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ABSTRACT

The CHAR module of the AUS reactor neutronics scheme solves the multiregion nuclide depletion equations using an analytic method. The module obtains cross section, flux and geometry data from AUS data pools, and uses the STATUS data pool which has been designed for the storage of nuclide compositions, spatial smearing factors and other miscellaneous information.

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A CODES; BURNUP; COMPUTER CALCULATIONS; CROSS SECTIONS; NEUTRON FLUX; NEUTRONS

CONTENTS

1. INTRODUCTION

The AUS scheme (Robinson 1975) is a system of computer codes for reactor neutronic computations which may be flexibly linked together in composite calculations. Data is passed between the modules (computer codes) of the scheme *via* data pools which are disk data sets of a defined structure.

The CHAR module has been developed to provide a method for solution of the nuclide depletion equations which may be applied to any burnup calculation in which individual nuclides are represented. The inclusion of a burnup capability in the AUS scheme has necessitated the addition of a new data pool, the STATUS data pool, which is used primarily for the storage of nuclide compositions. The data pool includes energy–dependent spatial smearing factors which are used to 'unsmear' any discrete materials which have been mixed together. A number of miscellaneous quantities are also stored in the data pool which has been designed as a general purpose data set to which any data of a fixed form may be added.

The entries added to the STATUS data pool by various modules form a record of the steps which make up a calculation and the current status of that calculation. The data pool serves to integrate more closely the modules of the AUS scheme and enables comprehensive editing of any calculation to be carried out.

Using input from the STATUS data pool along with cross section, geometry and flux data pools, the CHAR module applies an analytic solution of the nuclide depletion equations to burn up each discrete material of the system under study; this system may be either a single lattice cell or a whole reactor. The module adds the updated nuclide compositions to the STATUS data pool and optionally remixes macroscopic cross sections.

In this report, details of the STATUS data pool are given along with the standard use of the data pool by various modules. This is followed by a description of the CHAR module and the input data specification.

2. STATUS DATA POOLS

2.1 Introduction

STATUS data pools are FORTRAN sequential, unformatted data sets which are normally used as the pair of data sets ST1 and ST2 on DD38 and DD39 of the AUS system, respectively. The two STATUS data pools are used in combination, with ST2 acting as a pointer to the main ST1 data set. The data pools consist of a sequence of entries with each entry determining its own function. The form of the entries is fixed, however, so that a module may skip or copy entries without knowing the details of all entries. Each module of a calculation may add additional entries to the end of the data pool by using the sequence: search for end of file, backspace and write. That is, the data pools are 'add–on' data sets in which all entries are retained throughout a calculation sequence.

The data pool contains entries for isotopic compositions, spatial smearing factors and other miscellaneous data which together form a history of the functions that have been performed by the modules during a sequence of calculations. Its major purpose is to allow the automatic evaluation of nuclide reaction rates at any stage of a calculation. The data pool differs from other AUS data pools in several ways; it can embrace an entire calculation sequence, it can include general information, and it can take part in controlling the AUS calculation. Because of this generality, the use that each module makes of the data pool must be carefully defined and suitable labelling conventions must be established to differentiate between data generated within different subsections of the overall calculation. To be more specific, we wish to be able to calculate nuclide reaction rates in the components of a lattice cell which, together with other cells, forms a representation of a reactor core.

2.2 Spatial Smearing Factors

The spatial smearing of discrete materials is usually necessary in forming a neutronic model of a reactor. The STATUS data pool is used to store group-dependent smearing factors to enable these materials to be later unsmeared for editing purposes. The requirement that unsmeared fluxes and cross sections be available and not merely reaction rates leads to the definitions of smearing factors given below.

The macroscopic cross section Σ_{ig} for region i and group g is given by

$$\Sigma_{ig} = \underset{\ell}{\text{Sum}}\ N_{i\ell}\ \sigma_{ig\ell} \quad ,$$

where $\sigma_{ig\ell}$ and $N_{i\ell}$ are nuclide ℓ cross sections and concentrations respectively for components of region i.

