} = \frac{\overline{\chi_1} \overline{\nu \Sigma_1^f}}{\overline{\Sigma_1^t} + D_1 \overline{B_1^2}} \quad (7.5)$$

K_g^∞ is calculated in the same manner but with leakage ignored, that is, with

$\overline{\Sigma_g^t} + D_g \overline{B_g^2}$ replaced by $\overline{\Sigma_g^a} + \overline{\Sigma_g^r}$.

The fifth and final integration section edits the flux-weighted average macroscopic parameters $\overline{D_g}$, $\overline{\Sigma_g^a}$, $\overline{\Sigma_g^r}$, $\overline{\nu \Sigma_g^f}$, and

$$\overline{B_g^2} = \frac{1}{\overline{D_g} \tilde{\varphi}_g} \left(\frac{\chi_g}{\lambda} \sum_{j=1}^G \overline{\nu \Sigma_j^f} \tilde{\varphi}_j + \overline{\Sigma_{g-1}^r} \tilde{\varphi}_{g-1} - \overline{\Sigma_g^t} \tilde{\varphi}_g \right) , \quad (7.6)$$

where $\tilde{\varphi}$ designates the integral of the flux.

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.

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 $\Sigma \varphi$ is simply $\Sigma \varphi$. Given mesh rectangle r , bounded by columns $s-1$ and s , rows $t-1$ and t ,

$$\int_r \varphi dA = \frac{h_s h_t}{4} (\varphi_{s-1, t-1} + \varphi_{s-1, t} + \varphi_{s, t-1} + \varphi_{s, t}) \quad (7.7)$$

in x-y geometry and

$$\int_r \varphi dV = \frac{2\pi h_s h_t}{4} \left[r_s (\varphi_{s-1, t-1} + \varphi_{s-1, t} + \varphi_{s, t-1} + \varphi_{s, t}) - \frac{h_s}{6} (\varphi_{s-1, t-1} + \varphi_{s-1, t} - \varphi_{s, t-1} - \varphi_{s, t}) \right] \quad (7.8)$$

in r-z geometry. Here h_s is the interval between columns $s-1$ and s , h_t the interval between rows $t-1$ and t , and r_s the distance from column 0 to a point midway between columns $s-1$ and s . Similarly, given mesh triangle t ,

$$\int_t \varphi dA = \frac{h_1 h_2}{4\sqrt{3}} (\varphi_1 + \varphi_2 + \varphi_3) \quad (7.9)$$

in hexagonal geometry, where the fluxes are those at the vertices of the triangle and h_1 and h_2 are the lengths of the sides which form a 60° angle.

Pointwise Edit

Pointwise editing is done over a single region of the mesh specified in the input. Edits of the pointwise flux in each group and of the pointwise and quadrant (triangle) power values may be obtained. All quantities edited are normalized to unit power in a spatial problem and to the input power in a depletion problem.

The quadrant power values at point s, t are

$$P_{s, t, q} = \sum_{g=1}^G \kappa_{g, s, t, q}^f \varphi_{g, s, t} \quad (7.10)$$

for $q = 1, 2, 3, 4$, where $\kappa_{g, s, t, q}^f$ is the value associated with the mesh rectangle in quadrant q at point s, t . Quadrant values are edited only at those points at which any two nonzero values differ by more than 5%. The pointwise average power at point s, t is the arithmetic average of the nonzero quadrant values at the point and the pointwise peak power is the largest of these values.

VIII. OPERATING INSTRUCTIONS

On-Line Output

The case number is typed at the beginning of each case. If negative, this is the last case of the current job.

If the monitor toggle is set, the name of each segment of the program is typed when the segment is loaded. In addition, the omega segment types the overrelaxation factor for each group, the iteration segment types the convergence criterion and the iteration number, eigenvalue, and convergence achieved at the end of each outer iteration, and the depletion segment types the interval number at the beginning of each thermal flux renormalization.

Dynamic Monitor

During the coefficient segment the monitor memory location contains the current group number. During the omega and iteration segments this location contains the current group and number of inner iterations.

Force - Removal

The status of the force toggle is checked at the end of each outer iteration and if set, the iterations are terminated and the problem is edited. Similarly, the status of the removal toggle is checked at the end of each case and if set, no further cases are done.

Restart - Recovery

Initiation of a restart is not effective in the input segments and results in termination of the problem. In all other segments a restart causes the segment to be reloaded and execution to begin at the most recent restart point. In the iteration segment this is at the beginning of the current group or current fission source calculation. If an iteration restart fails, a second restart will return to the beginning of the current outer iteration. If the iteration cannot be restarted successfully, a restart with the force toggle set will edit the flux of the last complete iteration.

The job-case recovery option may be used with both programs. If a recovery is done at other than case one and if the output of the previous case is required as input, the recovery will terminate unless this output was saved on a filetape.

Filetapes

One or two input filetapes may be mounted at the beginning of a job. Input for the first case may be taken from one or both of these tapes and output of any case may be added to either tape.

One of the input filetapes may be designated a blank. The tape will then be labeled during some case of the job and does not contain useful information until that time. Care must be taken in doing a job-case recovery where there is a blank input filetape. If a tape has been labeled in a case preceding the one being recovered, it is this labeled tape and not a blank that must be mounted when the recovery is done.

At the beginning of each case in which output is to be saved, the programs search the proper filetape for the end-of-tape sentinel, erase this sentinel, and write a problem sentinel which contains the output identification for this case. Several program segments may add output to the tape and the end-of-tape sentinel is rewritten at the end of the case.

