MASTER

Argonne National Laboratory

GENERAL INPUT SPECIFICATIONS
FOR ANL REACTOR PROGRAMS

by

M. Butler and H. Greenspan

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS

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Applied Mathematics Division

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GENERAL INPUT SPECIFICATIONS FOR ANL REACTOR PROGRAMS

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M. Butler and H. Greenspan

I. INTRODUCTION AND ACKNOWLEDGMENTS

The necessity of reprogramming the reactor programs for the CDC-3600* permitted the review and subsequent reformulation of a standard form of problem specification. The use of such a form is designed to minimize the effort of problem preparation, at the same time reducing the possibility of error.

The standard-problem specifications described in this report are intended to cover input data of a sufficiently general nature to be applicable to both multigroup one- and two-dimensional diffusion and transport-theory programs.

Cross-section and related data are included only to the extent that provision is made for entry or modification of these data at run time. The assumption is made that cross-section data will usually be provided by an associated multigroup-library program.[†]

The purpose of this report is to describe in detail this common problem regarding input data, which has been organized into seven categories. Provision for input data, outside this common area, relative to a particular program has been included; however, no detailed specifications for this information are given. These specifications are determined by the particular program.

These specifications were designed preliminary to the programming of the CDC-3600 multigroup diffusion and transport programs. In implementing them, S. Sparck (CDC-ANL) contributed to their clarity. In addition, helpful comments were received from G. Duffy (ANL), S. Elkin (CDC), P. Kaestner and W. Sangren (CAI),^{††} and J. Zapatka (ANL).

II. INPUT SPECIFICATIONS

The seven categories chosen are:

1. identification and program-dependent input data;
2. geometry;
3. boundary and interface conditions;
4. material assignment;

*Control Data Corporation.

[†]S. Sparck, XLIBIT - An ANL Cross-section Library Code, ANL-7112 (1966).

^{††}Computer Applications Incorporated.

5. type designation;
6. initial source/flux values;
7. cross-section modification.

In addition, an end card is required to indicate the completion of input data for each problem.

Twelve-column fields have been used to designate floating-point quantities while fixed-point or integer data utilize 3- or 6-column fields. Program options are given a single column and are, in general, nonnumeric.

1. IDENTIFICATION AND PROGRAM-DEPENDENT INPUT DATA (1 Series)

Type 100000

PROBLEM NUMBER												IDENTIFICATION															
1	0	0	0	0	0																						
1						6	7					18	19													66	67

One type-100000 card must be present as the initial card in the problem input deck.

The problem number (cols. 7-18) is a floating-point quantity. The identification (cols. 19-66) is any combination of the 48-character IBM key-punch set. The problem number and identification will appear as the first line of printed output on each page.

Type 1XXXXX Program-dependent Input Data

All data pertaining to a particular program (i.e., additional input information necessary to operate the code) which is not covered by the general input specifications, categories 2 through 7.

It is intended that the individual program reports contain a description of the required type 1XXXXX input deck.

2. GEOMETRY (2 Series)

Type 200000

2						SLAB CYLINDER SPHERE												xy rz r0 xy--45° SYMMETRY rz--INVERTED																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
1-D Geom.						X _L						X _R						2-D Geom.						Y _B						Y _T																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
2	0	0	0	0	0																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											</

One type-200000 card should be included in an input deck. This card specifies the dimension of the problem and the associated geometry.

The geometry of the reactor for one-dimensional problems may be specified as a slab, cylinder, or sphere, that of two-dimensional problems may be specified as xy, rz, or r θ . The xy case permits selection of a 45-degree symmetry option. The rz case permits inversion of the r and z coordinates.

The quantities X_L , X_R , Y_B , and Y_T define the boundaries of the reactor in the coordinate system of the geometry specified. X_L is the left-most line of the one-dimensional coordinate or of the first coordinate in two-dimensional problems; X_R is the right-most. Y_B is the bottom (or lowest) line of the second coordinate in two-dimensional problems; Y_T is the top (or highest).

One Dimension

One and only one of columns 10, 11, and 12 should be nonblank. Both the quantities X_L and X_R must be given values by this card. Columns 37 on will be ignored by a one-dimensional program.

Two Dimensions

One and only one of columns 38, 39, 40, 41, and 42 should be nonblank. If both columns 38 and 41 are nonblank it will be interpreted as an xy geometry problem with 45° symmetry. If both columns 39 and 42 are nonblank the cylinder will be considered as lying on its side, parallel to its axis, while normally it is considered as upright.

r, z

z, r (r, z inverted)

All four of the quantities X_L , X_R , Y_B , and Y_T are given values by this card. Columns 10-12 will be ignored by a two-dimensional problem.

Type 2XXXXX

REGION NUMBER	x_L	NO. OF x INTERVALS	x_R	y_B	NO. OF y INTERVALS	y_T
2						
1 2	6 7	18 19	24 25	36 37	48 49	54 55
						66

The remaining 2XXXXX series cards are used to define regional interfaces or boundaries, and mesh structure.

