WIMS-CRNL
A USER’S MANUAL FOR THE CHALK RIVER VERSION OF WIMS

WIMS-CRNL
Un manuel d’instructions pour la version de Chalk River du code WIMS

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by

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Ce rapport décrit la préparation pour l'entrée des données du WIMS-CRNL, la version de Chalk River du code de réseau du WIMS. Aussi inclus sont les notes portant sur le fonctionnement du code, les contenus des bibliothèques associées, et la relation entre le WIMS-CRNL et les autres versions du code.

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This report describes the preparation of the input for WIMS-CRNL, the Chalk River version of the WIMS lattice code. Also included are notes on the operation of the code, contents of the associated libraries, and the relation of WIMS-CRNL to other versions of the code.
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1. Introduction

The Winfrith Improved Multigroup Scheme (WIMS)\(^1\) is a multigroup transport code for reactor lattice calculations, including burnup. It was created at the United Kingdom Atomic Energy Establishment, Winfrith, Dorset (AEEW), where it continues to evolve. The code has also been widely distributed, and exists in various versions and many countries. Some further notes on the history and versions of the code are given in Appendix A.

A copy of WIMS was transferred to Chalk River in 1971, where it has undergone extensive modifications. A standard version of this code is maintained on the CRNL computers. This version is designated 'WIMS-CRNL' to distinguish it from other versions within AECL, or elsewhere. The name WIMS-CRNL should be used in any reference to that code, and to results produced by it.

Over the years, AEEW has produced many publications relating to WIMS, including several input manuals\(^2\)\(^3\)\(^4\)\(^5\). CRNL users had 'made-do' with these manuals, and they will continue to be useful references for WIMS-CRNL. However, they have the drawback of describing options not available in WIMS-CRNL, while omitting some that have been added. A manual, AECL-7432\(^5\), was prepared to address this problem and reflected the state of development of WIMS-CRNL in 1979.

This report is intended to provide an up-to-date manual for WIMS-CRNL, reflecting the developments that have been made in WIMS-CRNL since those reported in AECL-7432. It is not intended to be a full description of the code or its operation, and novice users will probably want to consult other references for background information.

A user may prepare input for WIMS-CRNL directly, following the methods described here, or alternatively may use the CRNL input preparation code TESHOM\(^6\), which serves WIMS-CRNL as well as other lattice codes. For some cases, TESHOM may be useful, as a good deal of the WIMS-CRNL input is provided automatically by the default options. However, not all WIMS-CRNL options are available through TESHOM, and most types of input variation are more conveniently carried out using WIMS-CRNL input directly. Appendix B gives some information on using TESHOM for WIMS-CRNL cases.

WIMS-CRNL and its libraries are maintained on the permanent file system of the CRNL Computer Centre. The jobcards for attaching these files and running the code are given in Appendix C, and the libraries are described in Appendix D.

This report begins with a brief description of the organization and operation of WIMS-CRNL and an outline of the main calculational options available. The general organization of the input cards is described in Section 2. Section 3 describes the format of WIMS-CRNL input cards. In Section 4, the definition of the naming convention used in this report for geometry elements is given.
The keyword descriptions are in Section 5; on page 10 is an alphabetic index of the keywords. Section 6 consists of the notes referred to in Section 5, which enlarge on various points in the keyword definitions, and include some suggestions for input preparation.

The list of references in Section 7 is relatively brief, considering the vast amount that has been published about WIMS. However, the items included here contain more extensive bibliographies that will direct the interested user to most of the significant older items, while a current list of AEEW publications should be consulted for more recent reports. This is discussed further in Appendix A-1.

In Appendix E there is a simplified flowsheet for the code, showing the relationships of the various components and a brief description of the calculations performed in each section.

In Appendix F a number of sample WIMS-CRNL cases are presented, to give realistic examples of the use of facilities in the code.

In Appendix G a description of TAPE16 is presented. TAPE16 is the standard data interface that has been added to WIMS-CRNL for the transfer of data between WIMS-CRNL and user codes.

In developing WIMS-CRNL from WIMS-D2, much of the code has been rewritten, and several new options and features have been added. A number of options have been deleted because the options did not work, were related to machine dependent facilities not available at CRNL, or were irrelevant; for example, options that prepared input for other, obsolete codes. However, some of the options retained and described here are highly specialized and rarely, if ever, used. The descriptions of the input for these have been taken from the AEEW input manuals, and it is necessary to repeat their warning: the inclusion of an option in this report is not a guarantee that it will work well, or for that matter, that it will work at all. There is confidence that all the common options work properly. Users who have tested the less common ones are encouraged to evaluate the results and report their conclusions.

2. Input Preparation

2.1 General Considerations

WIMS-CRNL performs a multigroup transport calculation for a reactor cell, producing flux distributions, eigenvalues and reaction rates. In order to do this, the input data must describe the physical dimensions of the cell, its geometrical arrangement, and the composition, densities and temperatures of the cell materials. In addition, the code offers a choice for the basic method of the calculation, and the ability to vary a number of the parameters used, although default values are provided. The results of the transport calculations may be edited in a number of ways, and a great variety of output is available.

Figure 1 shows the main features of a WIMS-CRNL calculation. A basic principle in WIMS-CRNL is that it is possible for users to control the degree of detail in the various parts of a calculation, in order to optimize cost.
and accuracy requirements. For example, the SPECTROX calculation, prior to the main transport calculation, uses the full library energy group structure to determine the neutron spectrum for a simplified cell geometry. For the main transport calculation the library energy groups may be condensed to a smaller number of groups, but the computation is applied to the detailed cell geometry. Energy groups may be expanded and geometry de-homogenized as desired for the reaction rate output. This approach produces significant savings in cost with little reduction in the accuracy of the results.

The code offers the following main transport calculation options:

**DSN**
- The DSn\(^8\) 9 10 method in one dimensional annular geometry. Clusters of fuel pins are smeared into the appropriate annular geometry.

**PERSEUS**
- Collision probability calculation in annular geometry\(^11\). Clusters of fuel pins are smeared into the appropriate annular geometry.

**Pij**
- Collision probability calculation for a detailed, two-dimensional geometrical specification\(^12\). Because the Pij calculations may make relatively large demands on computer time and storage, Pij cases can be subdivided at a boundary (the "Pij" radius) that encloses all the non-annular geometry. The collision probabilities inside this boundary are calculated by the Pij method, while the remainder of the collision probabilities, outside this boundary, are computed using PERSEUS. The inner and outer regions are connected assuming a cosine current distribution at the interface.

The other major option is the cell geometry. There are three classes of cells treated by the code:

**Homogeneous**
- the entire cell consists of one material of uniform composition.

**Pin Cells and Plates**
- the cell structure is either purely annular or the analogous arrangement of parallel plates.

**Rod Clusters**
- arrays of fuel pins. The data formats are sufficiently flexible to describe most geometric arrangements.

After the main transport and edit calculations, the code may either proceed to the next set of input or perform a burnup calculation\(^13\). Details of all of the options are given with the keywords in Section 5 and the notes in Section 6.
Figure 1. WIMS-CRNL Calculations

1. Read Prelude Data
2. Read Main Data
3. Calculate Material Cross-Sections (non-Resonance)
4. Calculate Resonance Isotope Cross-Sections
5. Condense from Library Group Structure to Main Transport Group Structure

Homogenized Cluster

6. Calculate Cross-Sections for Rings of Fuel
7. Solve One Dimensional Flux Distribution with DSN or PERSEUS
8. De-homogenize Cluster

9. One Dimensional Problem
   a. DSN One Dimensional Flux Solution
   b. PERSEUS One Dimensional Collision Probability Calculation and Flux Solution

Not Homogenized Cluster

10. Two Dimensional Problem
    a. Calculate 2 Dimensional Collision Probabilities using Pij
    b. Calculate 1 Dimensional Collision Probabilities using PERSEUS, Link 1 and 2 Dimensional Collision Probabilities
    c. Solve 2 Dimensional Flux Distribution

11. Read Edit Data
12. Calculate Infinite and Effective Lattice Spectra for Homogenized Cell
13. Calculate Reaction Rates
14. Burnup Calculations (if required)
2.2 Input Data Groups

The input for a WIMS-CRNL case consists of at least three groups of data. This section describes these input groups in general terms, and indicates how they are used. The data groups are referred to as:

(a) Prelude data
(b) Main data
(c) Edit data

Figure 1 shows an outline of the sequence of calculations, and indicates where each data group is read in.

(a) Prelude Data

WIMS-CRNL is a variable dimension code, i.e. the dimensions of most of the arrays used within the code are functions of the case being calculated, and storage space within the computer's memory is allocated dynamically as required during calculations. In the version of WIMS received from Winfrith, the Prelude data consisted of those quantities necessary to assign storage areas throughout the WIMS calculation. The Prelude data has been simplified in WIMS-CRNL to that which is required to process the Main data and to define options in the method of problem solution.

(b) Main Data

The Main data consists of the information necessary to define the composition and geometry of the lattice cell, together with whatever additional information is necessary to proceed with the main transport calculation.

(c) Edit Data

As the name implies, this group specifies the editing operations to be performed on the results of the main transport calculation.

2.3 Input Format

All WIMS input is in free format, consisting of a keyword (significant to 4 characters), followed usually by alphanumeric data. These are described in detail in Section 5. Here we are concerned only with the grouping of the input.

Within each of the three groups, the keywords may occur in any sequence, except that the end of each group is indicated by a particular terminating keyword: PREOUT for the Prelude data, BEGIN for both the Main and the Edit data. Also, the first card of the Main data is the keyword INITIATE, except as discussed below for multiple cases.

Although keywords may occur in any order, grouping related information (such as materials, annuli and rod layouts) and adding meaningful comments is recommended and can make WIMS-CRNL input much easier to work with and understand. See Appendix F sample input cases.
2.4 Single Case Input

The minimum input for a single WIMS-CRNL case (i.e. one lattice cell calculation without perturbations or burnup) consists of the following:

Prelude  
[Prelude Data Cards]  
PREOUT - terminating keyword

Main  
[Main Data Cards]  
BEGIN - terminating keyword

Edit  
[Edit Data Cards]  
BEGIN - terminating keyword

2.5 Continuation of a Single Case

A single case as described above may be continued (for instance, in a burnup calculation or during perturbations) by simply adding more Main and Edit data cards as follows:

Prelude  
[Prelude Data Cards]  
PREOUT - terminating keyword

Main  
[Main Data Cards]  
BEGIN - terminating keyword

Edit  
[Edit Data Cards]  
BEGIN - terminating keyword

Main  
[Main Data Cards]  
BEGIN - terminating keyword

Edit  
[Edit Data Cards]  
BEGIN - terminating keyword

2.6 Multiple Case Input

A single WIMS-CRNL run may include several complete cases (i.e. a number of different lattice cells).

To run multiple cases in a single WIMS-CRNL run, each set of input data after
the first set must be preceded by the keyword PRELUDE, which causes the code to re-enter at the beginning of the computation. For example:

```
Prelude [Prelude Data Cards]
  PREOUT - terminating keyword

INITIATE - initiating keyword

Main [Main Data Cards]
  BEGIN - terminating keyword

Edit [Edit Data Cards]
  BEGIN - terminating keyword

Main PRELUDE

Prelude [Prelude Data Cards]
  PREOUT - terminating keyword

INITIATE - initiating keyword

Main [Main Data Cards]
  BEGIN - terminating keyword

Edit [Edit Data Cards]
  BEGIN - terminating keyword
```

3. WIMS-CRNL Input Format

All WIMS-CRNL input is in free format. Each item of the set of data begins on a separate card, and consists of a keyword followed by a data list. In some cases, there is no list and a keyword alone is sufficient. The keywords are significant to four alphabetic characters; more characters are normally appended to form a word for mnemonic purposes.

Valid separators between list items are blanks, commas or equality signs. Any characters following an asterisk (*) or oblique (/) are treated as comments. Continuation of a list to a subsequent card is indicated by a dollar sign ($) at the end of the entries on the current card. If the first character of a list item is numeric, the item is assumed to be a number. Numbers are all treated as real, and an exponent may be indicated by an 'E' between the mantissa and exponent. Both mantissa and exponent may be signed; if unsigned they are assumed positive. If the first character of a list item is a letter, the item is assumed to be a character string. Character strings may be delineated by quotes ("'). Embedded blanks, and special characters other than those mentioned above, are forbidden (except within delineated character strings).
Any unrecognized keywords will produce a diagnostic message and the contents of that card will be ignored. The code prints the images of all input cards, unless explicitly suppressed.

The following sections define all the WIMS-CRNL keywords, and an alphabetic index to them is given on page 10. The definitions are meant to be adequate for general use, but additional information is included in Section 6. Keywords marked with 'USER BEWARE' are considered to be incompletely tested, and users intending to use them should contact the author.

In the input description, repeated items or groups of items are delineated by round brackets (), and optional items are delineated by curly brackets {}. Note, however, that in many cases items are position dependent and so the optional items may be required.

4. Naming Convention for Geometry Elements

WIMS-CRNL treats the elements of cell geometry differently during different phases of its calculations. In the descriptions and notes that follow an attempt has been made to follow a consistent naming convention for the geometry elements used at different points by WIMS-CRNL.

Annulus and Rodsub: These names refer to the specific elements of geometry defined on the respective Main data cards.

Meshes: These refer to the elements of geometry into which the cell is divided during the main transport calculation. The exact relationship between these meshes and the annuli and rodsubs above depends on the method being used during the transport solution.

In pin cell cases using DSn or PERSEUS the meshes correspond to the annuli above after they have been subdivided according to the MESH card.

In homogenized cluster calculations using DSn or PERSEUS, the meshes also correspond to the annuli above after they have been subdivided according to the MESH cards, but the composition of the annuli containing rods is a homogenized mixture of rod and annular components.

In two-dimensional Pij calculations the meshes within the radius defined by the NPIJAN'sh ANNULUS are exactly as defined by the ANNULUS and RODSUB cards; outside of that radius, the meshes correspond to the annuli above after they have been subdivided according to the MESH card.

Zones: These refer to the elements of cell geometry for which there are distinct fluxes. Again, the exact relationship between the zones and the annuli, rodsubs, and meshes defined above depends on the method being used for transport solution.
In pin cell and Pij cases there is a one to one correspondence between the zones and the meshes above.

In homogenized cluster calculations, the zones correspond to the meshes defined above after the cluster has been de-homogenized. In each annulus that had been homogenized, the average flux is calculated, and the flux in each of the annulus components is calculated to form a zone. In those annuli that were not homogenized, the zones correspond to the meshes defined above.