While searching for the end-of-tape sentinel, the programs also examine each problem sentinel. If a problem sentinel is found which contains the same output identification as that for the current case, the programs stop after typing the comment "Current output ID found on input filetape. Advance only if certain that this case is being recovered after failure during previous run. Terminate otherwise." Normally, this indicates that the problem originator has chosen a duplicate identification, and if the problem is not terminated, a part of the filetape will be destroyed. If the current case did fail on a previous run, however, it may safely be continued because its output is the last information on the tape. In fact, it must be continued and completed successfully before other output may be added to the tape, since this is the only way the required end-of-tape sentinel will be rewritten. If the case is continued, the programs may also type the comment "Set force toggle on if failure was after flux filing routine, off otherwise, and advance." If the toggle is set on, the programs will obtain the converged flux and eigenvalue from the proper filetape and bypass the spatial calculation.

PDQ-5/6 INPUT FORM I

PROBLEM
PAGE OF

1 8 9 11 14 17 21 25 29 33 43 45
PROBLEM \$ PDQ 05 06 REQ. NAME CHARGE PRØDN AUTHOR.

FILETAPE 12	
FILETAPE 13	

TITLE

PROB. TYPE	TABLE INPUT	ADJOINT	GEOMETRY (PDQ-5 ONLY)	MESH INT.	TOTAL GROUPS	THERMAL GROUPS
010001						
FIXED-SOURCE	1 0	NO 0	NO 0	X-Y 1	CENT. 1	
EIGENVALUE	2 1	YES 1	YES 1	R-Z 2	INCHES 2	
ONE-ITERATION	3					

COMPS	EDIT REGIONS	COLUMN BOUNDARY	ROW BOUNDARY	DIAG. COLUMN (PDQ-6 ONLY)	BOUNDARY TOP	LEFT	BTM.	RIGHT	CONDITIONS
010002					0	0	0	0	ZERO FLUX
					1	1	1	1	ZERO DERIV.
					-1				ROT. SYMTRY.

λ_0	ϵ_1	ϵ_2	MACRO EDIT	ABSORP. RATE EDIT	COMP. PICTURE	EDIT REG. PICTURE
010003			NO <input type="checkbox"/>	NO <input type="checkbox"/>	NO <input type="checkbox"/>	NO <input type="checkbox"/>
			YES <input checked="" type="checkbox"/>			

X_1	X_2	X_3	X_4	X_5
010004				

PDQ-5/6 INPUT FORM II

PROBLEM _____
PAGE _____ OF _____

INPUT FLUX		INPUT CONCENTRATIONS		INPUT TABLES									
ID		ID		ID									
010006	CARDS FILETAPE 12 FILETAPE 13 PREV. CASE	1 2 3 4	NOT USED CARDS FILETAPE 12 FILETAPE 13 PREV. CASE	0 1 2 3 4	NOT USED CARDS ONLY FILETAPE 12 FILETAPE 13	0 1 2 3							
OUTPUT		QUANTITIES TO BE SAVED											
010007	DO NOT SAVE FILETAPE 12 FILETAPE 13 NEW MERGE	0 1 2 3	FLUX NO YES	POWER 0 1	CONC. 0 1	TABLES 0 1	INTEGRALS 0 1						
INITIAL TIME		FINAL TIME		$\Delta T_{MAX.}$		POWER		POWER FRACTION		MAX. XENON		REPL.	
010008										0 1	0 1	0 1	0 1
010009	RE-EDIT	1											
INPUT CHECK													
010010	STANDARD MACRO	1 2											

PDQ-5/6 INPUT FORM III
INTEGRATION SETS

PROBLEM _____
PAGE _____ OF _____

SUB-
SERIES SEQ.

BEGIN EACH SUBSERIES WITH SEQUENCE NUMBER 1

PDQ-5 : SUBSERIES 100 : EACH REGION AN EDIT

SUBSERIES 101 - 999 : EACH SUBSERIES AN EDIT

PDQ - 6 : SUBSERIES 100 - 199 : EACH SUBSERIES AN EDIT

SUBSERIES 200 - 299 : EACH FIGURE AN EDIT

SUBSERIES 300 - 399 : EACH REGION AN EDIT

SUBSERIES 400 - 499 : EACH FIGURE - REGION PAIR AN EDIT

PDQ-5/6 INPUT FORM IV
MACROSCOPIC DATA

PROBLEM _____
PAGE _____ OF _____

SUB-
SERIES SEQ.

D

Σ^a

Σ^r

$\nu \Sigma^f$

$\kappa \Sigma^f$

NOT USED

COMP.

SUBSERIES NUMBER IS THE GROUP NUMBER

BEGIN EACH SUBSERIES WITH SEQUENCE NUMBER 001

PDQ-5/6 INPUT FORM **V**
MISCELLANEOUS PARAMETERS

PROBLEM _____

PARAMETER	SERIES NUMBER	SUBSERIES NUMBER	PARAMETER	SERIES NUMBER	SUBSERIES NUMBER
REMOVAL FACTORS	03	GROUP NO. (1 DIGIT)	BUCKLING	08	GROUP NO. (1 DIGIT)
SOURCE	04	GROUP NO. (1 DIGIT)	COMP. AREAS	18	1
PDQ-5 MESH INT.	05,06	0	EDIT REG. AREAS	18	2
PDQ-6 MESH INT.	05,06	BASIC FIG. NO. (2 DIGITS)	FLUX	21	GROUP NO. (1 DIGIT)

BEGIN EACH SUBSERIES WITH SEQUENCE NUMBER 1

SEQUENCE NUMBER HAS TWO OR THREE DIGITS TO BRING CARD NUMBER TO SIX DIGITS

47

PDQ-5/6 INPUT FORM VI
OVERLAY DESCRIPTION

PROBLEM _____
PAGE _____ OF _____

SUB-
SER. SERIES SEQ.