To group condense and smear into group G and region I, the standard equation (except for the transport cross section) is

$$\Sigma'_{IG} = \left(\underset{g\in G}{\text{Sum}}\ \underset{i\in I}{\text{Sum}}\ V_i \phi_{ig}\ \Sigma_{ig}\right)/\left(\underset{g\in G}{\text{Sum}}\ \underset{i\in I}{\text{Sum}}\ V_i \phi_{ig}\right) \quad ,$$

where V_i and ϕ_{ig} are region volumes and fluxes.

If the nuclide cross sections are also condensed to the G group structure using

$$\sigma'_{iG\ell} = \left(\underset{g\in G}{\text{Sum}}\ \sigma_{ig\ell}\ \phi_{ig}\right)/\underset{g\in G}{\text{Sum}}\ \phi_{ig} \quad ,$$

then, defining the smearing factors as

$$f_i = V_i / V_I \tag{1}$$

and

$$d_{iG} = \left(V_I \underset{g\in G}{\text{Sum}}\ \phi_{ig}\right)/\left(\underset{g\in G}{\text{Sum}}\ \underset{i\in I}{\text{Sum}}\ V_i\ \phi_{ig}\right) \tag{2}$$

gives

$$\Sigma'_{IG} = \underset{i\in I}{\text{Sum}}\ f_i\ d_{iG}\ \Sigma_{iG} \quad ,$$

$$= \underset{i\in I}{\text{Sum}}\ f_i\ d_{iG} \underset{\ell}{\text{Sum}}\ N_{i\ell}\ \sigma'_{iG\ell} \ .$$

These smearing factors thus enable unsmearing in the G group structure.

Alternatively, if the nuclide cross sections are not condensed, the definition

$$d_{ig} = \left(V_I\ \phi_{ig}\right)/\left(\underset{g\in G}{\text{Sum}}\ \underset{i\in I}{\text{Sum}}\ V_i\ \phi_{ig}\right) \tag{3}$$

gives

$$\Sigma'_{IG} = \underset{i\in I}{\text{Sum}}\ f_i\ \underset{g\in G}{\text{Sum}}\ d_{ig}\ \text{Sum}\ N_{i\ell}\ \sigma_{ig\ell} \quad .$$

This allows an unsmearing in terms of the uncondensed groups provided the group structure is also stored in the data pool.

The second form (Equation(3)), unlike the first, may also be used for a subsequent group condense and smear to group H and region J as

$$\Sigma''_{JH} = \underset{I\in J}{\text{Sum}}\ f'_I \underset{G\in H}{\text{Sum}}\ d'_{IG} \underset{i\in I}{\text{Sum}}\ f_i \underset{g\in G}{\text{Sum}}\ d_{ig}\ \text{Sum}\ N_{i\ell}\ \sigma_{ig\ell} \quad .$$

The normal method is to use the second form of the factors and retain an uncondensed nuclide cross section library.

2.3 Data Pool Contents in Detail

2.3.1 Entry format

Each entry consists of two or more records, the first of which establishes the type of entry. This first 7–word record is

(A(I),I=1,5),N,M

where A is either a fully qualified material name of 20 characters or it has the form:

A(1 – 2) is $DATA ,

A(3 – 4) is the name of module writing the entry,

A(5) is the entry type, *e.g.* TIME, CELL, GRPS, and

|N| is the number of groups of information in the following records.

If N is negative, each information group begins on a new record thus enabling large quantities of data to be included easily. M is the maximum size of an information group in *4 words.

The trailing records have the form

(B(I,K),I=1,M),K=1,N) – one record for N positive, or

J,(B(I),I=1,J) – repeated |N| times for N negative.

2.3.2 Mixing rule entry

This is the basic entry in the data pool and it determines the entry format. Mixing rules describe either the mixing of nuclides to form a discrete material or the spatial smearing of materials. The name of any nuclide or material consists of 20 bytes as in the XSLIB data pool. The conventions for naming are given in Section 2.4.2.