If the ENDCAP option has been selected, WIMS-CRNL adds a zone to those defined above, whose properties and size are determined by the options chosen.

Regions:

For some editing operations (the printout of CHAIN 13, and in the calculation of diffusion coefficients) the zones above are contracted. Adjacent meshes (in the order of the list of zones) composed of the same material are added together to form a region.
5. The WIMS-CRNLF Keywords

5.1 Index of Keywords

5.1.1 Prelude Data Keywords

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<td></td>
</tr>
</tbody>
</table>
## 5.2 Prelude Data Group

**Keyword** | **Data** | **Use**
---|---|---
SEQUENCE n.m | Select main transport solution method:
| n = 1 | DSn (default) |
| n = 2 | PERSEUS |
| n = 3 | Pij |

m = order of integration in annular collision probability calculation, 2 to 5 (default 3). Pij and PERSEUS cases only

See note 21*. 

**CELL n** | Select cell type:
| n = 4 | Homogeneous |
| n = 5 | Pin cell, without energy condensation |
| n = 6 | Pin cell, with energy condensation |
| n = 7 | Rod cluster (default) |

See note 1.

**NGROUP n** | Define number of energy groups in the main transport calculation (equal to the number of entries on the FEWGROUPS card).

**NREGION n** | Define number of annuli or slabs (equal to number of ANNULI and the number of entries on the MESH card).

**NRODS n1 n2 n3 n4 n5 n6 n7 [n8]** | Define data for Pij calculation:

| n1 | number of rods in the cell |
| n2 | cluster symmetry factor: |
| n3 | number of lines in integration mesh |
| n4 | number of angles in integration mesh |
| n5 | number of rod types (default 5) |
| n6 | maximum number of RODSUBS in any rod type (default 5) |
| n7 | maximum number of unique sector angles in any rod type (default 2) |
| n8 | maximum number of annuli sectors (default 1) |

See note 2.

**TITLE s** | s is a string (delineated by quotes) of up to 130 characters to be used as a title in each CHAIN not suppressed.

* Notes on keywords can be found in Section 6.
SETS n  Specifies that there will be up to n sets of tracking lines specified in the Main data (on LINES cards) to be used in the integration of collision probabilities during the Pij calculation. The default is 1 set of lines specified on the NRODS card.

See example 3 in Appendix F.

NDSN n  Select the order of the DSn calculation (default 4).

NOPRINT  Suppresses all printout from CHAINS not explicitly activated on the SUPPRESS card.

PIFL n m { i j k }  Power iteration parameters for the collision probability flux solution (Pij and PERSEUS cases):

- n  - maximum number of outer iterations. If equal to 0, the code will set the maximum number of outer iterations to twice the number of non-thermal main transport groups (default 0)
- m  - maximum number of inner iterations per outer iteration (default 50)
- i  - number of inner iterations without variational acceleration (default 3)
- j  - number of inner iterations with variational acceleration (default 3)
- k  - rebalance control. If k=0, rebalancing will not be performed, if k>0 rebalancing will be performed and if k=2 rebalancing will be carried out over unconverged groups only (default 1)

NPLATE n  Selects slab geometry. The cell will be divided into n units for resonance shielding and SPECTROX calculations. Cylindrical geometry is default.

(USER BEWARE)

POISON n  Define number of regions in a subsidiary burnable poison pin cell calculation (default is 0). If n=1 the code sets the number of regions to n6+2 where n6 is the sixth number on the NRODS card.

See page 83 of Reference 4 (USER BEWARE).

PREOUT  Terminator for the Prelude data group.

Prelude Data
5.3 Main Data Group

INITIATE

Mandatory first card of this group for the beginning of a case. Should be omitted on re-entries within a case.

See note 3.

ANNULUS i j k or ANNULUS i j (k θ)

Defines the cell annuli:

- \(i\) - annulus number from cell center
- \(j\) - outer radius, (cm)
- \(k\) - MATERIAL number for all of the annulus not occupied by rods. For a Pij calculation with sectored annuli, \((k θ)\) are pairs of numbers giving material and final angle (radians, counterclockwise) for each sector. The number of pairs must not exceed \(n8\) on the NRODS card. The sector angles must be in increasing order.

See note 4.

POLYGON j n m r

Polygon geometry:

- \(j\) - 'annulus' number of the polygon
- \(n\) - number of sides of the polygon
- \(m\) - material number
- \(r\) - one half of the distance between cell centers (cm)

This option generates an annulus of equal area to the polygon, and is useful for specifying the pitch of square (\(n=4\)) and hexagonal (\(n=6\)) lattice cells.

ARRAY N (m n p θ)

Defines the locations of all rods of type N. Up to 12 sets of \((m n p θ)\) are allowed.

- \(m=1\) a ring of \(n\) rods with axes equally spaced around a circle of radius \(p\) (cm), one having an angular co-ordinate of \(θ\) (radians)
- \(m=2\) \((p θ)\) give the Cartesian co-ordinates (cm) of the axis of each of the \(n\) rods
- \(m=3\) a ring of \(n\) rods having a linear separation of \(p\) (cm) between centers, one with an angular co-ordinate of \(θ\) (radians)

For \(m=1\) or 3, \(0≤θ≤2π\), counterclockwise.
RODSUB N k r (m 0)  
Description of rod type N as located by the corresponding ARRAY:

- k - subdivision of the rod (concentric rings) counting from the center
- r - outer radius of the subdivision (cm)
- m - material number for the subdivision. For a sectored \( P_{ij} \) calculation, \((m \, 0)\) are pairs of numbers giving material and final angle (radians, counterclockwise) for each sector. The number of pairs must not exceed \( n_7 \) on the NRODS card. The sector angles must be in increasing order.

See note 5.

MATERIAL m d t n (list)  
Description of cell materials:

- m - material number
- d(\(\geq 0\)) - material density, \((g/cm^3)\). If the density is specified as zero, WIMS-CRNL will automatically calculate the saturation density of light or heavy water, whichever is the larger constituent.
- t - material temperature (K)
- n - material spectral type:
  
  \[
  \begin{align*}
  n=1 & \quad \text{fuel} \\
  n=2 & \quad \text{clad} \\
  n=3 & \quad \text{coolant} \\
  n=4 & \quad \text{moderator}
  \end{align*}
  \]

- (list) - Pairs consisting of the library nuclide identifier and its weight fraction in the material. The weight fractions are normalized by the code to 100\%. See Appendix D for the list of identifiers.

See note 6.

or

MATERIAL m -1 t n (list)  
As above, except that the list is pairs of nuclide identifiers and atom densities \((\text{atoms}/(\text{barn}\cdot\text{cm}))\).

or

MATERIAL m M  
If only two numbers are given, then new material \( m \) will be given the same specifications as previously defined material \( M \).

See note 7.
Definition of a material composed of water:

- **m** - material number
- **d** - water density (g/cm³). If the density is specified as zero, WIMS-CRNL will automatically calculate the saturation density of light or heavy water, whichever is the larger constituent.
- **t** - water temperature (K)
- **n** - material spectral type (see MATERIAL option)
- **i** - isotope identifier. The single isotope specified must be either hydrogen or deuterium
- **f** - atom fraction of isotope i. The isotope fraction is used as the molecular fraction of the light or heavy water.

Modify the existing set of material densities. The list is a string of constants by which the existing densities are to be multiplied. A truncated list will be filled out with l's.

Modify existing material temperatures. The list consists of a string of temperature increments, one for each material, to be added to the previously specified temperatures. A truncated list will be filled out with 0's.

The list specifies the number of mesh subdivisions to be used in each of the annuli or slabs during the transport solution in DSn and PERSEUS cases. In Pij cases only those annuli outside the NPIJAN'th annulus may be subdivided, and the first NPIJAN items on the MESH card are not used. The number of entries must equal the number on the NREGION card. The default subdivision is equal area; a negative number will select subdivision by equal width.

See note 8.

Select cluster annularization to be optimized by WIMS:

- **n=1** width homogenization: equal width of annulus on each side of rod pitch circles (recommended)
- **n=2** area homogenization: equal area of annulus on each side of rod pitch circle
- **n=3** displacement homogenization: minimize fuel displacement in a linearly varying flux field within each annulus.

See note 9.
FEWGROUPS (list)

Condensation of the library group structure into the main transport group structure. The number of entries is equal to the number on the NGROUPS card. Each entry gives the upper library group number for that particular condensed group (that is, the lower energy boundary). The last entry is thus always equal to the number of library groups.

See note 10.

SUPPRESS (list)

Normal printout control. The list consists of 16 switches that control the printout from the 16 CHAINS in the code. Settings are 1/0 to suppress/allow normal printout. Default values are all 0, i.e. full printout. Diagnostic messages cannot be suppressed. See Appendix E for CHAIN descriptions. A partial printout suppression is available with switch settings equal to -1, for CHAINS 7, 8 and 16.

TITLE s

s is a string (delineated by quotes) of up to 130 characters to be used as a title on the printout of each CHAIN not suppressed.

FISSION (i f)

Specification of fission spectrum. The fission yield spectrum will be made up with contributions from the isotopes:

- i - isotope identifier
- f - fission yield fraction of isotope

The fission spectrum will be automatically normalized to 1.0.

This option is only relevant if the nuclear data library in use contains isotope fission spectra.

NPJAN n

Definition of inner region of a Pij calculation:

- n - the number of annuli to be treated by Pij.
- All others, which lie outside this group, will be treated by PERSEUS.

In a Pij calculation, the first n numbers on the MESH card are not used by the code.

See note 11.

LINES ri ro n m

Defines a set of tracking lines to be used in Pij collision probability integration:

- ri = inner radius of set of lines
AUTOTRACK (r)

TRUNCATE (r)

s = neutron source spectrum, equal to number of calculation groups

BELL a

DANCOFF (a b n)

\( r \) = outer radius of set of lines

m = number of angles at which lines are to be constructed

n = number of radii at which lines are to be constructed

\( s \) = neutron source spectrum, equal to number of calculation groups

The inner and outer radii on all of the LINES cards must form a contiguous set, with the innermost inner radius equal to the radius of ANNULUS (NPIJAN). See SETS keyword, and example 3 in Appendix F.

The tracking line set used in PiJ collision probability integrations is to be found automatically by WIMS-CRNL. The code will successively increase the number of lines and angles used in the integration by a factor of 1.5 until the change in the mean chord length in any mesh path is less than \( t \). See SEIS and LINES options, and example 3 in Appendix F.

The Bell factor (default is 1.16).

Externally calculated Dancoff factors:

- **a**: infinite lattice Dancoff factor for a rod cluster.
- **b**: average Dancoff factor for a rod cluster.

If \( n \) is absent, the single values of \( a \) and \( b \) apply to all library groups up to \( n \).

In PiJ cases neutrons will be assumed to have collided after \( r \) mean free paths. The default value is 15 mean free paths, but 8 mean free paths have been found acceptable for some applications and results in worthwhile cost reductions during collision probability integrations.

The fixed source option. An independent neutron source will be present in mesh point 1. Valid for PiJ and PERSEUS cases only.

See note 12. (USER BEWARE)
REGULAR { a b }

Infinite lattice Dancoff factors are to be calculated by a tracking routine.

- a = fraction of infinite lattice Dancoff factor to be used as average cluster Dancoff factors (default 1.0)
- b = 0 hexagonal pincell lattice (default) = 1 square pincell lattice

See note 12.

RESXSECS r m (list)

Input resonance cross sections, if m is a number:

- r - nuclide identifier, e.g. U235
- m - number of cross section types: 1 for absorption, and 2 for absorption and fission yield

(list) - consists of the inner cross sections (barns) for each group, for each type in turn, followed by the corresponding set of outer cross sections

For an explanation of 'inner' and 'outer' see Appendix E.5.

or

RESXSECS r t m (list) if t is a string:

- r - nuclide identifier
- t - cross section identifier, either 'ABS' (list will be absorption cross sections) or 'NUF' (list will be fission yield cross sections).

- m - material number

(list) - resonance cross sections (barns) for each group

NORESONANCE

Bypass the resonance shielding calculation and use infinite dilution cross sections for all resonance isotopes.

NEWRES

This keyword selects the use of a newer, alternative resonance cross section calculation.

See note 13.

SKIN i

Selects calculation of skin effect for resonance capture in isotope i (i may be U238 or TH232). The model used in this calculation is only applicable to pin cell geometry.

Main Data
PINNER (m r)  
For each material m specified assign the fraction r of the cross sections in the resonance region to those calculated for the inner part of a cluster.

For an explanation of 'inner' and 'outer' see Appendix E.5.

POWER i q t nt  
{ eps ig (list)}  
Burnup control:  
i - specifies the rating units for q:  
i =1 q is W/g initial heavy elements  
i =2 q is cell averaged fissions/cm³/s  
i =3 q is fissions/cm³/s averaged over burnable materials  
i =4 q is total flux n/cm²/s  
i =5 q is flux in group ig n/cm²/s  
i =6 q is the thermal flux n/cm²/s  
If q=-1 the value reached by the previous burnup step is assumed. If i=0 burnup calculations are not performed (default).

t - the time step in days between homogeneous spectrum calculations and flux renormalization to the input power level.

nt - the number of time steps t between lattice calculations.

eps - local error tolerance during burnup integration (default 0.001).

ig - The number of the group used to normalize the flux level in the i=5 option (default is group 1).

(list) applies to i=4,5 or 6 and consists of a switch for each material. The switch may be set to 1/0 according to whether the material is to be included/omitted in the flux normalization (default values are all 1).

See note 15.

BUCKLING (list)  
The list consists of sets of:
$$B^2_r B^2_z \{ B'^2_r B'^2_z \}$$
to be used during burnup. If ($B'^2_r$) and ($B'^2_z$) are
given, a critical spectrum will be used with bucklings \( B_r^2 + \lambda \cdot B_r^2' \) and \( B_z^2 + \lambda \cdot B_z^2' \) with \( \lambda \) found to give \( k\text{-effective} = 1 \).

If the list consists of more than four numbers, it is assumed that the values are in sets of four for each main transport group.