<u>OVERLAY</u>	<u>SERIES NUMBER</u>	<u>SUBSERIES NUMBER</u>	<u>OVERLAY</u>	<u>SERIES NUMBER</u>	<u>SUBSERIES NUMBER</u>
PDQ-5 COMP.	17	1	PDQ-6 COMP.	8	INIT. FIG. NO. (3 DIGITS)
PDQ-5 EDIT REG.	17	2	PDQ-6 EDIT REG.	9	INIT. FIG. NO. (3 DIGITS)
			PDQ-6 FIGURE	17	0

BEGIN EACH SUBSERIES WITH SEQUENCE NUMBER 1
SEQUENCE NUMBER HAS TWO OR THREE DIGITS TO BRING CARD NUMBER TO SIX DIGITS

* LISTING OF INPUT DATA FOR CASE 1

* PDQ=5 SAMPLE PROBLEM FOR WARD+TM=477
010001,2,0,0,1,1,2,1
010002,4,0,21,14,1,1,1,1
010003,1+1,2+1,0+0,1,1,1,0
010004,1+1,0+0
010005,0,21,0,14,0,0,0,1
010006,1,0,0,0,0,0,0
010007,0,0,0,0,0,0,0
011001,1,+4
011011,2,+4
021001,11+1,11+0,11+1,0+0,0+0,1
021002,12+1,12+0,12+1,12+0,0+0,2
021003,13+1,13+0,13+1,13+0,0+0,3
021004,14+1,14+0,14+1,14+0,0+0,4
022001,21+1,21+0,0+0,0+0,0+0,1
022002,22+1,22+0,0+0,22+1,0+0,2
022003,23+1,23+0,0+0,23+1,0+0,3
022004,24+1,24+0,0+0,24+1,0+0,4
050001,1+0,21
060001,1+0,14
080001,1+2,4
911001,1+1,4
912001,1+1,4
171001,1,0,21,0,14,2,2,7,2,7,1,4,5,4,5
171002,2,2,4,7,12,3,8,11,2,12,1,10,11,5,9
171003,3,11,12,3,11,3,12,13,4,10,4,14,19,4,10
171004,4,15,18,3,11,4,16,17,2,13,1,14,17,5,9
171005,4,17,18,12,13

120040005 P0005 CADWL 10-21-64 10.7069

1

* PDQ-5 SAMPLE PROBLEM FOR WARD-TM-477

120040005 PDQ005 CADWL 10-21-64 10:7070 2

PROBLEM TYPE = EIGENVALUE

ADJOINT = NO

SYMMETRY = XY

MESH INTERVALS = CENTIMETERS

TOTAL NUMBER OF GROUPS = 2

NUMBER OF THERMAL GROUPS = 1

NUMBER OF MATERIAL COMPOSITIONS = 4

NUMBER OF EDIT REGIONS = 0

COLUMN BOUNDARY = 21

ROW BOUNDARY = 14

ROW 0 BOUNDARY CONDITION = SYMMETRY

COLUMN 0 BOUNDARY CONDITION = SYMMETRY

ROW 14 BOUNDARY CONDITION = SYMMETRY

COLUMN 21 BOUNDARY CONDITION = SYMMETRY

INPUT FIRENVALUE = 1000000+001

EPSILON 1 AND 2 = 200000-001 000000+000

CHT VALUES = 100000+004 000000+000

RE-EDIT = NO

INPUT CHECK = NO

EDIT 1 REGIONS
002 003 004

EDIT 2 REGIONS
001

EDIT 3 REGIONS
002

EDIT 4 REGIONS
003

EDIT 5 REGIONS
004

INTERVAL COL

1000000.000 21

DISTANCE FROM COLUMN 0 TO SUCCESSING COLUMNS

1000000.000	2000000.000	3000000.000	4000000.000	5000000.000	6000000.000	7000000.000	8000000.000	9000000.000	10000000.000
1100000.001	1200000.001	1300000.001	1400000.001	1500000.001	1600000.001	1700000.001	1800000.001	1900000.001	2000000.001
2100000.001									

INTERVAL ROW

1000000.000 14

DISTANCE FROM ROW 0 TO SUCCESSING ROWS

1000000.000	2000000.000	3000000.000	4000000.000	5000000.000	6000000.000	7000000.000	8000000.000	9000000.000	10000000.000
1100000.001	1200000.001	1300000.001	1400000.001						

GROUP	COMP	D	SIGMA A	SIGMA R	NU SIGMA F	K SIGMA F	BUCKLING
1	1	1100000.001	1100000.000	1100000.001	0000000.000	0100000.000	1000000.002
1	2	1200000.001	1200000.000	1200000.001	1200000.000	1200000.000	1000000.002
1	3	1300000.001	1300000.000	1300000.001	1300000.000	1300000.000	1000000.002
1	4	1400000.001	1400000.000	1400000.001	1400000.000	1400000.000	1000000.002