The entry is (for positive N)

(A(I),I=1,5),N,M+5

((B(I,K),I=1,5),(C(I,K),I=1,M),K=1,N)

where

A is the name of a material formed from N constituents,

B is the set of constituent names,

C is (a) the concentrations in atoms per barn cm of each nuclide, for M=1, or

(b) the spatial smearing factors for each material f_i, d_{ig} defined in Section 2.2, for M > 1, *i.e.* M is usually one more than the number of groups before energy condensation, but is one more than the number of groups after condensation if the nuclide data is condensed. In both cases d_{ig} is given for the same number of groups as the nuclide cross section data pool.

2.3.3 The TIME entry

The entry is

$DATAbbb MODNAM TIME 1 3

TNOW,TLAST,PTGRAL

where the underlined names are alphabetic data:

MODNAM is the A8 module name,

TNOW is the current time in days,

TLAST is the previous time in days,

PTGRAL is the integral of power of the total system with respect to time in watt days or watt days cm^{-3}.

2.3.4 The IRAD entry

The entry is

$DATAbbb MODNAM IRAD N 6

((A(I,J),I=1,5), B(J),J=1,N)

where

A is the set of names of discrete materials which are burnt up,

B is the integral of power density with respect to time in watt days cm^{-3} for each material.

2.3.5 The CELL entry

The entry is

$DATAbbb MODNAM CELL 1 3

CNAM NCELL

where

CNAM is the A8 name of the cell,

NCELL is a count of cell calculations for the current time step.

2.3.6 The GRPS entry

The entry is

$DATAbbb MODNAM GRPS 1 N

(IGB(I),I=1,N)

where

N is the number of condensed groups plus one,

IGB is a set of fixed point numbers giving the first group of condensed group 1, and the last group of each condensed group.

The numbers are in terms of the previous group set.

2.3.7 The GFAC entry

The entry is

$DATAbbb MODNAM GFAC 1 NG

(A(I),I=1,NG)

where
- NG is the number of energy groups,
- A(I) is the ratio of the k_{eff} flux for a cell calculation to the k_{inf} flux, for each group I.

2.4 Notes on Usage

2.4.1 General comments

The ST1 data set is the main data pool to which all entries should be added. The ST2 data set serves mainly as a pointer to the data in ST1 and, as such, contains the TIME and CELL entries which give structure to the data pool.

One TIME entry is given for each time step (including time zero) and precedes all other entries for that time. The TIME entry is followed by a single IRAD entry for times greater than zero. A CELL entry is given for each lattice cell calculation and immediately precedes entries written for that cell by a data preparation module.

Each set of mixing rule entries immediately follows an appropriate GRPS entry to define the group condensation. The mixing rules must be entered such that the order of materials on the STATUS data pool is the same as that on the cross section data pool. A further requirement is that the order of constituents within a spatial smearing rule be the same as the order of the definitions of those constituents on the STATUS data pool.

The GFAC entry which enables burnup of a cell in a critical spectrum is exceptional because it is written on the ST2 data set.

The use of STATUS data pools requires that materials be divided into two classes called materials and nuclides. A nuclide is present on the main cross section library of the data preparation module and has microscopic cross sections. It appears only on the right hand side of a mixing rule. A material is composed of nuclides and must be defined by a mixing rule. It may be macroscopic or microscopic and may even be identical in cross section to a nuclide. Materials and nuclides may be in the same cross section data pool, but more generally they are in different data pools which may have a different number of groups.

2.4.2 Material names

The materials and nuclides in an AUS calculation all have 20–byte names which are used to provide a unique identification. These names are constructed using the set of conventions detailed below.

The first requirement is that the name of a material or nuclide must be exactly the same on the STATUS and cross section data pools. The 20 bytes consist of two 8–byte words and one 4–byte word. The first word gives the simple name for a nuclide (*e.g.* U235) or the name of a material supplied by the user in defining that material. The second word gives the name of the cell calculation in which the cross sections were generated and, where necessary, a number to indicate the region of the cell to which the cross sections apply. The user–supplied cell calculation name must be different for different cells within the one system and should be restricted to six characters to allow for the cell region number. The last word is modified for a material (but

not a nuclide) each time the material is condensed. These four characters go through the sequence ORIG, MOD1, MOD2, *etc.*

2.4.3 Functions of the AUSYS supervisor program

The initialisation and simple editing features required for STATUS data pools are supplied by the AUSYS program (Robinson 1975) which supervises the AUS scheme.