The quantities x_L , x_R , y_B , and y_T give the region boundaries. They satisfy the following relations:

$$X_L \leq x_L < x_R \leq X_R \text{ and } Y_B \leq y_B < y_T \leq Y_T,$$

where X_L , X_R , Y_B , and Y_T are the reactor boundaries given on the 200000 card.

The set of regions defined by the 2XXXXX deck should cover the entire reactor.

For a one-dimensional problem each region is defined by the $[x_L, x_R]$; for a two-dimensional problem the rectangle whose sides are $[x_L, x_R, y_B, y_T]$ defines the region.

The regions may be defined either by a set of nonoverlapping (i.e., abutting) rectangles or by an "overlay" procedure. In the latter case overlapping rectangles may be used. The ordering of the region assignment information will determine the region interfaces or boundaries, with the latest region assignment taking precedence over previous assignments. The assignment of nonoverlapping (i.e., abutting) rectangles will be termed the "standard" assignment procedure.

The reactor is further subdivided along each coordinate axis by a number of mesh points, forming a one-dimensional or a two-dimensional grid of mesh lines. Two types of mesh assignment are possible, termed "constant" and "variable" structure. One or the other must be chosen for each coordinate axis.

One Dimension

1. Standard Region Assignment:

The region numbers are defined in integral order: 1, 2, 3, ..., etc. The 2XXXXX cards must be arranged by increasing region number. To reduce the amount of input information required, the regions are considered to be ordered by region number from the left boundary X_L to the right boundary X_R .

The right boundary x_R of each region must be given. The left boundary x_L may be omitted; if omitted, the x_L of a region will be assumed to be the x_R of the preceding region (or the left boundary of the reactor, X_L , for the case of the left-most region, i.e., region 1).

2. Overlay Region Assignment:

Both x_L (cols. 7-18) and x_R (cols. 25-36) must be given. The user is reminded that the ordering of the 2XXXXX cards will determine the final region configuration. *No region numbering restriction is imposed.*

3. Constant Mesh Structure:

If in each region a constant interval size is to be used, the number of intervals for the region may be provided in columns 19-24 on each 2XXXXX card. If the mesh in any region is specified in this manner, all regions must be specified similarly, and no further input information is required in category 2.

4. Variable Mesh Structure:

Leaving columns 19-24 blank on all type-2XXXXX cards implies the use of a variable mesh structure, and further input information (210000 or 220000 series cards) is required.

The two methods available for variable mesh definition are:

- a) increment method (210000 series cards), or
- b) ratio method (220000 series cards).

Care must be taken to insure that all region boundaries coincide with some mesh point.

NOTE: On the 2XXXXX cards, columns 37 on are ignored for one-dimensional problems.

Two Dimensions

1. Region Assignment:

For both the standard and the overlay procedures, all four region boundaries x_L (cols. 7-18), x_R (cols. 25-36), y_B (cols. 37-48), and y_T (cols. 55-66) are given on each 2XXXXX card.

For the standard procedure the ordering of the cards is immaterial. In the overlay method the program will determine region interfaces, with the latest region assignment taking precedence over previous assignments, and the regions so defined may or may not be "rectangular."

2. Mesh Structure:

In defining the mesh structure the following restrictions are imposed:

- a) All region interfaces must lie along mesh lines.
- b) Mesh lines in each coordinate must run from one coordinate boundary to the other (i.e., from X_L to X_R and from Y_B to Y_T).

In preparing two-dimensional problems it is advisable to construct a diagram laying out the problem regions. In order to assure conformance to requirements a) and b) above, the mesh lines should be superimposed on this diagram.

The mesh structure, if constant for either or both axes, may be specified on the 2XXXXX series cards by use of columns 19-24 for the "x" dimension and columns 49-54 for the "y" dimension. This implies a very simple geometry and requires the mesh structure of all regions to be specified in this same manner with a region and dimension-wise constant mesh spacing. Since condition b) must always be satisfied, the program will terminate the problem if the mesh specifications violate this condition.

Leaving columns 19-24 and 49-54 blank on all type-2XXXXX cards implies the use of a variable mesh structure, and further input information (210000 or 220000 series cards) is required.

The two methods available for variable mesh definition are:

- a) increment method (210000 series cards), or
- b) ratio method (220000 series cards).

Care must be taken to insure that all region boundaries coincide with some mesh line.

One axis may have a constant mesh while the other has a variable mesh, or both axes may have the same type of mesh structure.

Type 210000

NO. OF INTERVALS					x_i or y_i					NO. OF INTERVALS					x_i or y_i					NO. OF INTERVALS					x_i or y_i					AXIS	
2	1	0	0	0																											
1		6	7			12	13			24	25			30	31			42	43			48	49			60	61			67	68

The type-210000 cards are used if a *variable mesh spacing using the increment method* is specified for a coordinate axis.