GROUP	COMP	D	SIGMA A	SIGMA R	NU SIGMA F	K SIGMA F	BUCKLING
2	1	2100000.001	2100000.000	0000000.000	0000000.000	0000000.000	1000000.002
2	2	2200000.001	2200000.000	0000000.000	2200000.001	2200000.001	1000000.002
2	3	2300000.001	2300000.000	0000000.000	2300000.001	2300000.001	1000000.002
2	4	2400000.001	2400000.000	0000000.000	2400000.001	2400000.001	1000000.002

PDQ-5 SAMPLE PROBLEM FOR WAPD-TH-477

120040008 P0005 CADWL 10-21-64 10.7101

4

COMPOSITION OVERLAY

000 001 002 003 004 005 006 007 008 009 010 011 012 013 014 015 016 017 018 019 020 021
0 001
1 001
2 001 002 002 002 002 001 003 003 001 001 001 001 001 001 001 001 001 001 001 001 001 001 001
3 001 002 002 002 002 001 003 003 001 001 001 001 001 001 001 001 001 001 001 001 001 001 001
4 001 002 002 002 002 001 003 003 001 001 001 001 001 001 001 001 001 001 001 001 001 001 001
5 001 002 002 002 002 001 003 003 001 001 001 001 001 001 001 001 001 001 001 001 001 001 001
6 001 002 002 002 002 001 003 003 001 001 001 001 001 001 001 001 001 001 001 001 001 001 001
7 001 002 002 001 001 001 003 003 001 003 003 001 001 004 004 004 004 004 004 004 004 004 001
8 001 002 002 001 001 001 003 003 001 003 003 001 001 004 004 004 004 004 004 004 004 001 001
9 001 002 002 001 001 001 003 003 001 003 003 001 001 004 004 004 004 004 004 004 004 001 001
10 001 002 002 001 001 001 003 003 001 003 003 001 001 004 004 004 004 004 004 004 004 001 001
11 001 002 002 001 001 001 003 003 001 003 003 001 001 001 001 001 001 001 001 001 001 001 001
12 001
13 001
14 0

6 PDD-5 SAMPLE PROBLEM FOR WAPD-TM-477

120040006 PDD005 CADWL 10-21-64 10:7126

5

GROUP 1 OMEGA1(30) = 1.935618

OMEGA2(0) = 1.935618

E.R.B.(055,.075) = 925330=001

GROUP 2 OMEGA1(30) = 1.938493

OMEGA2(0) = 1.938493

E.R.B.(058,.075) = 909215=001

OUTER ITERATION 1

GROUP 1 R(1) = 372990=001

DELTA(001,055) = 1924186=001

GROUP 2 R(1) = 699135=001

DELTA(001,058) = 226021=001

RATIO = 10000=001 NORM = 378896=000 SIGMA EST. = 000000=000 DEGREE = 0 SIGMA = 000000=000

PT/AV = 11338=000 MAX. = 193454=000 MIN. = 300410=001 EPS. = 19926=000 LAMBDA = 410041=000

OUTER ITERATION 2

GROUP 1 R(1) = 249813=001

DELTA(001,055) = 145284=000

GROUP 2 R(1) = 550726=001

DELTA(001,058) = 146281=000

RATIO = 10000=001 NORM = 931473=000 SIGMA EST. = 76316=000 DEGREE = 0 SIGMA = 517828=001

PT/AV = 19231=001 MAX. = 386722=000 MIN. = 143004=000 EPS. = 29719=000 LAMBDA = 381942=000

OUTER ITERATION 3

GROUP 1 R(1) = 127132=002

DELTA(001,055) = 144406=000

GROUP 2 R(1) = 280768=002

DELTA(001,058) = 146247=000

RATIO = 10000=001 NORM = 996327=000 SIGMA EST. = 50966=001 DEGREE = 0 SIGMA = 509111=001

PT/AV = 56413=001 MAX. = 378442=000 MIN. = 343464=000 EPS. = 46073=001 LAMBDA = 378199=000

OUTER ITERATION 4

GROUP 1 R(1) = 643523=004

DELTA(001,055) = 144281=000

GROUP 2 R(1) = 143106=003

DELTA(001,058) = 146214=000

RATIO = 10000=001 NORM = 999814=000 SIGMA EST. = 50910=001 DEGREE = 0 SIGMA = 509008=001

PT/AV = 42503=001 MAX. = 377993=000 MIN. = 376025=000 EPS. = 24033=002 LAMBDA = 377981=000

OUTER ITERATION 5

GROUP 1 R(1) = 325506=005

DELTA(001,055) = 144217=000

GROUP 2 R(1) = 729233=005

DELTA(001,058) = 146176=000

RATIO = 10000=001 NORM = 999991=000 SIGMA EST. = 50895=001 DEGREE = 0 SIGMA = 508915=001

PT/AV = 42929=001 MAX. = 377970=000 MIN. = 377869=000 EPS. = 13340=003 LAMBDA = 377970=000

* PDD-5 SAMPLE PROBLEM FOR WAPD-TM-477

190040003 PDD05 CADWL 10-21-64 10:7229 6

INTEGRATION EDIT

NORMALIZATION FACTOR = 17269699+002

FLUX INTEGRALS FOLLOWED BY FLUX AVERAGES

EDIT	AREA	GROUP 1	2
1	11000000+001	83702898+001 76093544+001	44650334+000 40591213+000
2	18400000+001	13928744+002 75699697+001	74675043+000 40584262+000
3	34800000+000	25810174+001 75912275+001	13792364+000 40565778+000
4	40000000+000	30498088+001 76245221+001	16237690+000 40594224+000
5	36000000+000	27394637+001 76096213+001	14620280+000 40611889+000