The major STATUS data set ST1, like other data pools of the AUS scheme, has allocation and retrieval facilities provided by the AUS catalogued procedure. The allocation of a new data set includes the insertion of an end of file mark which serves to initialise the data set. The ST2 data set is not normally saved; it is initialised by AUSYS at the start of an AUS calculation by copying the last TIME entry and any following CELL entries from ST1 to ST2. If ST1 is new and simply has a file mark, this results in an ST2 data set consisting of a file mark also.

Cards to modify this standard option may be included in the AUSYS input stream following the STEP named or STOP directives. The data set is identified by the card

$DDnn DISP=NEW

or $DDnn DISP=OLD

where
- DDnn is the DD name of the data set,
- DISP=NEW causes an end of file to be written,
- DISP=OLD results in no action.

The identifying card may be followed by a card requesting an end of file to be inserted before a nominated entry. This assists recovery following an error. The card has the form

$EOF TIME = time CELL = cell name

If CELL = cell name is not given, the end of file is inserted before the nominated TIME entry, otherwise, it is inserted before the CELL entry for the cell name for the nominated time.

Cards to be added at the end of a data set may be included after a $DDnn or $EOF card. The layout of these free format cards is exactly the same as that of an entry in the data pool. However, no notice is taken of end of records. All 5–word alphanumeric names must be given as two words of length 1 to 8 characters and one word of length 1 to 4 characters. Special characters or blanks may be used to separate information. The layout of the cards is compatible with the punched output produced by the PSTAT subroutine of AUSYS. A $DD99 card is used to terminate the STATUS data cards if other AUSYS input is provided.

Example

```
$DD38    DISP=OLD
$EOF     TIME=200.  CELL=CORED
$DATA    MIRANDA CELL  1  3 / CORED  5
FUEL CORED001 ORIG 2  6 / U235 CORED ORIG .005, U238 CORED ORIG .03
MOD  CORED002 ORIG 1  6 / H2O  CORED ORIG .04
$DD99
```

2.4.4 Functions of a data preparation module

The details given here are those for the MIRANDA data preparation module (Robinson 1976). Any other data preparation module incorporated in the AUS scheme should provide similar features.

If the ST2 data set is empty, both ST1 and ST2 are initiated with TIME entries for time zero. The module then enters the write mode in which data comes entirely from input cards,and entries are added to ST1 and ST2 when an AUS cross section data pool is written. A CELL entry is added to ST2 and CELL,GRPS and material definition entries are added to ST1. A material definition is written for each output material which is not a nuclide on the input cross section library.

If ST2 is not empty, the last CELL entry there acts as a counter of calculations already carried out. If there are no more CELL entries for the current time on ST1 than on ST2, the module enters the write mode as above. If further CELL entries do exist, the first one sets the cell name and the following entries are used for material definitions which take precedence over the card input data. When data is obtained from ST1 in this way, the only entry written is a CELL entry added to ST2.

2.4.5 Functions of a cell editing module

The details given here have not been implemented as yet, but a general editing module EDIT (J.P. Pollard, AAEC unpublished report) which uses STATUS data pools is under development.

The current time and the latest cell name should be obtained from the ST2 data set. The definitions of materials which are required for any nuclide editing should be obtained from ST1 by skipping to the CELL entry for the current time and reading the remaining data. When a buckling search is performed, a GFAC entry should be added to both the ST1 and ST2 data sets.

When any mixing and/or condensing functions are performed, a GRPS entry followed by a mixing rule entry for each output material should be added to ST1. The mixing rule entry should still be made if the material is simply transferred from the input to the output cross section library. No entries should be made for any output nuclides and their names must remain unchanged. Only the last 4 characters of the 20–byte names of condensed materials should be changed whereas the names of mixed materials should be formed from a user–supplied name and the cell name.