In the increment method a sequence of pairs of numbers are given: (N_i, x_i) for the x-axis or (N_i, y_i) for the y-axis, where $i = 1, 2, \dots, I$. The numbers x_i and y_i must obey the relations

$$X_L \equiv x_0 < x_1 < x_2 < \dots < x_I \equiv \bar{X}_R \text{ and } Y_B \equiv y_0 < y_1 < y_2 < \dots < y_I \equiv Y_T.$$

The 210000 cards for the same axis must be grouped together, and must be ordered by increasing x_i or y_i .

Each pair of numbers (N_i, x_i) specifies that N_i equal mesh spaces are to be established in the interval $[x_{i-1}, x_i]$. Three pairs of numbers may be given on each card. The first blank pair will specify the end of the pairs of values for the given axis, when the number of pairs is not a multiple of three.

Example: One may wish to specify 6 intervals from $X_L = 0$ to $x_1 = 1.5$ cm, and 5 intervals from $x_1 = 1.5$ cm to $x_2 = 4.0$ cm. This indicates that mesh

lines are to be constructed at 0, 0.25, 0.5, 0.75, 1.0, 1.25, 1.5, 2.0, 2.5, 3.0, 3.5, and 4.0 cm. With the increment method, this would be specified as the pairs (6, 1.5) and (5, 4.0) on a series 210000 card.

NOTE: By making the x_i or y_i equal to region boundaries as defined on the type-2XXXXX cards, the variable mesh structure as established by 210000 cards may be used to simulate a constant mesh structure.

One Dimension

Column 68 is ignored. The preceding 2XXXXX cards must all contain blanks in columns 19-24. Type-220000 cards may not be used if 210000 cards are used.

Two Dimensions

Column 68 on each card must contain one of the letters "x" or "y." If 210000 cards are used for axis "x" (axis "y") the preceding 2XXXXX cards must all have blanks in columns 19-24 (cols. 49-54). If 210000 cards are used for an axis, type-220000 cards must not be used for that axis.

If 210000 cards are used for both axes, those for the y-axis may either follow or precede those for the x-axis.

Type 220000

x_i or y_i						r_{ij}		$r_{i,j+1}$		$r_{i,j+2}$		$r_{i,j+3}$		AXIS	CARD NUMBER		
2	2	0	0	0	0												
1	6	7	18	19	30	31	42	43	54	55	66	67	68	69	70	71	72

The type-220000 cards are used if a variable mesh structure using the ratio method is specified for a coordinate axis.

In the ratio method, sets of numbers $(x_i; r_{i1}, r_{i2}, \dots, r_{iJ})$ for the x-axis or $(y_i; r_{i1}, r_{i2}, \dots, r_{iJ})$ for the y-axis are given, where $i = 1, 2, \dots, I$. The numbers x_i and y_i must obey the relations

$$X_L \equiv x_0 < x_1 < x_2 < \dots < x_I \equiv X_R \text{ and } Y_B \equiv y_0 < y_1 < y_2 < \dots < y_I \equiv Y_T.$$

The 220000 cards for the same axis must be placed together, and must be ordered by increasing x_i or y_i . Four ratios r_{ij} may be given on the first card for the specified x_i or y_i and five on any subsequent cards for the same x_i (or y_i), if more than four ratios are used. The first ratio on these succeeding cards appears in columns 7-18, and a card number is required in columns 70-72 to ensure proper ordering. If four or fewer ratios are given for a single x_i or y_i value, the card number will be ignored.

The first blank ratio, r_{ij} , in the series for a given x_i (or y_i) terminates that series of ratios.

Each set of values $[x_i, (y_i); r_{i1}, \dots, r_{iJ}]$ specifies that the interval $[x_{i-1}, x_i]$ or $[y_{i-1}, y_i]$ is to be divided by establishing J mesh spaces along the $x, (y)$ axis according to the formula

$$I_{ij} = r_{ij} \frac{x_i - x_{i-1}}{\sum_{j=1}^J r_{ij}} \quad \text{or} \quad I_{ij} = r_{ij} \frac{y_i - y_{i-1}}{\sum_{j=1}^J r_{ij}}$$

NOTE: By definition $x_i = x_{i-1} + \sum_{j=1}^J I_{ij}$ and $I_{ij}/I_{i\ell} = r_{ij}/r_{i\ell}$, where

$j, \ell = 1, 2, \dots, J$.

Example: An illustration of the ratio method may be useful. Suppose one wishes to assign a variable mesh between $x_1 = 0.5$ cm and $x_2 = 4.14$ cm, using 5 intervals. The interval lengths $I_{21}, I_{22}, I_{23}, I_{24}$, and I_{25} are to be related by means of the ratios $r_{21} = 1, r_{22} = 2, r_{23} = 6, r_{24} = 6.2$, and $r_{25} = 3$. One would specify $x_2 = 4.14$ cm and the five ratios on two successive 220000 cards. $x_1 = 0.5$ cm would have appeared on the preceding card.

The program will compute the quantity $Z = \frac{x_2 - x_1}{\sum_{j=1}^5 r_{2j}} = \frac{4.14 - 0.5}{18.2} = 0.2$.