4 PDQ-5 SAMPLE PROBLEM FOR WARD-TM-477

12004000\$ PDQ05 CADWL 10-21-64 10:7230

7

INTEGRATED POWER EDIT

GROUP FRACTION OF EDIT POWER

EDIT	POWER FRACTION	GROUP 1	2
1	100000000+001	99065649+000	93435055+002
2	28432400+000	99029814+000	97018643+002
3	36382711+000	99066828+000	93317766+002
4	35184889+000	99093395+000	90660490+002

P00=5 SAMPLE PROBLEM FOR WARD=TM=477

12004000\$ P0005 CADWL 10-21-64 10.7230

8

INTEGRATED ABSORPTION EBIT

GROUP FRACTION OF TOTAL ABSORPTION FOLLOWED BY GROUP FRACTION OF EBIT ABSORPTION

EBIT	APSCRP. FRACT.	GROUP 1	2
1	41385005+000	37818138+000 91381258+000	35668668+001 86187421+001
2	58614995+000	53172737+000 90715246+000	54422582+001 92847541+001
3	11801757+000	10748715+000 91077242+000	10530422+001 89227578+001
4	15155520+000	13759427+000 91391239+000	12960938+001 86087613+001
5	14527727+000	13309997+000 91617885+000	12177308+001 83821150+001

PDQ=5 SAMPLE PROBLEM FOR WAPD-TM-477

120040005 PDQ05 CADWL 10-21-64 10:7230

9

TOTAL GROUP-INDEPENDENT BUCKLING, K INFINITY, AND K EFFECTIVE POINTS

K INFINITY FOLLOWED BY K EFFECTIVE

EDIT	Gp, IND, RUCK.	SUM	GROUP 1	2
1	-10203507*000	91818182*000 37796964*000	90909091*000 37443808*000	90909091*002 35315414*002
3	-10203507*000	91818182*000 37796964*000	90909091*000 37430263*000	90909091*002 34670101*002
4	-10203507*000	91818182*000 37796964*000	90909091*000 37444251*000	90909091*002 35271282*002
5	-10203507*000	91818182*000 37796964*000	90909091*000 37454295*000	90909091*002 34266912*002

* PBQ-5 SAMPLE PROBLEM FOR WARP-TM-477

120040708 80005 CADWL 10-21-64 10.7230 10

FLUX WEIGHT EDIT

GROUP 1

EDIT	R	SIGMA A	SIGMA R	NJ SIGMA F	BUCKLING
1	13018930*001	13018930*000	13018930*001	13018930*000	15606686*000
2	11000000*001	11000000*000	11000000*001	00000000*000	+11100000*000
3	12000000*001	12000000*000	12000000*001	12000000*000	15616350*000
4	13000000*001	13000000*000	13000000*001	13000000*000	15606370*000
5	14000000*001	14000000*000	14000000*001	14000000*000	15599208*000

* PDD-5 SAMPLE PROBLEM FOR WAPD-TM-477

12004000\$ P0005 CADWL 10-21-64 10:7230 11

FLUX WEIGHT EDIT

GROUP 2

EDIT	D	SIGMA A	SIGMA R	NU SIGMA F	BUCKLING
1	23018542+001	23018542+000	00000000+000	23018542+001	50262124+002
2	21000000+001	21000000+000	00000000+000	00000000+000	-32965553+002
3	22000000+001	22000000+000	00000000+000	22000000+001	10729736+002
4	23000000+001	23000000+000	00000000+000	23000000+001	51607303+002
5	24000000+001	24000000+000	00000000+000	24000000+001	83016321+002

* PDQ-5 SAMPLE PROBLEM FOR WAPD-TM-477

120040008 PDQ09 CADWL 10-21-64 10:7234 12

POINTWISE AVERAGE POWER

	0	1	2	3	4	5	6	7	8	9
0	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000
1	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000
2	00000+000	00000+000	91683+000	91843+000	91965+000	92054+000	92108+000	92122+000	99805+000	99855+000
3	00000+000	00000+000	91805+000	92003+000	92139+000	92275+000	92291+000	92292+000	99998+000	10007+001
4	00000+000	00000+000	91872+000	92083+000	92210+000	92312+000	92387+000	92395+000	10012+001	10021+001
5	00000+000	00000+000	91890+000	92103+000	92229+000	92329+000	92407+000	92424+000	10017+001	10027+001
6	00000+000	00000+000	91866+000	92068+000	92195+000	92279+000	92343+000	92377+000	10015+001	10027+001
7	00000+000	00000+000	91784+000	91973+000	92060+000	92107+000	92169+000	92243+000	10006+001	10021+001
8	00000+000	00000+000	91674+000	91838+000	91875+000	92000+000	92000+000	92000+000	99933+000	10012+001
9	00000+000	00000+000	91943+000	91688+000	91701+000	92000+000	92000+000	92000+000	99785+000	99996+000
10	00000+000	00000+000	91398+000	91530+000	91532+000	92000+000	92000+000	92000+000	99617+000	99842+000
11	00000+000	00000+000	91241+000	91359+000	91361+000	92000+000	92000+000	92000+000	99426+000	99642+000
12	00000+000	00000+000	91069+000	91161+000	91183+000	92000+000	92000+000	92000+000	99209+000	99393+000
13	00000+000	00000+000	90000+000	90000+000	90000+000	92000+000	92000+000	92000+000	90000+000	90000+000
14	00000+000	00000+000	90000+000	90000+000	90000+000	92000+000	92000+000	92000+000	90000+000	90000+000