**DBSQUARED 1 (list)**

Accounts for leakage by adding \( D^2 \) to \( \sum_a \) in the \( g \) main transport groups:

- \( i = -1 \): list consists of \( g \) values of \( B^2 \) \((\text{cm}^{-2})\) and \( B^2/(3 \cdot \sum_{tr}^a) \) is added to \( \sum_a \) for each material.
- \( i = 1 \): list consists of \( g \) values of \( B^2 \) followed by \( g \) values of \( D^2 \). \( D^2 \) is added to \( \sum_a \) for every material.
- \( i = 2 \): list consists of \( g \) values of \( B^2 \) followed by \( g \) values of \( D^2 \), and a switch \( j \) for each material, where:
  - \( j = -1 \) adds \( B^2/(3 \cdot \sum_{tr}^a) \) to \( \sum_a \)
  - \( j = 0 \) leaves \( \sum_a \) unaltered
  - \( j = 1 \) adds \( D^2 \) to \( \sum_a \)

The values of \( i = 1, -1 \) and \( 12 \) are treated the same as \( 1, -1 \) and \( 2 \), respectively, except that the \( D^2 \) absorption terms are removed before the Edit data are executed.

**PCELL 1 (list)**

Group-dependent albedos for the main transport calculation.

- \( i \) a dummy item
- (list) consists of \( g \) cell edge albedos, one for each main transport group

**FREE**

Specifies a free (vacuum) boundary condition at the cell edge. See PCELL above.

**BOUNDARY r**

Varies the boundary condition in DSn calculations between white \((r=0)\) to specular \((r=1)\). The default \((r=0)\) is recommended for lattice pitches large enough for neutrons to "forget" where they came from.
DIFFERENTIAL \{ i \}

Calculate individual condensation spectra for each fuel material in a cluster. Calculated if \( i=0 \) (default). If \( i=-1 \), a previous request for this option is cancelled.

TOLERANCE \( a \)

The convergence tolerance of the main transport routine eigenvalue (default 0.0001).

POISON \( i \ j \)

Burnup of highly absorbing pin cells in a rod cluster can be refined by a pin cell collision probability calculation at each criticality calculation. See reference 4 for more details.

\( i \) - number of regions in the pin cell calculation, POISON value in Prelude Data
\( j \) - number of regions in the poison pin itself.

(NOHOMOGENEOUS)

Prevents WIMS from doing homogenized cell spectrum calculations (in CHAINS 14 and 16), so that the main transport spectrum will be used throughout the calculation.

WPIJ \( m \)

Collision probabilities will be written on TAPE50 on record \( m \), to be read later using RPIJ. \( m \) may be an integer (*0) or a 1 to 10 character alphanumeric string.

RPIJ \( m \)

Collision probabilities will be read from TAPE50 on record \( m \), that were written using WPIJ. \( m \) may be an integer (*0) or a 1 to 10 character alphanumeric string.

WRITE \( m \)

Materials compositions at this point in a calculation will be written to TAPE50 on record \( m \), to be read later using READ. \( m \) may be an integer (*0) or a 1 to 10 character alphanumeric string.

READ \( m \)

Materials compositions, that were written using WRITE, will be read from TAPE50 on record \( m \). \( m \) may be an integer (*0) or a 1 to 10 character alphanumeric string. See WRITE.

RPHI \( m \)

Fluxes, that were written using WPHI, will be read from TAPE 50 on record \( m \). \( m \) may be an integer (*0) or a 1 to 10 character alphanumeric string. The fluxes read in will be used as the starting flux estimate in collision probability flux solutions (Pij and PERSEUS cases only).
WPHI m n
Fluxes will be written to TAPE50 on record m, that may be read later using RPHI. m may be an integer (*0) or a 1 to 10 character alphanumeric string. The fluxes will be written out during collision probability flux solutions (Pij and Perseus cases only), every n'th iteration. The default value of n is 100.

MATSIG
Selects the writing of material cross sections in the full library group structure to TAPE16

MTRFLUX
Selects the writing of the fluxes calculated by the main transport routine to TAPE16.

SCATTER n
Vary the frequency of scattering matrix re-calculation. An appreciable cost saving may be gained as the re-calculation of the scattering matrix before each main transport calculation is a significant cost in many cases, and as it varies slowly in many cases, savings can be gained by reducing this frequency. By default, the scattering matrices that have changed are re-calculated each main transport calculation.

CYCLE i km X dX RT IN w j
Perform automatic fuel cycle calculations:

- i - 1 or 2; see definition of X
- km - irradiation averaged value of k-effective at which burnup terminates
- X,dX - X±dX is the required initial k-effective if i=1, or the target irradiation if i=2.
- RT,IN - use these quantities as t and nt on POWER cards following the first burnup step
- w - irradiation at which plutonium will be extracted for recycle purposes (end of cycle if zero or blank)
- j =0 km is defined by averaging k-effective
- j =1 km is defined as the ratio of integrated neutron production to integrated neutron losses

Only a single set of input data is required for the complete fuel cycle calculation.

See note 16. (USER BEWARE)

RECYCLE j r
To continue a CYCLE run by recycling fuel:

j=1 add plutonium from the previous cycle plus specified enrichment to the basic fuel (specified by the MATERIAL card: to meet the objective specified by the CYCLE card
j=2 add only plutonium of the composition of the previous cycle to meet the objective.

j=3 add only the amount of plutonium from the previous cycle, ignore the objective, and terminate the cycle when the average k-effective = km from CYCLE option.

r - an estimate of the required enrichment relative to that required for the previous cycle. Default is 1.0.

See note 16. (USER BEWARE)

ENRICHMENT (list)
For the RECYCLE option, the list specifies the relative amounts of the following 6 isotopes to be used for enrichment:

1 - U235 (ID=235 or 1235)
2 - Pu239 (ID=3239)
3 - Pu241 (ID=241)
4 - Pu242 (ID=242)
5 - Am241 (ID=941)
6 - (non existent isotope ID=243)

See note 16. (USER BEWARE)

PROCESS t1 t2 f
The composition of the recycled plutonium is corrected for Pu241 decay and processing losses:

t1 - time in days between removing the fuel from the reactor and processing

f - fractional efficiency of plutonium extraction

See note 16. (USER BEWARE)

PRELUDE
In multiple case input, a complete new set of input data after the first case must begin with this card. Its function is to transfer the operation of reading Main data cards to reading Prelude data cards.

BEGIN
Terminator for the Main data group.
### 5.4 Edit Data Group

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Data</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIFFUSION</td>
<td>j k 1</td>
<td>Choice of method for the diffusion coefficient calculation:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>j=1 Benoist</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=2 Transport (default)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=4 Benoist and Transport</td>
</tr>
<tr>
<td></td>
<td></td>
<td>For the Benoist case, l is the number of edit regions forming the outer zone of a three-zone cell model.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>The middle zone is defined by k as follows:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>if k&gt;0 then:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>k=1 void with tubes on both sides</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=2 void with a tube on the inside</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=3 void with a tube on the outside</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=4 void only</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=5 tube only</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=6 tube with an infinitesimal void on the outside</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=7 tube with an infinitesimal void on the inside</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=8 two voids with a tube between them</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=9 three voids with two tubes between them</td>
</tr>
<tr>
<td></td>
<td></td>
<td>if k&lt;0, then</td>
</tr>
<tr>
<td></td>
<td></td>
<td>See note 17.</td>
</tr>
<tr>
<td>BUCKLING</td>
<td>r z</td>
<td>Input geometric buckling. If one or both of the values is 0.0, no buckling search(es) will be performed (defaults are 0.0).</td>
</tr>
<tr>
<td></td>
<td></td>
<td>r - radial buckling (cm$^{-2}$)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>z - axial buckling (cm$^{-2}$)</td>
</tr>
<tr>
<td>NOBUCKLING</td>
<td></td>
<td>No searches for critical bucklings are to be performed.</td>
</tr>
<tr>
<td>LEAKAGE</td>
<td>m</td>
<td>Select the leakage spectrum to be used during k-effective reaction rate edit, using the last diffusion coefficients.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>m=5 spectrum with input bucklings (default)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>=6 spectrum with critical bucklings, with</td>
</tr>
</tbody>
</table>
their ratio as given
=7 spectrum with critical bucklings, with
the radial buckling as given
=8 spectrum with critical bucklings, with
the axial buckling as given

If \( m > 0 \) (default) all three critical buckling searches
are carried out, although only the selected spectrum
is used in the reaction rate edit.

If \( m < 0 \), the \(|m|\) will be used as above, but only a
single critical buckling search will be performed.

BEEONE \( n \)

Selection of method of flux solution in the leakage
calculation:

\[
\begin{align*}
n = 1 & \quad \text{Bl theory} \\
= 0 & \quad \text{transport corrected diffusion theory (default)} \\
= -1 & \quad \text{both of the above}
\end{align*}
\]

REACTION (i t)

Specification of isotopes to be included in reaction
rate edits. The list consists of pairs: consisting
of a nuclide identifier \( i \), and a temperature \( t \) (the
temperature is not used by the code). The special
identifier 'ALL' may be used to select reaction rate
calculations for all isotopes present in the current
case.

PARTITION (list)

Specification of group structure to be used in
reaction rate edit. Each entry in the list gives
the last energy group for the interval; thus the
last entry is the number of library groups.

PRINT i j k l m n

Reaction rate printout control. The list consists
of six switches; the first four have the form
-1/0/1 for punch/print/suppress:

\[
\begin{align*}
i & \quad \text{reaction rates by zone} \\
j & \quad \text{reactions by zone} \\
k & \quad \text{reaction rates by material} \\
l & \quad \text{reactions by material}
\end{align*}
\]

The last two switches have the form 0/1 for
print/suppress:

\[
\begin{align*}
m & \quad \text{k-infinity spectrum} \\
n & \quad \text{k-effective spectrum}
\end{align*}
\]

Defaults for all switches are 0, full printout.

A reaction rate is the number of events per second
per unit volume that would occur if the isotope were
present in a concentration of $10^{22}$ atoms per cm$^3$. This is typically used to calculate foil reactions.

A reaction is the number of events per second that actually occur in a given zone or material.

The cell averaged flux spectrum used is that selected by the LEAKAGE card. The fine structure of the flux in the effective spectrum is that calculated by the main transport calculation, corrected by the ratio of the cell averaged effective lattice flux to the cell averaged infinite lattice flux. The normalization of reactions is either absorption or loss in the cell (see NORMALIZE option).

NORMALIZE s

Selects flux normalization to be used during leakage and reaction rate printouts:

s = 'ABS' The cell flux will be normalized so that there is one absorption in the cell (default).

s = 'LOSS' The cell flux will be normalized so that there is one absorption plus leakage in the cell.

ENDCAP m f t d n

An approximate treatment of bundle end regions will be carried out after the main transport calculation.

m - material number of end region material
f - length fraction of end region in the total of end region plus fuel
t - flux peaking factor of the central 'tie rod' (annulus); -1 for same value as d
d - flux peaking factor for the end region
n - outermost annulus occupied by the end region

THERMAL n

Define the number of thermal groups in the edits (default is the number of groups below 0.625 eV).

WESTCOTT i r t

Define the flux spectrum in region i to be a Westcott spectrum $\phi(w(r,t))$. This option should only be used in homogeneous cases, with the NOHOMOGENEOUS option selected.

OPTION n

Selects the WED edit (data for a code not available at CRNL), which consists of:

(a) flux per unit volume per mesh interval
(b) flux per unit volume times cross section for each material
(c) flux per mesh interval times cross section
sections for each material

n selects the quantities to be printed:

n=0 gives (a), (b) and (c)
=1 gives (a) and (c)
=2 gives (a)
=3 gives no printout (default)
=4 gives scattering cross sections for each region

MATERIAL {n} Punch material data cards for each burnable material (may be used for the restart of a burnup case).

n=0 or blank gives punched output
=-1 cancels request for output

TESTUBES This card causes tubes specified by the DIFFUSION card to be smeared with adjacent regions in the inner or outer zone if the tube thickness is greater than the tube material diffusion coefficient.

See note 18.

BEHADD (list) The 'Behrens slot' option. A list of 3*n numbers ($\leq$30) consisting of:

n values of hole volume
n values of hole radius
n values of Behrens shape factor

For rectangular holes, volumes are -1 and radii and shape factors are replaced by the lengths of the sides. A list of less than three numbers cancels this option.

See note 19 (USER BEWARE).

NOUT n A cylindrical fuel cluster may have more than one type of fuel pin in the outer ring, on the same pitch circle; n is the number of such pin types. It is assumed that there are equal numbers of each pin type, uniformly distributed. For example, if there are three pin types, A, B and C, these will be distributed A B C A B C etc. around the outer ring.

ALPHA i j Self shielding of Pu240 can be varied continuously during a burnup calculation:

i - first (highest energy) main transport group occupied by the Pu240 resonance at 1.06 eV
j - lowest such group

See note 20 (USER BEWARE).

**SATURATE n**

The library identifier of a single isotope required to be in equilibrium throughout burnup may be specified.

See note 20.

**CELLAV**

Selects the writing of cell average information to TAPE16, to be used in diffusion calculations.

**REGION**

Selects the writing of average cross sections and fluxes in each region in the main transport group structure and spectrum to TAPE16. As well, selects the writing of the flux spectrum in the full library group structure and reactions by selected isotopes to TAPE16.

**ISOCYL**

Selects the writing of information used in fuel recycle calculations to TAPE16.

**BEGIN**

Terminator for Edit data group.
6. Notes on the Keywords

These notes are referenced from the keyword descriptions of Section 5, and are intended to help clarify the meanings of the keywords, and to provide additional information on how to prepare the input, as well as pointing out some of the pitfalls that may be encountered.

Note 1: CELL

A pin cell is one in which all physical boundaries are concentric about the cell axis. Pin cell cases should include fuel clad, and coolant spectral type materials but not moderator materials.

The n=5 option indicates that the calculation is to be done in the full library group structure.

Note 2: NRODS

This card is required only for Pij cases in which there are rods, normally fuel bundles. The symmetry factors are well described in Reference 10.

The recommended method of finding the required number of lines and angles is to use the AUTOTRACK option, see example 3 of Appendix F.

The subdivision of portions of a rod into "sectors" is also best understood by referring to Reference 10. This option is used in determining cross-pin flux gradients, etc.

The proper definition for cell symmetry is given in Section E.10.

Note 3: INITIATE

This card initializes a number of variables at the start of a case. If the case is to be continued, as in a multiple step burnup calculation, this option should not be used, as these variables carry over values from previous steps.

Note 4: ANNULUS

The cell is described by a series of concentric annuli, numbered outward consecutively from the central cylinder, starting with 1 (but see also Note 6 on RODSUBS). Some annular boundaries will coincide with physical boundaries such as pressure tubes, calandria tubes, etc., but in addition there may be annular boundaries where no physical boundary exists.