Mesh interval lengths are then calculated as $I_{21} = r_{21}Z = 1(0.2) = 0.2$; $I_{22} = 2(0.2) = 0.4$; $I_{23} = 6(0.2) = 1.2$; $I_{24} = 6.2(0.2) = 1.24$; $I_{25} = 3(0.2) = 0.6$ cm.

The mesh points defining the 5 intervals in $[0.5$ cm, 4.14 cm] are calculated as follows:

$$\begin{aligned} x_1 &= 0.5 \text{ cm;} \\ x_{1,1} &= x_1 + I_{21} = 0.5 + 0.2 = 0.7 \text{ cm;} \\ x_{1,2} &= x_{1,1} + I_{22} = 0.7 + 0.4 = 1.1 \text{ cm;} \\ x_{1,3} &= x_{1,2} + I_{23} = 1.1 + 1.2 = 2.3 \text{ cm;} \\ x_{1,4} &= x_{1,3} + I_{24} = 2.3 + 1.24 = 3.54 \text{ cm;} \\ x_2 &= x_{1,4} + I_{25} = 3.54 + 0.6 = 4.14 \text{ cm.} \end{aligned}$$

Care is necessary to ensure that all region interfaces lie along mesh lines.

One Dimension

Column 68 is ignored. The preceding 2XXXXX cards must all have blanks in columns 19-24. Type-210000 cards may not be used if 220000 cards are used.

Two Dimensions

Column 68 on each card must contain either an "x" or a "y." If 220000 cards are used for the x axis (y axis), the preceding 2XXXXX cards must all have blanks in columns 19-24 (cols. 49-54). If type-220000 cards are used for an axis, type-210000 cards cannot be used for that axis.

If 220000 cards are used for both axes, those for the x axis may either precede or follow those for the y axis.

NOTE: By specifying equal ratios r_{ij} the mesh structure as established by the ratio method can be used to simulate the structure established by the increment method, and in this manner intermixing is possible.

Type 230000

AREA NUMBER						REGION NUMBER		REGION NUMBER												REGION NUMBER	
2	3	0	0	0	0																
1		6	7	12	13	18	19	24	25	30	31	36	37	42	43	48	49	54	55	60	61

Codes may provide as output information integrals evaluated over each region and each composition. If the user desires, he may specify certain combinations of regions for which these integrals may also be obtained. The type-230000 cards, specifying *area-region correspondence*, allow the definition of these areas.

The area numbers must be defined as 1, 2, 3, etc. The 230000 cards must be ordered by increasing area number. If more than one 230000 card is required for an area (i.e., if the area contains more than nine regions), the area number must be repeated on each such card.

The region numbers need not be ordered. A region number may be used in more than one area. It is not necessary that the set of all areas include all regions (i.e., a region number need not appear).

3. BOUNDARY AND INTERFACE CONDITIONS (3 Series)

Type 300000

DIFFUSION THEORY						TRANSPORT THEORY		DIFFUSION THEORY						TRANSPORT THEORY		SPECIAL INTERFACE CONDITION																									
$\phi = \text{CONSTANT}$ $\phi = 0$ $\phi' = 0$ LOG. DER. = CONST. PERIODIC GEN. B.C. INCOMING $\phi = 0$ REFLECTIVE PERIODIC WHITE								$\phi = \text{CONSTANT}$ $\phi = 0$ $\phi' = 0$ LOG. DER. = CONST. PERIODIC GEN. B.C. INCOMING $\phi = 0$ REFLECTIVE PERIODIC WHITE																																	
3	0	0	0	0	0																																				
1						6	7	8	9	10	11	12	13	14	15	16	17	19	20	21	22	23	24	25	26	27	28	29	30												
													X_L														X_R														
																	SPECIAL INTERFACE CONDITION																								
						32	33	34	35	36	37	38	39	40	41	42	43	45	46	47	48	49	50	51	52	53	54	55	56	59	60	61									
																	Y_B																		Y_T						

One type-300000 card specifying boundary and special interface conditions is to be included in an input deck.

The four sets of specifications (broken into diffusion and transport applications) refer to the left, right, bottom, and top boundaries, respectively. One and only one option should be nonblank in each of the four sets.

A one-dimensional problem will ignore columns 30-59 on the card.

If a boundary condition is chosen requiring the specification of constants, these must be given for each region along that boundary for each energy group, on type-3XXXXX cards.

In diffusion theory, periodic boundary conditions are applicable only if r0 geometry is used.

Type 3XXXXX

REGION NUMBER		INITIAL GROUP (j_i)			FINAL GROUP (j_f)			BOUNDARY-VALUE CONSTANT			j_i			j_f			BOUNDARY-VALUE CONSTANT			j_i			j_f			BOUNDARY-VALUE CONSTANT			L, R, B, or T		
3																															
1	2	6	7	8	9	10	11	12	13	24	25	26	27	28	29	30	31	42	43	44	45	46	47	48	49	60	61	67	68	69	

The 3XXXXX cards are optional, and are used only if any boundary condition specified on the 300000 card requires constants to describe that condition.

Boundary conditions requiring such constants are the following:

(a) $\phi = \text{constant}$ (the value of the constant C is to be specified).