POINTWISE AVERAGE POWER

	10	11	12	13	14	15	16	17	18	19
0	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000
1	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000
2	99839+000	99743+000	00000+000	00000+000	00000+000	00000+000	00000+000	10698+001	10689+001	00000+000
3	10007+001	99992+000	99847+000	00000+000	00000+000	10727+001	10727+001	10718+001	10698+001	00000+000
4	10023+001	10018+001	10009+001	99955+000	10755+001	10755+001	10752+001	10741+001	10724+001	10700+001
5	10029+001	10028+001	10024+001	10014+001	10775+001	10775+001	10767+001	10755+001	10741+001	10719+001
6	10028+001	10030+001	10031+001	10023+001	10786+001	10786+001	10775+001	10762+001	10751+001	10730+001
7	10024+001	10028+001	10032+001	10025+001	10789+001	10789+001	10775+001	10766+001	10756+001	10734+001
8	10017+001	10022+001	10026+001	10021+001	10786+001	10786+001	10777+001	10765+001	10755+001	10734+001
9	10009+001	10014+001	10015+001	10009+001	10774+001	10777+001	10772+001	10762+001	10749+001	10727+001
10	99957+000	99994+000	99964+000	99891+000	10754+001	10760+001	10760+001	10752+001	10736+001	10712+001
11	99752+000	99764+000	99700+000	00000+000	00000+000	10734+001	10740+001	10734+001	10716+001	00000+000
12	99492+000	99492+000	00000+000	00000+000	00000+000	00000+000	10717+001	10715+001	10699+001	00000+000
13	00008+000	00000+000	00000+000	00000+000	00000+000	00000+000	10700+001	10700+001	10687+001	00000+000
14	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000	00000+000

PDD-5 SAMPLE PROBLEM FOR WAPD-TM-477

120040005 PDD05 CADWL 10-21-64 10.7238 14

POINTWISE AVERAGE POWER

	20	21
0	00000+000	00000+000
1	00000+000	00000+000
2	00000+000	00000+000
3	00000+000	00000+000
4	00000+000	00000+000
5	00000+000	00000+000
6	00000+000	00000+000
7	00000+000	00000+000
8	00000+000	00000+000
9	00000+000	00000+000
10	00000+000	00000+000
11	00000+000	00000+000
12	00000+000	00000+000
13	00000+000	00000+000
14	00000+000	00000+000

***** END OF OUTPUT *****

* LISTING OF INPUT DATA FOR CASE 1

120040005 PDQ06 CADWL 10-21-64 10.7262 1

* PDQ=6 SAMPLE PROBLEM FOR WARD=TM=477
010001,2,0,0,1,2,1
010002,4,0,15,8,10,1,1,1,1
010003,1+1,2=1,0+0,1,1,1,0
010004,1+1,0+0
010005,0,15,0,8,0,0,0,1
010006,1,0,0,0,0,0
010007,0,0,0,0,0,0,0,0
011001,1,0,2,-4
013001,1,0,1,-4
021001,11+1,11+0,11+1,0+0,0+0,1
021002,12+1,12+0,12+1,12+0,0+0,2
021003,13+1,13+0,13+1,13+0,0+0,3
021004,14+1,14+0,14+1,14+0,0+0,4
022001,21+1,21+0,0+0,0+0,0+0,1
022002,22+1,22+0,0+0,22+1,0+0,2
022003,23+1,23+0,0+0,23+1,0+0,3
022004,24+1,24+0,0+0,24+1,0+0,4
050101,1+0,5
050201,1+0,8
050301,1+0,2
060101,1+0,8
060201,1+0,10
060301,1+0,1
080001,1+2,4
911001,1+1,4
912001,1+1,4
A01000,5,8
A01001,1,0,5,0,8,4,0,3,2,7,1,1,2,3,5,1,0,1,6,7
A02000,8,10
A02001,1,0,8,0,10,2,2,6,2,5,1,2,3,3,5,1,4,5,3,4
A02002,3,2,6,6,9,1,3,5,7,8
A03000,2,1
A03001,1,0,2,0,1
170001,1,10,0,10,0,0,0
170002,1,20,0,0,8,4,0
170003,1,30,0,12,6,5,0
170004,1,30,0,11,2,2,0
170005,1,30,0,5,3,3,0