In homogenized cluster calculations (CELL 7, SEQUENCE 1 or 2) separate types of rods should be in separate annuli. In Pij cases, annuli within the NPIJAN'th may not be subdivided using the MESH card and so an adequate spatial mesh must be defined by using a sufficient number of annuli (typically more than 2 per mean free path).
In Pij calculations, it is not necessary that a pin lie completely within an annulus, i.e. the boundary may cut through a pin and the code will then calculate the mesh areas appropriately. If annuli are sectored, however, the annuli sector divisions must either pass through no rods or bisect them.

All annuli in a case must be defined, the number of which is specified on the NREGION card.

Note 5  ARRAY

The ARRAY cards describe the number and position of the rods defined by RODSUB cards. The type numbers must be consecutive, starting with 1. All identical rods on the same pitch circle may be of the same type, but identical rods on different pitch circles should be of different types, as they will in general have different fluxes.

Note 6  RODSUBS

These cards describe annular rods distributed according to ARRAY cards. In Pij cases, the rods may be subdivided into concentric annuli as well as sectored for detailed material distributions or fine-structure calculations. As the cost of calculations increases with the number of meshes, rods should only be subdivided as required. Similarly, the calculation of collision probabilities for very small or optically thin meshes is difficult and so such meshes should be only used if they are actually required. The most frequent example of an expensive unnecessary mesh is the gap between fuel and clad: homogenizing it with the clad is an excellent approximation and in most cases the flux was poorly calculated in the gap. See Reference 10 for a good description of ARRAY and RODSUB input.

Fuel pins on the axis of the cell in a cluster should be represented as RODSUBS.

Note 7  MATERIAL

The materials must be numbered consecutively from 1. Materials in a cell that are initially the same composition but will change due to burnup should be specified as separate materials, to allow the compositions to vary independently.

In a cluster case (CELL 7) the fuel material in the outer ring, even if it does not undergo burnup, should be specified as a separate material from the fuel(s) in the inner part of the cluster, as WIMS-CRNL calculates separate resonance cross sections for the inner and outer part of the cluster.

Specification of the spectral type may cause some confusion; the general rule is to collect materials in similar regions. For structural materials, such as hanger rods and tubes, use the spectral type of their dominant surroundings.

Input Option Notes
Note 8  MESH

Each annulus must contain at least one mesh point. A general rule on the selection of the meshes is to consider the typical mean free paths of regions, and the spatial rates of change of the flux in those regions. More meshes are required in regions where the flux changes quickly with respect to mean free paths. A reasonable number of points is two or three per mean free path for general calculations, but where greater accuracy is required, more may be necessary.

See note 9, HOMOGENIZE

Note 9  HOMOGENIZE

This option automatically calculates optimized annuli radii for cluster homogenization. The model used in WIMS-CRNL for cluster homogenization is as follows:

- The material properties of each annulus in the cell containing RODSUBS are calculated from a flux (from the SPECTROX calculation) and volume weighted average of the rod materials and the remainder of the annulus.

- The flux distribution in the purely annular cell model is solved by DSn or PERSEUS. The number of mesh points in each of the homogenized annuli is determined by the MESH card.

- After the flux solution, the homogenized annuli are de-homogenized. The average flux in each homogenized annulus is calculated, and the fine structure from the SPECTROX calculation is used to calculate an average flux in each of the components of the annulus (the rod regions and the remainder of the annulus).

Although the homogenized cluster treatment in WIMS-CRNL produces results in very good agreement with explicit cluster models using Pij, the results are affected to some extent by the choice of annuli within the homogenized region. The recommended choice of annuli are a contiguous set of annuli containing rods, one annulus per 'ring' of rods. There should be no interstitial 'coolant' annuli. The annuli radii should be chosen in such a way that the results of Pij calculations are closely reproduced; in practice an equal width of annulus on either side of the rod pitch circle has been found to work well in most cases.

The restrictions on the HOMOGENIZE option are:

- all annuli containing rods must be in a group, with no interstitial annuli

- the annuli outer radii initially defined on the ANNULUS cards are arbitrary, but must fall between rings of rods

- as the outer radii of all of annuli to be homogenized will be
varied, there should be one coolant annulus between the last homogenized annulus and a fixed boundary such as a pressure tube.

Note 10  FEWGROUPS

Condensing the energy groups reduces both computing time and memory requirements, usually with little decrease in accuracy. The 89 group ENDF/B-V Library is commonly condensed to 20 groups for the main transport calculation. This is done by:

(Prelude) NGROUPS 20
(Main) FEWGROUPS 10 18 24 33 41 43 47 53 55 58 60 65 68 72 75 78 80 83 86 89

These are the default values produced in a case prepared by TESHOM (Appendix B).

Note 11  NPIJAN

The annular boundary that is specified by this card does not have to coincide with a physical boundary, but unlike the other annuli, it must not intersect any portion of the rods. The position of this boundary separates the cell into two domains, an inner one in which the collision probabilities will be calculated for the two dimensional geometry by $P_{ij}$, and an outer one in which the collision probabilities will be calculated for the one dimensional annular geometry by PERSEUS. The two domains will be connected by approximating the angular flux distribution at the boundary as a cosine distribution. The position of the boundary should be chosen to be at least a few mean free paths radially beyond the actual limit of the physically two-dimensional part of the cell.

Note 12  BELL
DANCOFF
REGULAR

These parameters are involved in the calculation of shielded resonance cross sections; see References 2 and 4. These options are only relevant to cases in which the new resonance treatment is not used (NEWRES).

Note 13  NEWRES

A new resonance treatment was developed for WIMS-CRNL. The resonance treatment is similar in theoretical basis to that originally in WIMS, but has been developed following the methods described in Reference 19. The method implemented is more straightforward, and the coding for it is easier to maintain and modify than that for the original treatment; future developments and maintenance of the resonance treatment in WIMS-CRNL will be in the NEWRES treatment.
Note 14 SKIN

This option is only applicable to pin cell geometry. For the isotope listed (U238 or TH232), the code redistributes the resonance captures through the pin (in each of the regions specified on ANNULUS cards within the fuel) according to an empirical prescription which gives good agreement with more accurate calculations. The average resonance capture rate calculated by WIMS-CRNL for the pin is preserved. The purpose of this option is to model the buildup of plutonium near the surface of a rod during burnup, the so-called skin effect.

Note 15 POWER

A burnup calculation follows the main transport and edit calculations. At the end of the main transport calculation, cell-averaged macroscopic cross sections are calculated in the condensed group structure from the flux weighted regional cross sections. The k-effective is calculated from the neutron balance in the equivalent homogeneous cell, using cell-averaged homogeneous cross sections, and a fundamental buckling mode. This calculation also gives cell-averaged condensed group fluxes. For the burnup calculation, the flux fine structure resulting from the (previous) main transport calculation is assumed to remain constant.

At the start of each burnup time step t, the cell-averaged fluxes are normalized to the quantity specified by the parameter i. The regional fluxes are determined from these normalized cell-averaged fluxes and the main transport calculation fine structure. The burnup equations are then integrated over the time step in each fuel region, using these constant regional fluxes. At the end of the time step, new isotope number densities and cell-averaged cross sections are determined. RTAU should be small enough so that the approximation of constant power to flux is good, about 10 days in a power reactor.

This process is repeated nt times, with the flux spectrum being renormalized at the beginning of each time step, but the fine structure remaining constant. To revise the fine structure, a new main transport calculation must be requested by additional sets of main data and edit data cards. If none of the case data are modified, the additional cards need consist only of a pair of terminators (BEGIN) for each main transport calculation, but other changes may be included. For example, a burnup case with 10-day time steps and main transport calculations at 0, 100, 400, 700 and 900 days would be as follows:

```
INITIATE
[Main Data]
POWER 1 37 10 10
BEGIN
[Edit Data]
BEGIN
BEGIN
POWER 1 37 10 30
BEGIN
BEGIN
```

input Option Notes
BEGIN
POWER 1 37 10 20
BEGIN
BEGIN

The main transport calculations should be more frequent during periods of rapidly changing spectra, such as with fresh fuel.

Note 16 RECYCLE CALCULATIONS

The four options CYCLE, RECYCLE, ENRICHMENT and PROCESS were designed to automate some parts of fuel cycle calculations; the coding for these options does not operate properly in WIMS-CRNL. The calculations that would be performed using these options are now carried out by an independent program, WIMCYCLP.

Note 17 DIFFUSION

The Benoist diffusion coefficient model implemented in WIMS-CRNL explicitly treats three annular regions, while the original Benoist model in WIMS used two outer regions plus a middle void.

The choice of the regions to be put in the three zones of the Benoist diffusion coefficient model should be based mainly on the relative transparency of the various regions. Relatively transparent materials such as gas or aluminum normally make up the middle zone. Note that zirconium is not transparent, and that geometries that are not well described by three annuli will not be well approximated in the diffusion coefficient calculation. The definition of 'regions' is made by CHAIN 13, in which adjacent 'zones' of the main transport solution are combined into a single 'region'.

Except for those cases using the TESTUBES option, the meaning of 'tubes' is of no significance, and k is simply related to the number of regions in the middle zone:

\[
k = \begin{cases} 
4 \text{ or } 5 & \text{1 region} \\
2, 3, 6 \text{ or } 7 & \text{2 regions} \\
1 \text{ or } 8 & \text{3 regions} \\
9 & \text{5 regions}
\end{cases}
\]

The data case produced by TESHOM for DIFFUSION may not be appropriate to all cases, and should be checked carefully.

Note 18 TESTUBES

This option tests if either of the 'tubes' on the inside or the outside of the middle zone defined on the DIFFUSION card is fairly transparent in each energy group. If the tube is not fairly transparent, it is grouped with the regions in the inner or outer zone as appropriate.
Note 19 BEHADD

A specialized geometry including "holes" in the cell materials; see Reference 12.

Note 20 ALPHA
SATURATE

These quantities are associated with the burnup calculation (see Note 15). For ALPHA, the default value associated with the "standard" 18-group condensation is i=j=10.

Note 21 SEQUENCE

The order of the annular collision probability integration in PERSEUS may be varied from 2 to 5. The accuracy of the calculation increases as the order is increased, as does the cost of the integration. For most calculations, a third order integration is sufficiently accurate and cost effective; for very accurate calculations, a fourth or fifth order integration should be applied.
References


(22) Carlvik, I., 'Integral Transport Theory in One-Dimensional Geometries', NUCLEONIK, 10 (1967), pp. 104-119.

8. Acknowledgements

I am indebted to G.J. Phillips for the original version of the WIMS-CRNL manual on which this manual was based. M.T. van Dyk prepared the original description of TAPE16, upon which Appendix G is based.
Appendix A
The History and Evolution of WIMS

A.1 Development of WIMS at Winfrith

WIMS was created at AEEW during the 1960's by linking together a group of independent multigroup lattice codes. The linked system provided common input and output sections, and optional choices for the flux calculation, which could be specified by the input cards. The system operated on the English Electric KDF-9 computer at Winfrith.

In most respects, the KDF-9 was a typical second-generation computer, with transistorized electronics, a 32-bit word size, and 32K of memory. Even the early versions of WIMS were far larger than the available core memory, but the hardware included a relatively advanced on-line disc system, on which large codes could be stored in what were essentially overlays. The operating system included a capability of allocating storage space after the start of execution, i.e. a "variable array dimension" scheme, and together these facilities allowed the execution of very large calculations for computers of that era.

Coding for the KDF-9 was done in EGTRAN, a version of FORTRAN II, and program operation was controlled by the Egdon Programming System. AEEW is located on Winfrith Heath, in Dorset, and the names Egtran and Egdon acknowledged the significance of this landscape to the literature of Thomas Hardy.

As WIMS was developed, various versions were given designations of WIMS-A, WIMS-B, etc. Once established, each version was "frozen" and no further modifications were made to it. All new developments, including correction of errors, were applied only to the latest version under development. This policy allowed, at least in principle, the exact reproduction of previous cases.

The status of WIMS in 1969 is summarized in Reference 13. In 1970 the current version at AEEW was WIMS-D2, and in 1971 this code was transferred to CRNL. The present version of WIMS-CRNL has developed from this code, and although the structure of the code has been extensively modified, most of the physics of the calculations remains intact.

During the early 1970's, WIMS-D3 was developed at AEEW. By this time the code was operating on the Winfrith ICL/4-70 computer, and the main changes in the D3 version were machine-dependent ones to make more efficient use of the newer hardware.

In 1975 WIMS-D4 was established. This is a significant extension of previous versions and includes a large number of new options, as indicated in Reference 5. This version is written in IBM FORTRAN, and has not been translated to the Control Data machines at CRNL. Members of the WNRE staff have run cases on a commercial computer utility.

AEEW is also developing WIMS-E, which was intended to be a successor to WIMS-D but has turned out to be a parallel development. WIMS-E is an example of "modular coding", a fashionable development of the late 1960's as the
"third generation" of digital computers was becoming available. Modular coding was intended to exploit the new storage technologies and more sophisticated operating systems of these machines to provide easier maintenance and more flexible operation of very large systems of computer codes.

Briefly, modular coding implies that the large codes are divided into more-or-less independent modules, each of which performs a single (but not necessarily simple) calculation. The modules communicate only through online disc files, called "interfaces". Providing that the interfaces have been rigorously but flexibly defined, it is then possible (at least in principle) to couple the modules in various ways to perform a variety of calculations.

During 1970, WIMS-E duplicated most of the calculations of WIMS-D2, and was put into operation on the Winfrith ICL/4-70. It quickly became apparent, due in part to limitations of that machine's original operating system, that WIMS-E was significantly slower than WIMS-D2, and used excessive amounts of disc storage. It was also evident that for the modules then available there were only a very few combinations of the modules that were logical, and so the flexibility of the modular scheme offered no advantages. For these reasons, development of WIMS-D was continued in parallel with WIMS-E.

Since that time, the relative position of WIMS-E has improved significantly. Better operating systems have become available, and a large number of additional modules have been added for the system. WIMS-E is now established as an important reactor design tool, and is capable of many computations not available in WIMS-D, although the latter will continue in existence as a cheaper and more convenient code for some applications.

It had been anticipated that WIMS-E would eventually be made publicly available through the National Energy Software Center (Argonne National Laboratory). It is now understood that commercial considerations have delayed this action, and may preclude it.

A.2 Development of WIMS at CRNL

A recent summary of the developments that have been made to the WIMS code since it was received at CRNL can be found in Reference 16. A few of the more important areas of improvement in user applications of the code are noted below.