(b) Logarithmic Derivative = constant. This is the condition $\vec{n} \cdot \text{grad } \phi = -\frac{C}{D}$, where D is the diffusion coefficient and C is to be specified. D and C may be energy-dependent; $\vec{n}$ is the outward-pointing normal to the surface.

(c) General boundary condition (Gen. B. C.). This is a condition of the type $B_1 \vec{n} \cdot \text{grad } \phi + B_2 \phi = B_3$, where B_1 , B_2 , and B_3 may be energy-dependent and are to be specified.

A triplet of numbers (j_i, j_f, C) is used to specify the constant C for the set of energy groups whose group numbers are j_i, j_i+1, ..., j_f. Three such triplets may be given on each 3XXXXX card (in cols. 7-24, 25-42, and 43-60). The boundary to which the constants apply is indicated in column 68 on the card by using one of the letters L, R, B, or T. The region number to which the information applies is given in columns 2-6 on each card.

For the general boundary condition B_1 is given in columns 13-24, B_2 in columns 31-42, and B_3 in columns 49-60. The (j_i, j_f) in columns 7-12 applies to all three values. Columns 25-30 and 43-48 are ignored.

If more than one card is required to specify the constants for a given boundary and region, the information in columns 2-6 and 68 must be repeated on each card used.

If special interface condition data are necessary, these are to be specified in the program-dependent input. In such cases column 60 of the type-300000 card is nonblank.

4. MATERIAL ASSIGNMENT (4 Series)

Type 400000000000

SET NAME																	
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18

One of these cards is included in an input deck. The name given in columns 14-18 is the name of the set of cross sections to be used for the problem. The name must correspond to that of one of the sets in the cross-section library, and may be numeric and/or alphabetic, as desired.

NOTE: The substances for which cross sections are supplied on the cross-section-library tape will be referred to as "isotopes" whether they represent isotopes or materials.

Two levels of mixing are provided: "isotopes" from the cross-section-library tape or from 700000 cards are mixed to form "materials," and materials are mixed to form "compositions." It is also possible to bypass the material level and mix isotopes directly to form compositions. It is the compositions that are used by the reactor programs.

Type 400000

MATERIAL NUMBER						ISOTOPE NAME						NUMBER DENSITY						ISOTOPE NAME						NUMBER DENSITY						ISOTOPE NAME						NUMBER DENSITY																	
4	0	0	0	0	0																																																
1						6	7					12	13					18	19					30	31					36	37					48	49					54	55					66					

The 400000 cards define "materials" as a combination of one or more "isotopes." Isotope names may be numeric and/or alphabetic, as desired.

It is possible to bypass materials and directly define compositions in terms of isotopes; in this case the type-400000 cards are to be omitted.

The materials are to be numbered sequentially as 1, 2, 3, etc. with the 400000 cards ordered by increasing material number. The ordering of "isotope" names on the cards is immaterial.

Three isotope names, each with its associated number density, may be given on each card. If more than one 400000 card is required for a single material definition, the material number is to be repeated on each such card. The first blank in the list of isotope names for a material terminates the list, when the number of isotopes contained in a material is not a multiple of three.

Type 410000

COMPOSITION NUMBER						MATERIAL NO. OR ISOTOPE NAME						VOLUME FRACTION						MATERIAL NO. OR ISOTOPE NAME						VOLUME FRACTION						MATERIAL NO. OR ISOTOPE NAME						VOLUME FRACTION																	
4	1	0	0	0	0																																																
1						6	7					12	13					18	19					30	31					36	37					48	49					54	55					66	67				

The 410000 cards define compositions as combinations of either materials or isotopes. If type-400000 cards are used to define materials in terms of isotopes, then the compositions are defined in terms of these materials and material numbers are used on the 410000 cards. If type-400000 cards are omitted, then the compositions are defined in terms of isotopes and isotope names are used on the 410000 cards.

The compositions are to be numbered sequentially: 1, 2, 3, etc., with the 410000 card ordered by increasing composition number. The ordering of the material/isotope identifiers is immaterial.

Three material/isotope identifiers, each followed by its associated volume fraction, may be given on each card. If more than one card is required for a single composition, the composition number is to be repeated on each such card. The first blank in the list of identifiers for a composition terminates the list.

Type 420000

The 420000 cards assign a single composition to each region defined. The order of the cards is immaterial. Each region number defined by a type-2XXXXX card is used only once in the set of all 420000 cards. The ordering of the region numbers on these cards is immaterial.

Nine region numbers may be given on each 420000 card. If more than one card is required for a single composition, the composition number is to be repeated on the additional cards.

5. TYPE DESIGNATION (5 Series)

Type 500000

One 500000 card is to be included in an input deck. This card specifies whether a real or an adjoint problem is to be solved, and specifies the type of problem.

A real solution is indicated by leaving column 8 blank; column 8 non-blank specifies an adjoint solution.

Columns 10-12, 26-30, and 44 specify the problem type, which falls into one of the following three categories: source calculation, flux convergence, and criticality search.