* PDQ=6 SAMPLE PROBLEM FOR WAPD=TH=477

190040008 PDQ06 CADWL 10-21-64 10.7263 2

PROBLEM TYPE = EIGENVALUE

ADJOINT = NO

MESH INTERVALS = CENTIMETERS

TOTAL NUMBER OF GROUPS = 2

NUMBER OF THERMAL GROUPS = 1

NUMBER OF MATERIAL COMPOSITIONS = 4

NUMBER OF EDIT REGIONS = 0

COLUMN BOUNDARY = 15

ROW BOUNDARY = 8

DIAGONAL COLUMN = 10

ROW 0 BOUNDARY CONDITION = SYMMETRY

COLUMN 0 BOUNDARY CONDITION = SYMMETRY

ROW 8 BOUNDARY CONDITION = SYMMETRY

COLUMN 15 BOUNDARY CONDITION = SYMMETRY

INPUT EIGENVALUE = 100000+001

EPSILON I AND R = 200000+001 000000+000

CHT VALUES = 100000+001 000000+000

REGEDIT = NO

INPUT CHECK = NO

EDIT 1 FIGURES 01
REGIONS 02 03 04

EDIT 2 FIGURES 01
REGIONS 01

EDIT 3 FIGURES 01
REGIONS 02

EDIT 4 FIGURES 01
REGIONS 03

* PDQ-6 SAMPLE PROBLEM FOR WAPD-TH-477

120040005 PDQ06 CADWL 10-21-64 10,7265 3

EDT 5 FIGURES 01

REGTNS 04

BASIC FIGURE 1

INTERVAL COL

1000000000 5

INTERVAL ROW

1000000000 8

BASIC FIGURE 2

INTERVAL COL

1000000000 8

INTERVAL ROW

1000000000 10

BASIC FIGURE 3

INTERVAL COL

1000000000 2

INTERVAL ROW

1000000000 1

FINAL FIGURE	INITIAL COMP FIGURE	INITIAL EDIT FIGURE	ORIGIN X , Y	ANGLE OF ROTATION	REFLECTED 0 NO 1 YES
1	10	0	10 0	0	0
1	20	0	0 8	240	0
1	30	0	12 6	300	0
1	30	0	11 2	120	0
1	30	0	9 3	180	0

PDQ-6 SAMPLE PROBLEM FOR WAPD-TM-477

120040005 P0006 CADWL 10-21-64 10:7284

4

6 PDQ-6 SAMPLE PROBLEM FOR WAPD-TM-477

12004000\$ PDQ06 CADWL 10-21-64 10.7286

5

GROUP	COMP	D	SIGMA A	SIGMA R	NU SIGMA F	K SIGMA F	BUCKLING
1	1	110000+001	110000+000	110000+001	000000+000	000000+000	100000+002
1	2	120000+001	120000+000	120000+001	120000+000	120000+000	100000+002
1	3	130000+001	130000+000	130000+001	130000+000	130000+000	100000+002
1	4	140000+001	140000+000	140000+001	140000+000	140000+000	100000+002
GROUP	COMP	D	SIGMA A	SIGMA R	NU SIGMA F	K SIGMA F	BUCKLING
2	1	210000+001	210000+000	000000+000	000000+000	000000+000	100000+002
2	2	220000+001	220000+000	000000+000	220000+001	220000+001	100000+002
2	3	230000+001	230000+000	000000+000	230000+001	230000+001	100000+002
2	4	240000+001	240000+000	000000+000	240000+001	240000+001	100000+002

* PDD-6 SAMPLE PROBLEM FOR WAPD-TM-477

120040008 P0006 CANNL 10-21-64 10:7300 6

GROUP 1 MAX = 1.944697 OMEGA = 1.943956 MIN = 1.943316 20 ITERATIONS

GROUP 2 MAX = 1.947193 OMEGA = 1.946471 MIN = 1.945847 20 ITERATIONS

OUTER ITERATION 1

GROUP 1 R(1) = 433004+000 DELTA(001,117) = 109462+000

GROUP 2 R(1) = 509581+000 DELTA(001,123) = 121454+000

RATIO = 10000+001 NORM = 276813+000 SIGMA EST. = 000000+000 DEGREE = 0 SIGMA = 000000+000

PT/AV = 44984+001 MAX. = 769722+001 MIN. = 614318+002 EPS. = 13765+000 LAMBDA = 257288+000

OUTER ITERATION 2

GROUP 1 R(1) = 454765+001 DELTA(001,117) = 239854+002

GROUP 2 R(1) = 588919+001 DELTA(001,123) = 272584+002

RATIO = 10000+001 NORM = 977046+000 SIGMA EST. = 11173+000 DEGREE = 0 SIGMA = 922564+002

PT/AV = 47891+001 MAX. = 252222+000 MIN. = 159585+000 EPS. = 18003+000 LAMBDA = 251382+000

OUTER ITERATION 3

GROUP 1 R(1) = 146523+003 DELTA(001,117) = 280907+002

GROUP 2 R(1) = 153027+003 DELTA(001,123) = 210475+002

RATIO = 10000+001 NORM = 999949+000 SIGMA EST. = 28701+002 DEGREE = 0 SIGMA = 235157+002

PT/AV = 81767+001 MAX. = 250544+000 MIN. = 250178+000 EPS. = 73126+003 LAMBDA = 250538+000

OUTER ITERATION 4

GROUP 1 R(1) = 109210+005 DELTA(001,103) = 121484+001

GROUP 2 R(1) = 304746+006 DELTA(001,109) = 320083+002

RATIO = 10000+001 NORM = 100000+001 SIGMA EST. = 46631+002 DEGREE = 0 SIGMA = 324304+002

PT/AV = 53986+001 MAX. = 250536+000 MIN. = 250535+000 EPS. = 15658+005 LAMBDA = 250536+000

6 PROBLEM SAMPLE PROBLEM FOR WARD-TM-477

120040005 PROB04 CADWL 10-21-64 10:7437

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INTEGRATION EDIT

NORMALIZATION FACTOR = 25927145+002

FLUX INTEGRALS FOLLOWED BY FLUX AVERAGES

EDIT	AREA	GROUP 1	2
1	25914737+000	19011751+001 75699585+001	10049276+000 40013464+000
2	78808312+000	59479214+001 75473275+001	31531219+000 40010017+000
3	73612159+001	55514005+000 75414179+001	29445911+001 40001423+000
4	82272413+001	62343665+000 75777120+001	32920602+001 40014144+000
5	95262794+001	72259844+000 75853165+001	38126249+001 40022182+000