2.4.6 Functions of a reactor editing module

All the details for a cell editing module also apply here except that no particular cell is involved, but all cells for the current time. A buckling search is not applicable. If any cross section mixing is performed, a suitable material name modifier may be obtained from the geometry data pool.

2.4.7 Functions of the CHAR burnup module

A summary of the use of the STATUS data pool by the CHAR module is included here for completeness.

The ST1 data set is read in the same manner as for a reactor editing module. After the burnup calculation, the ST2 data set is restarted with an updated TIME entry. A TIME entry, an IRAD entry, and updated mixing rules for all materials defined directly in terms of nuclides are added to ST1. Any $DATA entries for the previous time which have the same module name as the previous TIME entry (*i.e.* the data preparation module) are added to ST1 with the mixing rules in the same order as before. If the option of remixing the macroscopic cross sections is used, all entries on ST1 for the previous time are added to ST1 as it is assumed that the modules which wrote these entries are to be bypassed.

2.4.8 Other modules

Any module which modifies cross sections should make the appropriate entries in the STATUS data pool. In particular, if a poison search calculation is performed, the following actions should be taken.

A new cross section library which includes the poisoned material should be written. A definition of the poisoned material should be added to ST1 in the form of a smearing rule. This implies that the poison must be a material not a nuclide. The 20–byte name of the poisoned material should be the same as the unpoisoned material except for a modification of the last 4 characters. This feature has not yet been implemented.

2.5 A Simplified Example

To burn up a reactor consisting of two fuelled regions plus a reflector. Each fuel region consists of simple cylindrical cells and the flux is assumed constant over each fuel region for burnup purposes.

The modules used are:

- MIRANDA to generate cross sections for each cell component;
- ANAUSN to compute fluxes within the cell;
- EDIT to condense and smear cell cross sections;
- MERGEL to combine cross section data pools;
- POW to compute fluxes for the overall system; and
- CHAR to burn up the reactor.

The first three modules constitute a lattice calculation which is performed for both cell types (CORE and BLNK). The whole process is repeated after each burnup step.

Brief details of job	ST1 data as updated to the currently indicated stage
AUSYS	new data set
MIRANDA –	$DATA,MIRANDA,TIME,1,3 / 3*0
produces a 20–group XS library of	$DATA,MIRANDA,CELL,1,3 / CORE , 1
FUEL,MOD,REFL,U235,U238,FP	$DATA,MIRANDA,GRPS,1,21 / 1,...127
	FUEL,CORE,ORIG,3,6 / U235,CORE,ORIG,.005
	U238,CORE,ORIG,.03
	FP ,CORE,ORIG, 0.0
	MOD,CORE,ORIG,1,6 / H2O, CORE,ORIG,.04
	REFL,CORE,ORIG,1,6 / C , CORE,ORIG,.08
ANAUSN	–

Brief details of job	ST1 data as updated to the currently indicated stage
EDIT –	$DATA,EDIT,GRPS,1,5 / 1,...20
produces a 4–group XS library	CELL,CORE,MOD1,2,26 / FUEL, CORE, ORIG, ...
of CELL,REFL	MOD,CORE,ORIG, ...
	REFL,CORE,MOD1,1,26 / REFL,CORE,ORIG, ...
MIRANDA –	
produces a 20–group XS library of	$DATA,MIRANDA,CELL,1,3 / BLNK, 2
FUEL,MOD,U235,U238,FP	$DATA,MIRANDA,GRPS,1,21 / 1, ... 127
	FUEL,BLNK,ORIG,3,6 / U235,BLNK,ORIG,.0001
	U238,BLNK,ORIG,.03
	FP ,BLNK,ORIG, 0.0
	MOD,BLNK,ORIG, 1,6 / H2O,BLNK,ORIG, .04
ANAUSN	–
EDIT –	$DATA,EDIT,GRPS,1,5/ 1,...20
produces a 4–group library of	CELL,BLNK,MOD1 , 2,26/FUEL,BLNK,ORIG, ...
CELL	MOD,BLNK,ORIG, ...
MERGEL	–
POW	–
CHAR	$DATA,MIRANDA,TIME,1,3 / 50., 0., 1000.
	$DATA,MIRANDA,IRAD,2,6 / FUEL,CORE,ORIG, 10000.
	FUEL,BLNK,ORIG, 3000.
	$DATA,MIRANDA,CELL,1,3 / CORE, 1
	$DATA,MIRANDA,GRPS,1,21 / 1,...127
	FUEL,CORE,ORIG,3,6 / U235,CORE,ORIG .0047
	U238,CORE,ORIG 0.02999
	FP ,CORE,ORIG 0.0006
	MOD,CORE,ORIG, 1,6 / H2O,CORE,ORIG .04
	REFL,CORE,ORIG,1,6 / C ,CORE,ORIG .08
	$DATA,MIRANDA,CELL,1,3 / BLNK , 2
	$DATA,MIRANDA,GRPS,1,21/ 1,....27