Information relating to each of the problem types is given below, together with the columns on the 500000 card to be completed in each case.

(a) Source Calculation

The flux is computed from a given external source distribution, specified on the 61XXXX cards. Nonblank columns: 10, 13-24.

(b) Flux Convergence

Iterations are performed until successive values of the flux meet the specified flux-convergence criterion, δ . Nonblank columns: 11, 13-24.

(c) Criticality Search

A search procedure is incorporated to obtain $k_{\text{eff}} = 1.0$ to a desired accuracy, ϵ (cols. 31-42), by varying material concentration (col. 26), x or y dimension, or both (col. 27-28), or transverse buckling (col. 29) in all or specified regions of the reactor.

Space is provided on this 500000 card for an initial critical parameter guess, columns 46-57, and a quantity (modifier or second guess) which may be used by some programs to construct a second or succeeding estimate of this parameter, columns 58-69.

In programs having the facility to search for parameter values corresponding to a $k_{\text{eff}} = k_0 \neq 1$, or $\alpha = \alpha_0 \neq 0$, the k_0 or α_0 value is to be specified in the problem-dependent input section.

1. Concentration Calculation (col. 26)

The amount of certain specified materials in one or more compositions is changed to achieve criticality. The 5XXXXX series cards are used to describe modifications of the composition material to be made.

2. Critical-dimension Calculation (cols. 27-28)

The entire x dimension, y dimension, or both dimensions, of the reactor can be varied to achieve criticality. In such cases no further information is necessary. It is also possible to vary the dimensions of selected regions to achieve criticality. In this case column 44 is nonblank, and the additional input required is given on the 5XXXXX cards.

3. Buckling (B^2) (col. 29)

The transverse buckling of the reactor is uniformly varied to achieve criticality. In this case the buckling is region-independent. If region-dependent bucklings are desired, column 44 must be nonblank and further input using the 5XXXXX cards is required.

4. α Calculation (col. 30)

This calculation applies to the reactor as a whole and simulates its time behavior.

Type 5XXXXX

The type-5XXXXX cards are used for a concentration calculation, and for regional specifications in a critical-dimension or buckling calculation.

Concentration Calculation:

COMPOSITION NUMBER						MODIFIER						MATERIAL NO. OR ISOTOPE NAME						MODIFIER						MATERIAL NO. OR ISOTOPE NAME						MODIFIER						MATERIAL NO. OR ISOTOPE NAME																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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Spectrum Average:

If column 9 is nonblank, the initial source/flux data will be distributed among the energy groups according to the fission-spectrum fractions considered as a vector (i.e., independent of incident neutron energy).

Surface Source/Distributed Source:

Column 10 is used to specify the form of the external source in a source calculation. If blank, a distributed source is indicated; if nonblank, a surface source is specified. Type-61XXXX cards contain the external source values.

Region/Interval:

If column 11 is blank, the value given on each 61XXXX card is constant for that region.

If column 11 is nonblank, each of the values supplied on the 61XXXX cards is the distributed source value for a single mesh interval or space.

Type 6XXXXX

REGION NUMBER					SOURCE/FLUX VALUE										SOURCE/FLUX VALUE										GROUP NUMBER		CARD NUMBER	
6																												
1	2		6	7	18	19	30	31	42	43	54	55	66	67	69	70	72											

The 6XXXXX cards are optional. If omitted, initial values are assigned to all mesh points or intervals, or spaces, by the program.

The type-6XXXXX cards contain initial source or flux values, and have a different format, depending upon whether the assigned values are for regions or for each mesh point or interval.

If the initial values are specified for each region, the region number appears in columns 2-6; the source/flux value is then given in columns 7-18. If these values are to be group-independent, columns 67-69 are left blank. For group-dependent values the group number is required in columns 67-69. When source or flux is specified in this manner, no ordering of the 6XXXXX cards is necessary for the one-dimensional case. For two dimensions, all cards without group numbers should come first, followed by those cards having group numbers. The latter cards are arranged by increasing group number.

If the source/flux is to be specified for each mesh point or interval, the region number, columns 2-6, on the 6XXXXX series cards is ignored. The source/flux values are then given for all values of the x coordinate in increasing order for a given value of the y coordinate. The process is started with the lowest y coordinate and continued in increasing y order.

A series of N initial values (where $1 \leq N \leq$ total number of mesh points or intervals) is to be supplied in columns 7-66, five values per card. The first blank value terminates the series. The i th value is assigned to the i th mesh point or interval either for all groups or for the group specified by columns 67-69. The mesh points or intervals are numbered as shown below. If the cards for a group are omitted, the initial values for all mesh points or intervals in that group will be zero.

If there are more than five mesh intervals or points, columns 70-72 must be given sequential values. Cards having the same group number should be kept together and ordered by increasing card number. In one dimension the groups may appear in any order. For two dimensions the cards must be ordered by increasing group number.

Type 61XXXX

The type-61XXXX cards give values for an external source. These cards are optional and are used if column 10 on the 500000 card is nonblank. These cards are used for specifying either a distributed source or a surface source.