The WIMS code, as received from Winfrith, was written in IBM FORTRAN and was designed to run on an IBM computer. While these facts did not preclude its implementation on a CDC computer, they made a significant amount of effort necessary to make the code work well on the CRNL computer system. As well, the implementation of the code in the CDC operating environment was not an optimum in cost.

The initial developments (prior to about 1979) were:

- WIMS was converted to CDC FORTRAN 4 and OVERLAY loading.
- Variable names were changed to improve the consistency throughout the
code. The variable name inconsistencies were due, in large part, to the fact that WIMS was initially built by bringing together a number of independent codes.

- In order to implement an anticipated improvement in the code, the number of subroutines was reduced until each of the major subdivisions of the WIMS-CRNL calculation was carried out by one, or a few, routines. This lengthened many of the routines to a few thousand lines of source code.

The developments to the code implementation since that time have been:

- WIMS-CRNL was converted to FORTRAN 5 to make it more portable. As far as is possible the code is now written in ANSI standard FORTRAN 77.

- The variable storage scheme was changed from 'extensible blank common' to dynamic memory allocation when this became available in the CDC operating system. This change significantly improved the efficiency of memory use, which had been limiting the turn around time and the size of cases that could be calculated. Currently the main limit on storage in WIMS-CRNL is due to the central memory size of the CRNL system, about 100 thousand sixty bit words.

- File processing has been improved, especially of the nuclear data library. Random access files, rather than sequential, are now used where appropriate; when implemented efficiently on the CDC system this has resulted in an 8 fold reduction in Input/Output time (79% reduction in cost) in a typical burnup case.

- Extended Semiconductor Memory (ESM), which is about half a million sixty bit words of memory that can be indirectly addressed, is now used as a fast substitute for disk files in the processing of the nuclear data library and as storage for collision probability matrices if required. ESM is used as available and required, in a manner that is transparent to the user. In a typical burnup case, the use of ESM results in a 30% reduction in Input/Output time (7% cost reduction). In some applications, such as two-dimensional full core models of small reactor designs, it has allowed detailed calculations that would have otherwise been impossible.

- Changes have been made to the code to simplify some parts of input preparation, and the handling of data produced by WIMS-CRNL.

- To improve the structure of the code and to ease its maintenance, the code has been divided up into smaller subroutines.

Improvements have been made to the numerical methods and physics of WIMS-CRNL. Some of the main areas of change have been:

- Integration of isotopic compositions during burnup was changed from a simple Simpson's rule to a Gear integration using STIFFZ. This change allowed greater control of the accuracy of burnup calculations and non-equilibrium transients to be simulated, without any significant increase in cost.

History of WIMS
- To improve the evaluation of the Bickley function used in the integration of collision probabilities. A method of speeding up the evaluation has reduced the cost of integration by a factor of 2.5 relative to the method originally used in WIMS. The method currently used is to evaluate the function using a second order Chebyshev polynomial, which is tabulated at 2500 points. The trade-off of a large table in central memory and a very short calculation to evaluate the function has been made against the cost of evaluating rational polynomials; it has proven to be cost effective. The cost reduction has had a significant impact on the cost of performing detailed two-dimensional calculations with WIMS-CRNL.

- The approximate method of calculating collision probabilities in annular geometry (ring transmission probabilities using a cosine current approximation) was replaced by an accurate calculation. A small increase in cost for most cases was considered an acceptable tradeoff.

- The method of calculating Benoist diffusion coefficients was changed from a two region plus void model to an explicit three region model. The accuracy of the Benoist diffusion calculation was improved with no significant cost increase.

- An alternative resonance treatment was incorporated into WIMS-CRNL. The new treatment, although very similar in general principles to the original treatment in WIMS, was based on simpler physical models and allows changes and improvements to be incorporated more easily.

- The two-dimensional collision probability calculation, Pij, has been extended to allow sectored annuli to be modelled in WIMS-CRNL. This option had been incorporated into a later version of the Winfrith WIMS (WIMS-E), but this version of the code is not available.

- An approximate treatment of the resonance skin effect in annular geometry has been incorporated into WIMS-CRNL. This extension allows more accurate distributions of fissile isotopes produced during resonance capture (for instance Pu239 production) to be calculated, which has proven to be an important component in the calculation of fuel temperature distributions and fuel performance.
The TESHOM input code may be used to run WIMS-CRNL cases. TESHOM operates by reading its own free-form input and preparing the corresponding WIMS-CRNL input in the form described in this report. This input is then delivered to the permanent file copy of WIMS-CRNL for execution, or it may be saved on file and later used for separate input to WIMS-CRNL.

In addition to the "standard" WIMS-CRNL input produced by TESHOM, some of the default values may be overridden using appropriate TESHOM keywords.

For some input parameters, such as the locations of annuli, or the specification of burnup runs, the TESHOM default values will rarely be optimum. Since not all of the default values can be overridden, TESHOM is probably best used to prepare an initial deck of WIMS-CRNL input. This deck may then be revised to best represent the particular lattice for the WIMS-CRNL calculations.

TESHOM does not produce correct isotope identifiers or group condensation schemes for the ENDF/B-V library.
Appendix C

Jobcards

The following show the jobcards that are currently required to execute WIMS-CRNL on the CDC computers at CRNL.

(a) Direct execution of WIMS-CRNL input:

    JOBCARD, ------
    LIBRARY(APPLICS)
    WIMS(options)
    LIBRARY.
    /EOR
    [WIMS Input Cards]

The 'options' available for the execution of WIMS-CRNL are controlled through the optional parameters on the control card as follows:

    WIMS(input,output,punch,ABS=a,LIB=x,LIMIT=n)

Where

   'input' is the local file name of the WIMS-CRNL case input (default is INPUT)

   'output' is the local file name for WIMS-CRNL printout (default is OUTPUT)

   'punch' is the local file name for punched output from WIMS-CRNL (default is PUNCH)

   'a' is a flag: - if equal to YES (default) the 'frozen' version of WIMS-CRNL will be used
       - if equal to 0 the current developmental version of WIMS-CRNL will be used. This version will have been tested, and will include any recent modifications, but will change without notice.

   'x' is a flag: - if equal to 0, no library will be attached and so the user is responsible for attaching a library as local file TAPE2.
       - if equal to 1 (default) the Winfrith library will be attached automatically.
       - if equal to 5 the ENDF/B-V library will be attached automatically. If the user is not validated for use of this restricted library, the run will be aborted.

   'n' is the maximum number of printout lines from the WIMS-CRNL case (default is 10000)

The options input, output, and punch are position dependent.

Executing WIMS-CRNL at CRNL
(b) Execution of WIMS-CRNL with TESHOM input:

```
JOBCARD, ------
ATTACH,TESHOM,TESHOM,ID=TESHOM.
TESHOM.
RETURN(WIMS)
LIBRARY(APPLICS)
WIMS,TAPE4,options.
LIBRARY.
/EOR

[TESHOM Input Cards]
```

In this case, TAPE4 contains the WIMS-type input, which may be saved on file to use for direct input as in (a).

In Pij (and PERSEUS) cases requiring large numbers of meshes and or groups, the available central memory on the computer system at CRNL may not allow the case to be run. WIMS-CRNL will use Extended Semiconductor Memory (ESM) to store the Pij matrices as required and available, allowing much larger problems to be solved.
Appendix D

The WIMS-CRNL Libraries

There are two standard libraries of nuclear data used in WIMS-CRNL calculations, which reside on the permanent file system of the central site computers at CRNL. The two libraries are the 'Winfirth' library, and the 'ENDF/B-V' library.

The Winfrith library contains 69-group data for 110 nuclides, as listed in Table D-2. For a few isotopes the library contains more than one set of data, and for these the recommended sets are indicated by an asterisk (*). Table D-2 gives the energy group structure.

The Winfrith library has the following history. In 1971 January, G. Phillips transferred an 80-nuclide, 69-group library from AEEW to CRNL. In 1973 D. Hamel obtained another 69-group library that contained data for 13 additional nuclides, and Hamel merged the two libraries. After some modifications to the data that related to thorium calculations, this became the current library, except for a later, minor correction to the uranium-234 data.

Recently, an 89 group library has been created for WIMS-CRNL from ENDF/B-V nuclear data. The library represents the state of the art in nuclear data, and has been found to be in good agreement with experiment when used with WIMS-CRNL. The isotopes contained in the library are listed in Table D-3. The energy group structure in the ENDF/B-V library is shown in Table D-4.

The code WILMA is available for library listing, additions, deletions and condensations.
<table>
<thead>
<tr>
<th>ISOTOPE</th>
<th>ISOTOPE NAME</th>
<th>WEIGHT (AMU)</th>
<th>TEMPERATURE TABULATIONS</th>
<th>RESABS TABLES</th>
<th>RESFIS TABLES</th>
<th>FISSILE</th>
<th>BURNABLE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) 2001</td>
<td>H1A</td>
<td>1.0078</td>
<td>5</td>
<td>0</td>
<td>0</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>2) 6001</td>
<td>H1</td>
<td>1.0078</td>
<td>5</td>
<td>0</td>
<td>0</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>3) 8001</td>
<td>H1H2O</td>
<td>1.0078</td>
<td>9</td>
<td>0</td>
<td>0</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>4) 9001</td>
<td>H1HBO</td>
<td>1.0078</td>
<td>9</td>
<td>0</td>
<td>0</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>5) 2002</td>
<td>D2</td>
<td>2.0141</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>6) 8002</td>
<td>D2A</td>
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Table D-2: Energy Group Boundaries in Winfrith Library

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3.6726E+02 > 21 > 1.4873E+02 > 22 > 7.5501E+01 > 23 > 4.8052E+01 > 24 > 2.7700E+01
2.7700E+01 > 25 > 1.5968E+01 > 26 > 9.8770E+00 > 27 > 4.0000E+00 > 28 > 3.3000E+00
3.3000E+00 > 29 > 2.6000E+00 > 30 > 2.1000E+00 > 31 > 1.5000E+00 > 32 > 1.3000E+00
1.3000E+00 > 33 > 1.1500E+00 > 34 > 1.1230E+00 > 35 > 1.0970E+00 > 36 > 1.0710E+00
1.0710E+00 > 37 > 1.0450E+00 > 38 > 1.0200E+00 > 39 > 9.9600E+01 > 40 > 9.7200E+01
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Table D-4
Energy Group Boundaries in ENDF/B-V Library
( Electron Volts )

WIMS-CRN Library
Appendix E
The Structure of WIMS-CRNL

The structure of WIMS-CRNL has changed with time since the code was received from Winfrith, as the computers and operating systems have evolved. Because the structure has changed, some of the terminology used in its descriptions has been inconsistent. The following description will attempt to present a clear picture of the past and present structure of WIMS-CRNL.

WIMS-CRNL is a large code and it was not possible to load all of the code at once into the computer(s) on which it was developed and run. This is still the case for the computers at the central site of CRNL, although it is no longer a problem for virtual memory computers. The technique used to load sections of the WIMS-CRNL code as they are required during a case has changed with operating systems:

- The original scheme (on a KDF-9 computer) was called CHAINS, and this name has stuck with the code although they are not necessarily the fundamental units of WIMS-CRNL as they once were. Each CHAIN was loaded as a unit, and was a basic unit of the WIMS-CRNL calculation.

- The next scheme used was based on OVERLAYS in the CDC operating system. The sequence and composition of the overlays closely followed that of the CHAINS.

- Currently a SEGMENT scheme is used. In this scheme the code has been divided into many sections to minimize the central memory field length required by the code while not adding significantly to the cost.

For most purposes, the system used for loading the different sections of the code is not important for the understanding of code operation, and it is sufficient to know that the sequence generally follows the flow of the calculations. In the following discussions 'CHAINS' are used to refer to major units of the WIMS-CRNL calculation, as opposed to 'Segments' which refer to the units of code loaded together.

The code consists of 16 CHAINS. Figure E-1 is a simplified flowsheet showing the sequence of execution through these CHAINS. The following notes briefly describe the contents and function of each CHAIN. The numbering of the CHAINS requires some explanation. At one time there were 15 secondary CHAINS, numbered more-or-less in their order of execution, except for CHAIN 12, the burnup calculation. When the code was transferred to CRNL, CHAIN 12 was split into two parts, and the second part became a new CHAIN, number 16. Two CHAINS were deleted, so the actual total of CHAINS was then 14. Since the name of the CHAIN is also associated with the particular calculation the burnup calculation is now referred to as "CHAIN 12A" and "CHAIN 12B", residing in "CHAIN 12" and "CHAIN 16", respectively.

In the Main data group of the input, the SUPPRESS keyword controls the output from the CHAINS. This card retains the format of 16 switches, corresponding to the original CHAINS, although CHAINS 9 and 10 no longer exist, and dummy values must be supplied for these two switches when using the SUPPRESS
In the following descriptions, Sections E.1 through E.16, the level of detail has been geared to the requirements and interests of most users: greater detail is presented in those areas where more understanding may be required for effective application of WIMS-CRNL.

**FIGURE E-1. WIMS-CRNL Flowchart**

```
Base

→ CHAIN 0 Prelude
→ CHAIN 1 Main Data
→ CHAIN 2 Cross Sections
→ CHAIN 3 Resonance Calculations
→ CHAIN 4 SPECTROX Calculations
→ CHAIN 5 Condensation

\/

CHAIN 6 DSn

\/

CHAIN 7 PERSEUS

\/

CHAIN 8 Pij

ECHAIN 11 Unsmear
→ CHAIN 13 Multi-Region Few Group Edit
→ CHAIN 14 Leakage
→ CHAIN 15 Reaction Rates
→ CHAIN 12 Burnup A
→ CHAIN 16 Burnup B
```

**E.1 Base**

This controls the sequence of execution of the main segments in WIMS-CRNL.
E.2 CHAIN 0 Prelude

This reads the Prelude data group cards. Central memory storage that will be required to process the Main data, or will be required throughout the case, is allocated.

E.3 CHAIN 1 Main Data Preparation

This reads the Main data group cards and sets initial conditions. The subroutine RESTART, which controls the automatic fuel cycle calculations is executed if required. The initial processing of the cell geometry is carried out, which includes: calculation of cluster homogenization model if required, calculation of region volumes and some initial checks of the cell geometry definition.

E.4 CHAIN 2 Cross Section

The microscopic cross sections are read from the library, and macroscopic cross sections for all the cell materials are computed. During the calculation of material cross sections in the thermal range, linear interpolation in temperature is performed between the available temperature tabulations. Therefore, if an isotope cross section tabulation does not span a range of interest, those cross sections, when used by WIMS-CRNL, will not vary with material temperature.