* PDQ-6 SAMPLE PROBLEM FOR WAFD-TM-477

120040008 PDQ-6 CADWL 10-21-64 10,7437

8

INTEGRATED POWER EDIT

GROUP FRACTION OF EDIT POWER

EDIT	POWER FRACTION	GROUP 1	2
1	10000000+001	99076234+000	92376595+002
3	26782927+000	99036923+000	96307700+002
4	32872087+000	99074404+000	92559584+002
5	40644986+000	99103604+000	89439559+002

6 PNO=6 SAMPLE PROBLEM FOR WARD=TH=477

120040006 P0006 CADWL 10-21-64 1017437 9

INTEGRATED ABSORPTION EXIT

GROUP FRACTION OF TOTAL ABSORPTION FOLLOWED BY GROUP FRACTION OF EDIT ABSORPTION

EXIT	ABSORP, FRACT.	GROUP 1	2
1	27407914+000	25070402+000	23375115+001
		91471399+000	85266017+001
2	72892086+000	65920590+000	66714961+001
		90809610+000	91903903+001
3	73646192+001	67119234+001	65269587+002
		91137412+000	88625881+001
4	89286869+001	81658024+001	76288449+002
		91455804+000	85441959+001
5	11114608+000	10192676+000	92193117+002
		91705230+000	82947703+001

6 PDD-6 SAMPLE PROBLEM FOR WAPD-TM-477

120040008 PDD06 CADWL 10-21-64 1017437 10

TOTAL GROUP-INDEPENDENT BUCKLING, K INFINITY, AND K EFFECTIVE FRITS

K INFINITY FOLLOWED BY K EFFECTIVE

EFIT	GP, IND, RUCK,	SUM	GROUP 1	2
1	+10202301+000	91818182+000 25053620+000	90909091+000 24822183+000	90909091+002 23143681+002
3	+10202301+000	91818182+000 25053620+000	90909091+000 24812334+000	90909091+002 24128565+002
4	+10202301+000	91818182+000 25053620+000	90909091+000 24821724+000	90909091+002 23189524+002
9	+10202301+000	91818182+000 25053620+000	90909091+000 24829040+000	90909091+002 22457954+002

6 PDD-6 SAMPLE PROBLEM FOR WADD-TH-477

120040005 P0006 CADWL 10-21-64 10:7437 11

FLUX WEIGHT FDIT

GROUP 1

EDIT	N	SIGMA A	SIGMA R	NU SIGMA F	BUCKLING
1	13088082+001	13088082+000	13088082-001	13088082+000	29186546+000
2	11000000+001	11000000+000	11000000-001	00000000+000	-11+00000+000
3	12000000+001	12000000+000	12000000-001	12000000+000	29202537+000
4	13000000+001	13000000+000	13000000-001	13000000+000	29187290+000
5	14000000+001	14000000+000	14000000-001	14000000+000	29175419+000

4 PDC-6 SAMPLE PROBLEM FOR WAPD-TM-477

120040005 P0006 CADWL 10-21-64 10,7437 12

FLUX WEIGHT EDIT

GROUP 2

EDIT	D	SIGMA A	SIGMA R	NU SIGMA F	BUCKLING
1	23086378*001	23086378*000	00000000*000	23086378*001	62525285*002
2	21000000*001	21000000*000	00000000*000	00000000*000	-21906933*002
3	22000000*001	22000000*000	00000000*000	22000000*001	18738576*002
4	23000000*001	23000000*000	00000000*000	23000000*001	60785158*002
5	24000000*001	24000000*000	00000000*000	24000000*001	95578896*002

6 PDQ-6 SAMPLE PROBLEM FOR WAPD-TM-477

120040008 PDQ06 CADWL 10-21-64 10:7442 13

POTNTWISE AVERAGE POWER

	0	1	2	3	4	5	6	7	8	9
0										
1										
2		91295+000	91427+000	91498+000		99274+000	99351+000	99333+000		
3		91285+000	91432+000	91584+000	91632+000	99360+000	99457+000	99510+000	99454+000	
4		91192+000	91392+000	91525+000	91631+000	99369+000	99474+000	99553+000	99575+000	
5		91038+000	91228+000	91378+000	91499+000	99275+000	99442+000	99535+000	99586+000	
6		90840+000	91013+000			99057+000	99266+000	99408+000	99493+000	
7										
8										

* PDD-6 SAMPLE PROBLEM FOR WAPD-TM-477

190040009 PDD06 CADWL 10-21-64 1017445 14

POINTWISE AVERAGE POWER

	10	11	12	13	14	15
0						
1						
2		10696*001	10704*001	10701*001		
3	10703*001	10717*001	10717*001	10711*001		
4	10720*001	10725*001	10722*001	10713*001		
5	10726*001	10729*001	10725*001	10708*001		
6	10722*001	10724*001	10718*001	10699*001		
7		10710*001	10704*001	10686*001		
8						

***** END OF OUTPUT *****

ACKNOWLEDGMENT

In addition to the authors, programming contributions were made by D. Liappas, G. J. Peters, and A. J. Vigilotti. The inner-outer iteration strategy is due to L. A. Hageman and the PDQ-6 difference equation derivation to R. B. Kellogg. The basis for the implementation of variable mesh hexagonal geometry was developed by A. A. Gonzalez and B. H. Ruth.

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