Distributed Source:

In the case of a distributed source the data are supplied in the same manner as the values on the 6XXXXX cards. The card number appears in columns 70-72.

Surface Source:

When a surface source is used, the location of the surface, or shell source for a particular group, is obtained either from the region number (cols. 3-6) or from the x and y coordinates (cols. 7-30). If the region number on a 61XXXX card is nonblank, the coordinates must be blank, and vice versa.

For a one-dimensional problem, columns 19-30, 55-66, and 70-72 are ignored.

If the region number is given, the location of the shell source is, for one dimension, the right-most mesh interval in the region. For two dimensions the location depends on column 72 of the card: if column 72 is blank the shell source occupies the set of mesh spaces just inside the top and the right-hand boundaries of the region; if column 72 is nonblank, the shell source occupies the top-most, right-most mesh space in the region.

If the coordinates are given, the location of the shell source is, for one dimension, the mesh interval in which the x coordinate lies. For two dimensions the location again depends on column 72 of the card: if column 72 is blank the shell source occupies the set of mesh spaces which contain the two line segments $y = y_i$, $X_L \leq x \leq x_i$ and $x = x_i$, $Y_B \leq y \leq y_i$; if column 72 is nonblank, the location is the single mesh space in which the point (x_i, y_i) lies.

NOTE: For this application in specifying x and y coordinates, a mesh interval is considered to include its left-hand endpoint but exclude its right-hand endpoint; a mesh space includes its left and bottom sides but excludes its top and right sides.

If it is desired to have the same initial shell-source values apply to all groups, then only one 61XXXX card is used; the group number of this card must be zero or blank.

The 61XXXX cards must be arranged by increasing group number when group numbers are used. A card need not be used for all groups; if the 61XXXX card for a group is omitted, zeros will be assigned as the values for all components of the surface source for that group. Columns 70-71 are ignored in surface-source application.

7. CROSS-SECTION MODIFICATION (7 Series)

Type 700000

ISOTOPE NAME													
7	0	0	0	0	0							9	
1					6	7					12	13	14

The 700000 cards are optional and need not be included in an input deck.

The 700000 cards need not be ordered in any way.

A type-700000 card must be followed by one or more cross-section data cards. If the isotope whose name is given in columns 7-12 is new and is being added, the isotope name must not duplicate the name of any isotope already in the cross-section set being used, and the entire data deck for the isotope must follow the 700000 card. If the isotope name duplicates that of an isotope already in the set, it is assumed that only a modification of the existing cross-section values for that isotope is desired; in this case the complete isotope data deck is not required.

The data cards that add an isotope must be arranged in the same order required as input to the cross-section library program.

The data cards which act as change cards for an isotope already in the cross-section library must be ordered as they would be if they occurred embedded in an isotope data deck.

Notes Concerning the Use of Change Cards with the XLIBIT Program:

On all change cards the SETNAME (cols. 1-5), MATNAME (cols. 6-11), and TYPE (col. 13) must be given. In addition, the quantities: special character (col. 12), group number (cols. 13-16), card number (cols. 17-19), and ℓ -number (col. 20) must be given if they are applicable to cards of a given TYPE.

If a data field on a change card is left blank, the original existing value will be used. Any nonblank value (including zero) given will be substituted for the original value.

1. If it is desired to transform a fissionable isotope into a nonfissionable isotope, then those type-1 cards having nonzero or nonblank values for either ν or the fission cross section σ_f must be altered by inserting zeros for these values of ν and σ_f .

2. If it is desired to transform a nonfissionable isotope into a fissionable isotope, then *nonblank*, *nonzero* values must be inserted for ν and/or σ_f on one or more type-1 cards. The user must also supply a set of type-2 cards for the "isotope" as change cards.

3. If it is desired to transform the fission spectrum of an isotope from group-dependent to group-independent or from group-independent to group-dependent, the new type-2 cross-section-change cards of the appropriate form must be supplied. The original fission spectrum of the isotope will be disregarded in this case and a new fission spectrum will be formed from the type-2 cards supplied.

NOTE: If type-2, -4, -6, or -8 change cards are used, the card numbers (cols. 17-19) to be placed on these cards may not match the card numbers used on any corresponding, original cross-section-data cards. See paragraph 7, below.

4. If no type-3, -5, or -7 cards occur in the data deck for an isotope, they may be added simply by including them among the change cards for the isotope. Likewise, individual cards of type-3, -5, or -7 that do not occur in the original data deck may be added by including them among the change cards. Note that the addition of a card of type-3 (or -5 or -7) may necessitate the addition of one or more corresponding (i.e., having the same group number and ℓ -number) cards of type-4 (or -6 or -8, respectively).

5. If it is desired to add a card of type-4, -6, or -8 to the deck for an isotope, this may be accomplished by merely including the card among the change cards for the "isotope."

Note that the addition of a card of type-4 (or -6 or -8) necessitates the altering of values on the corresponding card of type-3 (or -5 or -7, respectively), or the addition of a corresponding type-3, -5, or -7 card if none already exists.