The bulk of the work performed by CHAIN 2 is associated with the manipulation of the scattering matrices. As the matrices are large (up to 89·89 elements) and contain many zeros, they are treated as sparse matrices, complicating the addition of isotopes and temperature interpolations as materials are made up from their components. The matrices are too large to be all stored in central memory, and are stored in ESM as available or in a random access file.

E.5 CHAIN 3 Resonance Calculation

Additional library data are used for the calculation of the resonance cross sections, for isotopes having those tabulations. The resonance treatment in WIMS-CRNL is based on equivalence relations that relate mixtures of isotopes and heterogeneous geometries to an equivalent dilution of each resonance isotope. The method has proven to be efficient and accurate for normal applications of WIMS-CRNL.

The geometries that can currently be treated are homogeneous, pin-cell and cluster. A treatment is available for slab geometry in the 'old' resonance treatment. For cluster geometry, the fuel is separated into two parts: the fuel in the outer ring in the cluster, and the rest of the fuel in the inner part of the cluster. Separate resonance cross sections are calculated for the materials in the inner and outer parts of the cluster.

E.6 CHAIN 4 SPECTROX

The cell geometry is approximated in a simplified model and the spectra are calculated in the full library group structure for the "fuel", "can",
"coolant" and "moderator" regions.

For pin cell geometry, the cell materials are collected into fuel, clad and coolant. The flux spectrum in a simplified three region annular cell model is calculated.

In cluster geometry, the treatment is more complicated to better approximate the effects due to the complex geometry. The cell materials are collected into fuel, clad, coolant and moderator regions. Collision probabilities are calculated for a three region annular cell of fuel, clad and coolant of average size and composition. The cluster is formed by linking together the pin cells in the cluster, reducing the collision probabilities to those for four regions: all of the fuel, all of the clad, all of the coolant and the surface of the cluster. The cluster surface is then linked to the moderator and the flux spectrum in the four region model is calculated. In addition to the treatment of cluster geometry, a model exists (DIFFERENTIAL) to approximately calculate the spectrum in different fuel materials within a cluster.

E.7 CHAIN 5 Condense

The spectra calculated by SPECTROX are used to condense the group cross sections in the library group structure to a smaller group structure (specified by FEWGROUPS) for the main transport calculation. In homogenized cluster calculations, cross sections for materials that are the spectrum and volume average of fuel, clad and coolant in each annulus are calculated.

E.8 CHAIN 6 DSN

Main transport calculation in annular geometry by the Carlson Sn method. When completed, the code continues to CHAIN 11.

E.9 CHAIN 7 PERSEUS

Main transport calculation by collision probabilities in annular or slab geometry. In annular geometry collision probabilities are calculated using the Carlvik method. The power iteration method, with variational acceleration and rebalancing, is used to solve the neutron flux distribution and spectrum.

When completed, the code continues with CHAIN 11.

E.10 CHAIN 8 PIJ

Calculation of collision probabilities in two-dimensional geometry, within the inner area defined by the "Pij radius". The main portions of the Pij calculation are as follows:

1. The cell geometry is checked and divided up into the meshes defined by the ANNULUS and RODSUB cards. The information that will be required during the tracking to follow is collected.

2. The tracking required for the calculation of collision probabilities is
performed. The tracking is performed in a similar fashion to that used in many Monte Carlo codes, defining a large number of lines and determining the intersections with individual meshes.

The symmetry number of the cell defined on the NRODS card is used to reduce the size of the tracking problem. A simplified explanation of the symmetry (defined by n2 on the NRODS card) is as follows:

The symmetry number defines that number of planes in the radial direction spaced equally around the cell, one placed at $\theta=0$. If the cell symmetry is rotational, then the geometry within each of the sectors bounded by the planes is identical. If the cell symmetry is reflectional, the sectors on either side of each plane are mirror images of each other.

The cell symmetry partially determines the placement of lines in the tracking mesh, explained below.

3. The code constructs a number of lines during tracking, determined by the NRODS, SETS and LINES cards. The placement of the lines is determined by the number of lines and angles as follows:

   Tracking line centers are placed at equal radial increments within the radial limits defined by the LINES card, or if LINES cards are not used between the cell center and the outer limit of the Pij region. The number of tracking line radial positions is equal to the 'number of lines' on the data cards.

   At each radial position, tracking line centers are placed at the number of angles defined by the data cards. The tracking line centers will be placed at equal angular increments within a sector of $2\pi/(\text{the symmetry number})$. The placement of the sector is determined by the sign of the symmetry number: if positive, the sector begins at 0 and if negative the sector is centered on 0.

4. Once the center of each line has been defined, lines are 'constructed' that are normal to the radial direction. The points along the line at which cell boundaries are crossed are calculated, and this 'track' is written to a file. During this calculation, although the lines only originate within the symmetry sector defined above, the lines extend throughout the two dimensional region in which all geometry subdivisions are explicitly represented.

5. After all tracks have been completed, the code begins the integration of the collision probabilities from the track. The file of tracks is read once for each energy group. The collision probabilities are evaluated by a series of Bickley functions involving the track segment lengths and material cross sections, consuming the bulk of the time required for a Pij calculation. The method used for the evaluation of the Bickley function has been carefully optimized to produce accurate results at the least cost.
When the calculation of the collision probabilities in the two-dimensional region is completed, the code continues with CHAIN 7, where the PERSEUS calculation is applied to the remaining outer area of the cell, and the flux solution is carried out.

E.11 CHAIN 11 Unsmear

Does a variety of preliminary calculations related to the neutron balance and reaction rates, including the "unsmearing" of rod clusters from their annular approximations.

[Chain 12 - see below]

E.12 CHAIN 13 Regional and Cell Edit

This is the first stage of the edit operations performed on the results of the main transport calculation. Flux distributions, cross sections, etc. are printed for the main transport groups (i.e. the condensed groups specified by FEWGROUPS) and also in a two-group presentation. The Edit Data group of input cards is read in by this CHAIN.

E.13 CHAIN 14 Leakage

This CHAIN performs the diffusion coefficient calculations, leakage calculations and buckling searches on the homogenized lattice cell.

E.14 CHAIN 15 Reaction Rates

Calculates reactions and reaction rates by mesh and by material for any combination of library energy groups and for any library nuclide. The reaction rates can be computed over spectra with and without leakage.

At the end of CHAIN 15, the code enters the burnup calculation in CHAIN 12 if requested, but otherwise returns to CHAIN 1 to read a new set of Main Data group cards.

E.15 CHAIN 12 Burnup A

The first part of the burnup calculation. Reads burnup data from the Library, prepares cross sections, etc.

E.16 CHAIN 16 Burnup B

Continues the burnup calculation, integrates the burnup equations, determines the new nuclide number densities, etc., and prints the burnup output. When complete, the code returns to the Main data input in CHAIN 1. If the burnup case is to continue, the next Main data group will (probably) consist of only a new POWER card, and a new flux distribution corresponding to the revised nuclide number densities will be computed by a new pass through the entire code.
Sample WIMS-CRNL Cases

In the following sample WIMS-CRNL cases, input cards to be mentioned in the following discussions are marked with a sharp (#).

F.1.1 Homogeneous Cell Case

#1 TITLE "SAMPLE CASE FOR A HOMOGENEOUS WIMS-CRNL CALCULATION"
#2 SEQUENCE 2 * PERSEUS FLUX SOLUTION
   CELL 4 * HOMOGENEOUS CALCULATION
   PREOUT
   INITIATE
   *
   * HOMOGENEOUS SOLUTION OF NATURAL URANIUM IN HEAVY WATER
#3 MATERIAL 1 1.105 293 1 D2=20.06 H1=.028 O16=79.91 U235=.0310 U238=4.375
   *
   SUPPRESS 1 1 1 1 1 1 1 1 1 1 0 0 1 * PRINT CHAINS 14 AND 15
   BEGIN
   PARTITION 69 * ONE GROUP REACTION RATE PRINTOUT
#4 LEAKAGE -6 * PRINT REACTION RATES AT CRITICAL BUCKLING
   PRINT 1 1 1 0 1 0 * PRINT CRITICAL REACTIONS BY MATERIAL
   REACTION U235=0 U238=0
   BUCKLING 5E-5 5E-5 * STARTING GUESS FOR BUCKLINGS
   BEEONE 1 * B1 LEAKAGE
   BEGIN

F.1.2 Notes for Sample Homogeneous Cell Case

The above sample homogeneous case is one of the simplest WIMS-CRNL calculations that can be performed, but is useful in showing some recommended ways of preparing input. The first card in the case (#1) is the case title. The title, while not required, is a very useful way of identifying the case, as it will appear at the start of the printout of each CHAIN not suppressed, and as a record on TAPE16.

The method of transport solution selected (#2) was the PERSEUS collision probability solution. This method has been found to be the most efficient for homogeneous cases.

In the definition of the cell material (#3), isotope names rather than numbers have been used, as they are much clearer in meaning and more portable between nuclear data libraries. An equals sign (=) has been used as a delimiter between the isotope names and their weight fraction; a space would be functionally the same, but would not show the connection between the data items as clearly.

The leakage card (#4) selects that the reaction rates in the effective cell spectrum will be chosen as those at critical buckling with the input ratio of axial to radial buckling. This is the normal way to select a critical spectrum where the bucklings are not known in advance. A single critical buckling search has been selected as the other two were not required; in
cases in which a number of searches will be done using the Bl leakage treatment the extra, unused, buckling searches are just wasting computer time.

F.2.1 Pin Cell Case

```
TITLE "ZEEP ROD IN HEAVY WATER, SAMPLE CASE"
#1 SEQUENCE 2.4
CELL 5
NREGION 3
NMATERIAL 3
INITIATE
  *
  ANNULUS 1 1.6285 1 * FUEL
  ANNULUS 2 1.7470 2 * CLAD
#2 POLYGON 3 6 3 10.0 * MODERATOR, 20 CM HEXAGONAL PITCH
  *
#3 MESH 4 1 -12
  *
  *NATURAL URANIUM METAL
  MATERIAL 1 -1 293 1 U238=4.760E-2 U235=3.454E-4
  MATERIAL 2 -1 293 2 AL=5.128E-2 016=7.4E-6
  MATERIAL 3 -1 293 3 O16=3.324E-2 D=D2O=6.633E-2 H-H2O=1.529E-4
  *
#4 NEWRES
#5 FISSION U235=1.143 U238=.090
#6 TOLERANCE 1E-5
  SUPPRESS 111111111111111001
  BEGIN
  DIFFUSION 1 5 1
#7 BEEONE 1
  PRINT 1 1 0 0 1 0
  LEAKAGE 5
#8 NORMALIZE LOSS
  BUCKLING .0003495 .0003495
#9 NOBUCK
#10 REACTION ALL=0
  BEGIN
```

F.2.2 Notes for Sample Pin Cell Case

The above sample pin cell case is a real case for a natural uranium metal 'ZEEP' rod in heavy water moderator. The case input has been prepared to perform a benchmark quality calculation with the ENDF/B-V library. The method of transport solution selected (#1) was PERSEUS, with a fourth order collision probability calculation. A relative convergence tolerance of 1.E-5 in the transport solution (#6) selected to insure a high degree of self-consistency in the solution.

The physical size of the unit lattice cell was defined (#2) as hexagonal, at 20 cm pitch. The radius of an equivalent circular cell could have been computed by hand and used in an ANNULUS card, but the hexagonal description

Sample Cases
is much more straightforward and less prone to error.

A relatively fine spatial mesh (#3) was chosen by successive refinement, to ensure that the answers were not mesh-dependent. If the lattice cell pitch were changed, the mesh card ought to be changed at the same time; generally once a sufficient mesh has been found at one lattice pitch, the appropriate number of moderator meshes at other pitches is simply proportional to the moderator thickness in thermal mean free paths.

The 'new' resonance treatment has been selected (#4). The two resonance treatments generally give very similar results, but the new treatment is recommended and being actively maintained, and therefore is less likely to have problems.

The relative fission yields in the fissile isotopes have been specified (#5). The default spectrum is pure U235 fissions, adequate for most calculations, but for benchmark calculations it is better to use the more realistic spectrum. The relative fission yields in U235 and U238 were found from reaction rates calculated by CHAIN 15 in a previous calculation of this lattice cell; in most cases a single iteration is sufficient.

The Bl flux leakage treatment was selected (#7) as it is the more accurate method. The Bl leakage treatment, although more accurate than the diagonal corrected transport treatment, is more expensive and so its use is not always justified. In general the two methods give quite good agreement in heavy water and graphite cases, but will have some differences in light water cases. For most production calculations, the absolute value of a buckling used or calculated is not important as it is used only to get a critical spectrum; in comparisons against experiment, however, the absolute buckling is significant. No buckling searches (#9) will be performed as the only important buckling in this case is the measured one.

The flux normalization in leakage and reaction rate calculations (#8) was chosen as one neutron absorbed or leaked from the cell, to make it consistent with calculations by another code of the same lattice cell. All of the reactions in the cell (#10) will be printed to allow detailed comparisons.