6. If a user wishes to delete a card of type-3, -4, -5, -6, -7, or -8 from the data deck of an isotope, he may do it by including a change card having a type, group number, card number (if applicable), and ℓ -number (if applicable) that match those of the card to be deleted, and with blanks in columns 21-80. Note that deleting a type-3 (or -5 or -7) card necessitates deleting as well any corresponding type-4 (or -6 or -8, respectively) cards. Conversely, deleting a type-4 (or -6 or -8) card necessitates altering values on the corresponding type-3 (or -5 or -7) card.

7. The card number used on a change card of type-2, -4, -6, or -8 must obey the following rule: Suppose that the data on a set of type-2, -4, -6, or -8 cards occupy N such cards, and suppose that it is desired to change one or more values on the Ith (e.g., 3rd) of these cards. Then the card number used on the change card must be I (e.g., 3). This may differ from the card number appearing on the original cross-section-data card.

APPENDIX A
Input Data Forms

73							8

2. GEOMETRY

2a. REGION DEFINITIONS

[illegible]

2b. INCREMENT MESH DEFINITIONS

73									80

NO. OF INTERVALS						NO. OF INTERVALS						NO. OF INTERVALS						NO. OF INTERVALS					
x_i OR y_i						x_i OR y_i						x_i OR y_i						x_i OR y_i					
1	6	7	12	13		24	25	30	31		42	43	48	49		60							
2	1	0	0	0	0																		
2	1	0	0	0	0																		
2	1	0	0	0	0																		
2	1	0	0	0	0																		
2	1	0	0	0	0																		
2	1	0	0	0	0																		
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2	1	0	0	0	0																		
2	1	0	0	0	0							</											

REACTOR CODE INPUT FORM

2d. AREA ASSIGNMENT

73							8

[illegible]

IF MORE THAN ONE CARD IS REQUIRED AREA NUMBER MUST BE REPEATED ON NEXT CARD(S).

32	
80	

60 ☐ SPECIAL
INTERFACE COND.

L/R/B/T

68

[illegible]

EXCEPT FOR FIRST j_i ALL FOLLOWING j_i 's MUST = PRECEDING $j_f + 1$.

1

12

--	--	--	--	--

14

18

SET NAME AND ISOTOPE NAME CANNOT INCLUDE THE CHARACTERS . OR ,

--	--	--	--	--	--	--	--

73

80

NUMBER DENSITY

7

12 13

18 19

30 31

36 37.

48 49

54 55

66

[illegible]

73							80

IF MORE THAN ONE CARD IS REQUIRED TO SPECIFY A COMPOSITION OR ASSIGN REGIONS TO A COMPOSITION, THE COMPOSITION NUMBER HAS TO BE REPEATED ON THE SUCCEEDING CARDS.

73							80

73 80

IF MORE THAN ONE CARD IS REQUIRED TO SPECIFY A COMPOSITION OR ASSIGN REGIONS TO A COMPOSITION, THE COMPOSITION NUMBER HAS TO BE REPEATED ON THE SUCCEEDING CARDS.

6. INITIAL SOURCE / FLUX VALUES

FLUX
INTERVAL 60
SPECTRUM AVERAGE
SURFACE SOURCE
INTERVAL 61

COL. 7 BLANK FOR SOURCE DATA
NON-BLANK FOR FLUX DATA

COL. 8 BLANK FOR SPECIFICATION BY REGION
NON-BLANK FOR SPECIFICATION BY INTERVAL

73							80

6	0	0	0	0	0				
1						6	7	8	9

[illegible]

APPENDIX B Sample Problems

Problem 1: OLD FAITHFUL--a 2-dimensional rz geometry, diffusion-theory calculation for k_{eff}

Ten intervals in each region, along each coordinate for a total of 400 spaces over the one-quarter reactor.

Material Vol. Fraction	U_1	U_2	M	S
Composition 1	0.14	0.157	0.123	0.315
Composition 2	0.0019	0.833	0.0731	0.0227

Initial source guess of 1.0 for reactor

Initial k_{eff} guess of 0.9.

Flux convergence criterion $\delta = 0.0001$.

A listing of the input deck for this problem follows:

100000	1.0		OLD FAITHFUL				OLDF0001
200000		0.0	50.05	x	0.0	50.4	OLDF0002
200001	0.0		50.05	0.0		50.4	OLDF0003
200002	0.0		20.05	0.0		20.4	OLDF0004
210000	10	20.05	10	50.05			x OLDF0005
210000	10	20.4	10	50.4			y OLDF0006
300000	x		x		x		OLDF0007
400000000000		397					OLDF0008
410000	1	U1	.14	U2	.157	M .123	OLDF0009
410000	1	S	.315				OLDF0010
410000	2	U1	.0019	U2	.833	M .0731	OLDF0011
410000	2	S	.0227				OLDF0012
420000	1	2					OLDF0013
420000	2	1					OLDF0014
500000	x	.0001			.9		OLDF0015
600000							OLDF0016
600001	1.0						OLDF0017
600002	1.0						OLDF0018