F.3.1 Pij Cluster Calculation

```
TITLE "19 ELEMENT UO2 FUEL ASSEMBLY, D2O COOLANT --- ENDF/B-V DATA"
SEQUENCE 3.5
#1 SETS 3
 NRODS 19 -12 10 10 3 2 1
 CELL 7
 NGROUP 33
 NREGION 10
 NMATERIAL 10
 PREOUT
 INITIATE
 ANNULUS 1 1.32 1 * COOLANT
 ANNULUS 2 1.88 1
 ANNULUS 3 2.44 1
 ANNULUS 4 3.01 1
```
ANNULUS 5 3.57 1
ANNULUS 6 4.1275 1
ANNULUS 7 4.3975 2  * AL PRESSURE TUBE
ANNULUS 8 5.08 3
ANNULUS 9 5.222 4  * AL CALANDRIA TUBE
POLYGON 10 6 5 9.0  * 18.0 CM PITCH
*
ARRAY 1 1 1 0 0
RODSUB 1 1 .7105 6
RODSUB 1 2 .7609 9
*
ARRAY 2 1 6 1.65 0
RODSUB 2 1 .7105 7
RODSUB 2 2 .7609 9
*
ARRAY 3 1 12 3.19 0.2618
RODSUB 3 1 .7105 8
RODSUB 3 2 .7609 9
*
NEWRES
#2 NPIJAN 9
#3 LINES 0 1.5 1 1
LINES 1.5 3 1 1
LINES 3 5.222 1 1
#4 AUTOTRACK 0.1
TOLERANCE 1E-5
SUPPRESS 1 0 1 1 1 1 1 1 1 1 1 0 0 1
MESH 1 1 1 1 1 1 1 1 1 1 -7
FEWGROUPS 4 8 12 16 20 22 24 26 28 31 35 39 41 44 47 50 53 56 59 $
62 65 67 69 71 73 75 77 79 81 83 85 87 89
FISSION U235=.632 U238=.036
*
#5 WATER 1 0.0 298.2 3 D-D2O=99.630
MATERIAL 2 2.7193 298.2 4 AL=98.79992 CU=0.3 SI=0.6 CR=0.3 B10=6.9E-8
MATERIAL 3 0.0012172 298.2 4 O16=23.47 N14=76.49 C=0.0139
MATERIAL 4 2.7193 298.2 4 AL=98.79992 CU=0.3 SI=0.6 CR=0.3 B10=6.9E-8
WATER 5 0.0 298.2 4 D-D2O=99.63
MATERIAL 6 10.45 298.2 1 U235=0.62677 U238=87.52069 U234=0.00476 $
016=11.84778 017=.00508
MATERIAL 7 6
MATERIAL 8 6
MATERIAL 9 5.8157 298.2 2 ZIRC-II=100
* ENDCAP
#6 MATERIAL 10 4.057 298.2 -3 H-H2O=.0083 D-D2O=4.481 016=17.86 $
    ZIRC-II=77.65
BEGIN
NORMALIZE LOSS
DIFFUSION 1 1 1
BEEONE 1
ENDCAP 10 .034 -1 1 6
LEAKAGE 5
BUCKLING 7.035E-5 7.035E-5
NOBUCK

Sample Cases
F-5

REACTION U235=0 U238=0
PARTITION 65 89
PRINT 1110 10
BEGIN

F.3.2 Notes for Sample Pij Cluster Case

The above sample Pij cluster case is a case for a natural uranium oxide 19 element cluster in heavy water moderator. The case input has been prepared to perform a benchmark quality calculation with the ENDF/B-V library.

The geometry of the cluster in this example is shown in Figure F-1. The figure was prepared automatically from the WIMS-CRNL input, by the code DRAWPIJ. For information about DRAWPIJ, contact the author.

One of the more difficult parts of the input preparation for a Pij calculation is the choice of the proper integration mesh to be used during the calculation of collision probabilities within the two dimensional cluster. The recommended method to use for accurate calculations is the AUTOTRACK option (#4). The method used is similar to what a user might do by hand to check if an integration mesh was sufficiently refined: increase the number of lines and angles and check if the important results of the calculation change significantly. WIMS-CRNL can simplify this task, because it is not necessary for the code to perform the complete transport solution to determine if the integration mesh was adequate: WIMS-CRNL can evaluate the adequacy of the integration mesh by monitoring the amount the mean chord length in each mesh changes as the number of lines or angles is increased. The mean chord length in a mesh is very closely related to the self collision probability, and related to all of the collision probabilities to and from that mesh. The cost of calculating collision probabilities and fluxes is avoided for the inadequate meshes. The method is not foolproof, as some small but perhaps important meshes may not be traversed by many lines and so will not contribute to the error estimate, or an unimportant mesh may require a denser mesh of lines and angles than the important meshes.

The value of the tolerance to be used in the AUTOTRACK option depends on the required accuracy of the calculation: 0.3 should be accurate normally, but smaller values such as 0.1 or even smaller may be used if needed. Once a WIMS-CRNL calculation has been completed, and an adequate set of lines and angles have been found, it is best to substitute the selected number of lines and angles on the NRODS or LINE(s) cards to avoid the expense of another search. At the same time, the selected set should be inspected to ensure that it is reasonable for the application. If changes are made to the materials in a cell, it is not necessary to change the tracking mesh. Similarly, if the number or size of the meshes in the annular zone outside of the Pij zone are changed, it is not necessary to change the tracking mesh.

The collision probability integration mesh has been divided into three parts (#2, #3) to simplify the calculation for the code. The last set of lines is completely outside of the two-dimensional region of the problem; one angle will be sufficient because of the pure annular geometry in this region (AUTOTRACK will detect this), while more will be required in the inner region. The inner region has been divided into two zones, so that should the
required density of lines and angles be different in the two zones, they will only be used as required.

The definition of the heavy water (#5) was taken from the measured temperature and purity. The calculation of density and detailed isotopic composition has been left to WIMS-CRNL.

The material of the end-region (#6) has been calculated from a volume weighted average of all materials beyond the fuelled length of the bundle, within the calandria tube.

**Figure F-1: Geometry of Sample 19 UO₂ Cluster Case**

![Diagram of sample geometry]

**Scale 1:1**

- Fuel pin outer radius = 0.7105 cm
- Fuel clad outer radius = 0.7609 cm
- 1 Pin at center
- 6 Pins on a circle of 1.65 cm radius
- 12 Pins on a circle of 3.19 cm radius
- Pressure tube: inner radius = 4.1275 cm, outer radius = 4.3975 cm
- Calandria tube: inner radius = 5.08 cm, outer radius = 5.222 cm

Sample Cases
Appendix G

TAPE16 Description

G.1 Introduction

Options exist for saving data that are calculated by WIMS-CRNL on a file, TAPE16. The method of data transfer that has been implemented has proven to be flexible and general in its application. There are currently a significant number of applications that receive data produced by WIMS-CRNL on TAPE16, and process it into a form for more specialized data requirements. The data written to TAPE16 is produced independently of the printout of WIMS-CRNL.

G.2 TAPE16 Contents

TAPE16 is written with FORTRAN unformatted binary writes. The records are written as follows:

\texttt{WRITE (16) KEY1, KEY2, N, ( DATA(I), I=1,N )}

The key to the contents of each record is contained in the first two elements of the record, each containing ten display code characters. The first element generally indicates the WIMS input option used to cause the record to be written to TAPE16 (e.g. 'CELLAV' indicates that the WIMS input keyword CELLAV was used). The second element describes the type of data on the record (e.g. 'FLUX'). The third element contains an integer value equal to the number of data items contained in the record.

Several input keywords may be used to select information to be written to TAPE16. These are:

- \texttt{MTRFLUX} - Main data input, causes infinite lattice fluxes calculated by the main transport routine to be written.
- \texttt{CELLAV} - Edit data input, causes cell averaged information to be written.
- \texttt{ISOCYCL} - Edit data input, causes burnup information to be written.
- \texttt{REGION} - Edit data input, region and reaction data is written. The reaction data written will be determined by the PRINT and REACTION edit data keywords.
- \texttt{MATSIG} - Main data input, material cross sections in the full library energy group structure are written.

G.3 Description of TAPE16 Records

A list and description follows of all records associated with each WIMS input
keyword. Unless otherwise stated, integer data items begin with the characters I to N and real data items begin the characters A to H or 0 to Z.

G.3.1 General Information Records

The general information records are always written to TAPE16.

'TITLE ','CARD 14,(CASETL(J),J=1,14)

CASETL - case title (character*10)

Written by CHAIN 0.

'WIMS ','CONSTANTS ',23+2*NEL,NEL,NG,NGFISS,NGFAST,NGRES,
NGTHML,NIFISS,NIFISP,NRODTY,MAIN,NGMTR,dummy,dummy,
NMT,NANROD,dummy,NMATZ,NM,dummy,NRDSB1,NRDCSP,NRDSCP,
NPLATE,(NUMBER(J),J=1,NEL),(NAME(J),J=1,NEL)

NEL - number of isotopes in library
NG - number of library energy groups
NGFISS - number of library fast groups
NGRES - number of library resonance groups
NGTHML - number of library thermal groups
NIFISS - number of fissile isotopes in library
NIFISP - number of fission products in library
NRODTY - number of rod types
MAIN - main transport calculation method used:
1 = DSn
2 = PERSEUS
3 = Pij
NGMTR - number of main transport groups
NMT - number of slabs or annuli
NANROD - number of annuli containing rods
NMATZ - number of materials
NM - number of burnable materials
NRDSB1 - maximum number of rod sub-divisions in any rod type plus one
NRDSCP - maximum number of sectors in any rod type plus one
NPLATE - non-zero for slab cases
NUMBER - isotope numeric identifiers
NAME - isotope character identifiers(character*10)
dummy - these elements do not contain usable values

written by CHAIN 0

'TITLE ','CARD2 ',14,(CASETL(J),J=1,14)

CASETL - case title (character*10)

Written by CHAIN 1 if a TITLE card was encountered in the Main data.
G.3.2 MATSIG Records

'MATSIG ', 'SIZES ', 5, NMAT, NG, NGFAST, NGFISS, LSCAT

NMAT - number of materials in the case
NG  - number of library groups
NGFAST - number of groups that may contain n,2n cross sections
NGFISS - number of groups with fission spectra yields
LSCAT - maximum length of packed scattering matrices

Written by CHAIN 4.

'MATSIG ', 'ENERGIES ', NG, (E(I), I=1, NG)

E - upper energy limit of each group (eV)

TAPE16 Description
Written by CHAIN 4.

'MATSIG', 'FISSINSPEC', NGFISS, (S(I), I=1, NGFISS)

S - fission yield into each group

Written by CHAIN 4.

'MATSIG', 'ABSORPTION', NG, (ABS(I,J), I=1, NG)

ABS - absorption cross section for material j (cm⁻¹)

Written by CHAIN 4.

'MATSIG', 'NUFISSION', NG, (FIS(I,J), I=1, NG)

FIS - nu*fission cross section for each material j (cm⁻¹)

Written by CHAIN 4.

'MATSIG', 'NU', NG, (RNU(I,J), I=1, NG)

RNU - yields per fission for each material j

Written by CHAIN 4.

'MATSIG', 'N2N', NGFAST, (RN2N(I,J), I=1, NGFAST)

RN2N - n,2n cross section for each material j (cm⁻¹)

Written by CHAIN 4.

'MATSIG', 'SCATTERPO', LP0, (SPO(I,J), I=1, LP0)

SPO - packed PO scattering matrix for each material j (cm⁻¹). The format of the packed matrix for each group G is as follows:

RK, RL, (X(M), M=1, RL)

X(RK) is the self-scattering cross section in group G. RL is the number of non-zero elements.

Written by CHAIN 4.

'MATSIG', 'SCATTERP1', LP1, (SP1(I,J), I=1, LP1)

SP1 - packed P1 scattering matrix for each material j (cm⁻¹). Format is the same as SPO in the previous record.

Written by CHAIN 4.

TAPE16 Description
The records 'MATSIG ','ABSORPTION' through 'MATSIG ','SCATTERPI' are repeated for each material in turn.

G.3.2 CELLAV Records

'CELLAV ', 'MODERATOR ', NGMTR*(2+NGMTR), (ABSN(I), I=1, NGMTR), (TOTL(I), I=1, NGMTR), ((SCAT(I, J), J=1, NGMTR), I=1, NGMTR)

cross section data for the moderator region of cell
ABSN - absorption cross sections (cm⁻¹)
TOTL - transport cross sections (cm⁻¹)
SCAT - scattering cross sections (cm⁻¹)

Written by CHAIN 13.

'CELLAV ', 'BALANCE ', 3, TABS, TNUF, TRLEAK

TABS - total cell absorptions
TNUF - total cell fission yields
TRLEAK - total cell radial leakage

Written by CHAIN 13.

'CELLAV ', 'NGROUPS ', 1, NGMTR

NGMTR - number of groups in main transport calculation

Written by CHAIN 13.

'CELLAV ', 'F-FACTOR ', 2, FFACTOR, WFACTOR

FFACTOR - ratio of fuel thermal flux / cell thermal flux
WFACTOR - ratio of fuel irradiation / cell irradiation

Written by CHAIN 13.

'CELLAV ', 'ABSORPTION', NGMTR, (ABSORB(I), I=1, NGMTR)

ABSORB - cell averaged absorption cross sections (cm⁻¹)

Written by CHAIN 13.

'CELLAV ', 'NU-FISSION', NGMTR, (NUFISS(I), I=1, NGMTR)

NUFISS - cell averaged nu*fission cross sections (cm⁻¹)

Written by CHAIN 13.

'CELLAV ', 'TOTAL-X ', NGMTR, (TOTAL(I), I=1, NGMTR)

TOTAL - cell averaged transport cross sections (cm⁻¹)

TAPE16 Description
Written by CHAIN 13.

'CELLAV ', 'FLUX ', NGMTR, (DRTED(I), I=1, NGMTR)
DRTED - cell averaged fluxes, main transport spectrum

Written by CHAIN 13.

'CELLAV ', 'SCALE ', 1, SCALE
SCALE - flux scale factor (Main transport flux/Edit flux)

Written by CHAIN 13.

'RADIAL ', 'LEAKAGE ', NGMTR, (RLEAK(I), I=1, NGMTR)
RLEAK - radial leakage in main transport calculation

Written by CHAIN 13.

((SCAT(M,K), M=1, NGMTR), K=1, NGMTR)
SCAT - cell averaged scattering cross sections (cm$^{-1}$)

Written by CHAIN 13.

'CELLAV ', 'FISSPECT ', NGMTR, (FISPEC(I), I=1, NGMTR)
FISPEC - cell averaged fission spectrum

Written by CHAIN 13.

'CELLAV ', 'Q ', NGMTR, (SLOWD(I), I=1, NGMTR)
SLOWD - cell averaged slowing down density

Written by CHAIN 13.

'CELLAV ', 'DIFFUSION ', 5*NGMTR+5, B1, JDIFFUS, ENDCAP,
(XDR(I), I=1, NGMTR), (XDZ(I), I=1, NGMTR), (PHIEFF(I), I=1, NGMTR),
(PHIINF(I), I=1, NGMTR), BR2INI, BZ2INI, (CUR(I), I=1, NGMTR)

B1 - leakage treatment, logical variable:
  .TRUE. = B1
  .FALSE. = Diagonal Transport corrected
JDIFFUS - type of diffusion coefficients,
  1 = Benoist
  2 = transport
ENDCAP - logical variable indicating that endcap correction
  has been used (ENDCAP = .TRUE.).
XDR - radial diffusion coefficients
XDZ - axial diffusion coefficients
PHIEFF - effective flux

TAPE16 Description
PHIINF  - infinite flux
BR2INI - input radial buckling (cm$^{-2}$)
B2ZINI - input axial buckling (cm$^{-2}$)
CUR   - cell leakage

Written by CHAIN 14.

'CELLAV ','CRITICALB ',NGMTR+4,
IBUCK, BR2, BZ2, BR2BZ2, (PHIEFF(I), I=1, NGMTR), (CUR(I), I=1, NGMTR)

IBUCK - type of critical buckling search performed,
1 = radial/axial ratio as given
2 = radial buckling as given
3 = axial buckling as given
BR2   - critical radial buckling (cm$^{-2}$)
BZ2   - critical axial buckling (cm$^{-2}$)
BR2BZ2 - total critical buckling (cm$^{-2}$)
PHIEFF - effective flux
CUR   - cell leakage

Written by CHAIN 14 if a critical buckling search is performed.

'CELLAV ', 'K ', 4, XKINF, XKEFF, XKINF2, XKEFF2

XKINF - k-infinity (NGMTR groups)
XKEFF - k-effective (NGMTR groups)
XKINF2 - k-infinity (2 groups)
XKEFF2 - k-effective (2 groups)

Written by CHAIN 14.

'CELLAV ', 'SIGMAF ', NGMTR, (RNUCEL(M), M=1, NGMTR)

RNUCEL - cell averaged fission cross sections (cm$^{-1}$)

Written by CHAIN 12.

'CELLAV ', 'POWERDENS ', NM+1, B, (P(I), I=1, NM)

NM   - number of burnable materials
P    - relative power densities (power per unit volume)

Written by CHAIN 12.

'CELLAV ', 'AVG-ENERGY', 4, RTIME, ENERGY, RIRRAD, CUMFLX

RTIME   - time (days)
ENERGY  - average energy per fission (MeV)
RIRRAD  - total fuel burnup (MWd/t)
CUMFLX  - total cell irradiation (n/kb)

Written by CHAIN 16.
'CELLAV ','PINBURNUP ',3*NM+1,RIRRAD,(PINBRN(I),I=1,NM),
(POWR(I),I=1,NM),(NPINSX(I),I=1,NM)

written only for cluster cases:
RIRRAD  - total fuel burnup (MWd/t)
PINBRN  - burnup per fuel ring, inner to outer (MWd/t)
POWR    - power per fuel ring (MW/t)
NPINSX  - number of pins per ring

Written by CHAIN 16.

'CELLAV ','IRRADSTEP ',1,STEP

STEP  - size of irradiation burnup step (days)

Written by CHAIN 16.

G.3.4 ISOCYCL Records

'WIMCYCLE ','YIELDS ',1,YOAINT,YOINT

YOAINT  - integrated yields over absorptions
YOINT   - integrated yields over absorptions plus leakage

Written by CHAIN 16.

'WIMCYCLE ','BURNUP ',4,RTIME,RIRRAD,NNB,NM

RTIME   - time (days)

'WIMCYCLE ','BURNUP ',4,RTIME,RIRRAD,NNB,NM

RTIME   - time (days)
RIRRAD  - burnup (MWd/t)
NNB     - total number of isotopes that appear in the burnable materials
NM      - number of materials that undergo burnup

Written by CHAIN 16 and is followed by NM 'WIMCYCLE','DENSITY' records.

'WIMCYCLE ','DENSITY ',2*NNB+1,RV,(IR(I),RN(I),I=1,NNB)

written once for each burnable material
RV      - material volume
IR      - isotope numeric identifier
RN      - isotope number density

Written by CHAIN 16.

G.3.5 MTRFLX Records

'MTRFLX ','FLUX ',(2+NGMTR)*MTRMSH+2,NGMTR,MTRMSH,

TAPE16 Description
\[(\text{MATMSH}(I), \text{VQLE}(I), (\text{PHI}(I,J), J=1, \text{NGMTR}), I=1, \text{MTRMSH})\]

- **MATMSH** - material number associated with mesh point I
- **VQLE** - volume associated with mesh point
- **PHI** - main transport routine fluxes associated with mesh point

Written by CHAIN 11.

### G.3.6 REGION Records

- **'REGION ','DESCRIPTOR',1+3*\text{NZONE}, \text{NZONE},**
  
  \((R(J), J=2, \text{NZONE}+1), (\text{VOLS}(J), J=1, \text{NZONE}), (\text{ICQDU}(J), J=1, \text{NZONE})\)

  - **NZONE** - number of zones
  - **R** - outer radii of zones, inner to outer (cm)
  - **VOLS** - areas of zones (cm\(^2\))
  - **ICQDU** - material number of zones

Written by CHAIN 13.

- **'REGION ','DIMENSIONS',2,\text{NREGON},\text{NGMTR}**

  - **NREGON** - number of edit regions
  - **NGMTR** - number of main transport groups

Written by CHAIN 13.

- **'REGION ','FLUX ',3+\text{NGMTR}, K, \text{KA}, V\text{A}, (R\text{AF}(I), I=1, \text{NGMTR})**

  - **K** - region number
  - **KA** - region material number
  - **VA** - region volume
  - **RAF** - region fluxes

Written by CHAIN 13. This record occurs once for each region and is always followed by \text{NGMTR} 'REGION','SIGMAS' records.

- **'REGION ','SIGMAS ',3+\text{NGMTR}, \text{ABSN}, \text{FISS}, \text{TOTL},**
  
  \((\text{SCAT}(I,J), J=1, \text{NGMTR})\)

  for region specified on most recent 'REGION','FLUX' card and for main transport group 'I' for the I'th 'REGION','SIGMAS' record:

  - **ABSN** - absorption cross section (cm\(^{-1}\))
  - **FISS** - fission cross section (cm\(^{-1}\))
  - **TOTL** - transport cross section (cm\(^{-1}\))
  - **SCAT** - scattering cross section (cm\(^{-1}\))

Written by CHAIN 13.

The presence of the following records that use the keyword 'REACTION' is determined by the options selected through the use of the Edit data keywords.

TAPE16 Description
BEEONE, DIFFUSION, PRINT and REACTION. The Edit data keyword REGION must be used for these records to be written to TAPE16.

'REACTION ','FLUX ','NZONE*NG+6+NGREAC,KWORD2,KWORD3,KWORD,
NZONE,NG,NGREAC,(FF(J,L),J=1,NZONE),L=1,NG),
(IPV(J),J=1,NGREAC)

KWORD2 - leakage treatment used, character*10:
'DIAGONAL' - transport corrected diffusion theory
'B1' - B1 flux solution

KWORD3 - type of diffusion coefficients used (k-effective edits only), character*10:
'BENOIST' - Benoist diffusion coefficients
'TRANSPORT' - transport coefficients

KWORD - reaction edit requested, character*10:
'K-INFINITY' - reactions in infinite spectra
'K-EFFECTIV' - reactions in effective spectra

NZONE - number of zones
NG - number of library groups
NGREAC - number of groups used for reaction edits
FF - fluxes used for reaction edits by zone in full library group structure
IPV - few group structure used for the reaction edits

Written by CHAIN 15.

'REACTION ',FILTY,7+(NGREAC+1)*NITEMS,'ABSORPTION',
NAME,KWORD2,KWORD3,KWORD,NGREAC,NITEMS,
((ABSTAB(I,NZ),I=1,NGREAC),NZ=1,NITEMS),
(KSPEC(I),I=1,NITEMS)

FILTY - reaction type, character*10:
'RATES-MESH' - reaction rates by zone
'MESH' - reactions by zone
'RATES-MAT' - reaction rates by material
'MATERIAL' - reactions by material

NAME - isotope name, character*10
KWORD2 - as for 'REACTION ','FLUX '
KWORD3 - as for 'REACTION ','FLUX '
KWORD - as for 'REACTION ','FLUX '
NGREAC - number of reaction edit groups
NITEMS - number of zones for edits by zone or number of materials for edits by material
ABSTAB - absorption reactions
KSPEC - spectral type associated with each zone or material

Written by CHAIN 15.

'REACTION ',FILTY,7+(NGREAC+1)*NITEMS,'FISSION ',
NAME,KWORD2,KWORD3,KWORD,NGREAC,NITEMS,
((FISTAB(I,NZ),I=1,NGREAC),NZ=1,NITEMS),
(KSPEC(I),I=1,NITEMS)

TAPE16 Description
The order of the 'REACTION' records is relatively complicated. The reaction data set could be considered to be a large block of records that can be subdivided into smaller sub-blocks. The k-infinity spectra records all appear in the first sub-block with the k-effective records following in the
second sub-block.

For the k-infinity block, all data for one isotope appear together. This isotope block contains four sub-blocks, these being, in order of appearance on TAPE16, reaction rates by mesh, reactions by mesh, reaction rates by material and reactions by material. Each reaction edit block contains from one to four records, these being the absorption edit (always present), the fission and nu*fission edits (present for fissile isotopes) and the n,2n edit (if n,2n data is present in data library).

The k-effective block can be divided into two blocks, the first for the diagonal transport flux solution data and the second for the Bl flux solution. These flux solution blocks each contain two blocks for the diffusion coefficients used, in order of appearance, Benoist and transport. Each of these blocks is divided into isotope blocks whose structure is the same as that described for the k-infinity records.

G.4 Retrieving Data from TAPE16

The relative order of records on TAPE16 will not change, but future additions to WIMS-CRNL may mean that two currently adjacent records may not always be so and therefore codes written to process TAPE16 should be written to search for records before reading them. Similarly, when TAPE16 is being searched, only the keys should be read, as the data length could exceed the allocated storage on records not anticipated.

The subroutine FIND listed below may be used to search for and position TAPE16 at the required record. For example, if one wanted to read the number densities the following FORTRAN code could be used:

```fortran
SUBROUTINE EXAMPLE (DN,NEL,NMATZ)
REAL DN(NEL,NMATZ)
LOGICAL FOUND, FIND

C FIND RECORD 'NUMBER' 'DENSITY'
FOUND = FIND (16,'NUMBER ','DENSITY ')
IF ( FOUND ) THEN
  READ (16) (DUM,1=1,3),NEL,NMATZ,
  > ((DN(I,J),J=1,NMATZ),I=1,NEL)
ELSE
  PRINT *, ' UNABLE TO FIND RECORD'
ENDIF

LOGICAL FUNCTION FIND (UNIT,N1,N2)
C
C FIND RECORD TYPE N1, N2 ON DEVICE 'UNIT'
```

TAPE16 Description
INTEGER UNIT
CHARACTER*10 I, J, N1, N2
C
10 CONTINUE
READ (UNIT,END=20) I, J
IF ( .NOT.(I.EQ.N1.AND.J.EQ.N2) ) GO TO 10
BACK SPACE UNIT
FIND = .TRUE.
RETURN
C
20 CONTINUE
PRINT 30, N1, N2, UNIT
30 FORMAT ('OE-O-F ENCOUNTERED ON FIND (',A10,',',A10,
> ') ON TAPE',I4/)
FIND = .FALSE.
RETURN
END

When multiple cases appear on one file, separated by end-of-file marks, the following logical function may be used to skip to the next case:

LOGICAL FUNCTION SKIPE (UNIT)
C
C SKIPS OVER END OF FILE MARK AND POSITIONS
C TAPE 'UNIT' AT START OF NEXT CASE.
C RETURNS TRUE IF ANOTHER CASE IS FOUND
C
LOGICAL FIND, FOUND
C
CHARACTER*10 EOFMRK, TAPE16
C
DATA TAPE16,E:,'^.."",/TAPE16',E-O-F'/
C
FOUND = FIND(UNIT,TAPE16,EOFMRK)
IF ( FOUND ) THEN
READ (UNIT)
READ (UNIT,END=100)
100 X = EOF(UNIT)
READ (UNIT,END=200)
BACK SPACE UNIT
SKIPE = .TRUE.
RETURN
ENDIF
C
200 CONTINUE
PRINT 300, UNIT
300 FORMAT ('NO MORE CASES ON TAPE ',I3)
SKIPE = .FALSE.
RETURN
END

TAPE16 Description
Appendix H

H.1 Introduction

TAPE50 is a file that is used within WIMS-CRNL for the storage and retrieval of information between cases, under user control. The main application of this feature is in the 'restart' of previous cases. TAPE50 may be cataloged as a permanent file after a WIMS-CRNL run, to be later attached and used in another WIMS-CRNL run. As TAPE50 is a random access file, any operations besides cataloging and attaching the file are not recommended.

The WIMS-CRNL input keywords controlling the reading and writing of information to TAPE50 are: WRITE, READ, WPIJ, RPIJ, WPHI and RPHI. Each record on TAPE50 is uniquely identified by an alphanumeric key; the key may be a one to 10 character string or a number not equal to zero. Up to 63 different records may be used on TAPE50 (this number can be increased if required). The record keys are shared by all of the options using TAPE50, but it would be incorrect to try operations such as to read a record with WPIJ that was written using WRITE.

H.2 READ and WRITE

These keywords control the reading and writing of material properties. The properties stored for each case material are:

- isotopic composition
- temperature and spectral type
- burnup

The information stored about the cell are:

- average fuel burnup, irradiation and irradiation time
- integral eigenvalue

As the cell geometry is not stored on TAPE50 during WRITE operations, it is important to perform READ's and WRITE's at the appropriate point in a WIMS-CRNL calculation; the operations are performed at the time WIMS-CRNL encounters the card in the Main data input. A WRITE should only be performed after all of the Main data concerning the materials has been completed, and cell geometry and options must be defined in cases using READ. A READ will change all of the case materials, and so modifications should be performed after the READ. The number of materials and nuclear data library must not change between cases using READ and WRITE.

An abbreviated example of the use of READ and WRITE cards follows. The example is a simple burnup case in which the cell is irradiated and a number of perturbations are performed on the cell with the fuel at its final composition.

[Prelude Data Cards]
PREOUT

TAPE50 Description
H.3 WPIJ and RPIJ

These keywords control the reading and writing of collision probability matrices. Because of the relative cost of their calculation, only the collision probabilities within the 'Pij' radius are saved. The main application of this option is in Pij cases whose collision probabilities are very expensive to calculate, and it is desired to save them in case the flux solution does not complete.

H.4 WPHI and RPHI

These keywords control the reading and writing of main transport routine fluxes in collision probability cases. If a flux solution is very time consuming, it may be carried out in a number of separate WIMS-CRNL runs, by saving the flux at the end of one run, and using that as the initial flux guess for the next run. In normal applications, there is little advantage to starting the flux solution with a previous one on TAPE50, as a significant part of the cost of a run is outside of the flux solution.
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