Brief details of job	ST1 data as updated to the currently indicated
	FUEL,BLNK,ORIG, 3,6 / U235,BLNK,ORIG .000095
	U238,BLNK,ORIG .02998
	FP, BLNK,ORIG .00001
	MOD,BLNK,ORIG , 1,6 / H2O,BLNK,ORIG .04
MIRANDA	–
ANAUSN	–
EDIT	$DATA,EDIT,GRPS , 1,5 / 1, ... 20
	CELL,CORE,MOD1 , 2,26/ FUEL,CORE,ORIG ...
	MOD,CORE,ORIG ...
	REFL,CORE,MOD1, 1,26/REFL,CORE,ORIG ...
MIRANDA	–
ANAUSN	–
EDIT	$DATA,EDIT,GRPS, 1,5 / 1, ... 20
	CELL,BLNK,COND , 2,26/ FUEL,BLNK,ORIG ...
	MOD,BLNK,ORIG ...
MERGEL	–
POW	–
etc.	

3. THE CHAR MODULE

3.1 Introduction

The CHAR module solves the isotope depletion equations for any number of spatial divisions of a system in which any number of isotopes have been represented. The module may be used, in combination with any diffusion or transport module which writes one of the AUS flux data pools, to undertake burnup calculations of a single cell (including cluster geometry) or a complete reactor core. Use of the spatial smearing factors on the STATUS data pool allows unsmearing of materials so that each discrete material may be burnt in the correct flux. The module has been written in a general form in order to accommodate any scheme for solving reactor burnup problems which involves the explicit calculation of individual nuclide concentrations.

The module has been written in the FORTRAN IV language, except for one small subroutine in IBM360 assembler language at the heart of the solution of the depletion equations. As the module makes dynamic use of all available core storage, no storage problems are anticipated with any feasible calculation. The functions performed by the various routines of the module and the input data specification are set out in the following sections.

3.2 Details of the Method

3.2.1 Evaluation of nuclide reaction rates

The average group fluxes Φ_{IG} and volumes V_I for each material I of the geometry data pool are obtained from either the FLUXA or FLUXB data pool. Other types of flux input could be incorporated with minor modifications to the module. If a suitable GFAC entry is present on the ST2 STATUS data pool, it is used to adjust the fluxes to a critical spectrum.

It must be stressed that a geometry material defines a region of constant flux for burnup purposes. No generation of additional materials is carried out.

The entries on the ST1 STATUS data pool for the current time are used to unsmear any smeared materials and to obtain the nuclide composition of discrete materials. If f_i and d_{ig} are the smearing factors defined in Section 2.2, the volume V_i and the flux in group g ϕ_{ig} of a material i smeared to form material I are given by

$$V_i = f_i \, V_I$$

$$\phi_{ig} = d_{ig} \, \Phi_{IG} \quad \text{for} \quad g \in G \quad .$$

The group condensation vector is obtained from the GRPS entry on ST1. The CHAR module can unsmear a material that has passed through any number of spatial smearing and condensation stages. The group structure of the nuclide cross section data pool may be the same as the flux data pool or it may correspond to any higher stage.

The required microscopic reaction rates for fission emission, fission, absorption, and the two possible production processes are given by simple summation:

$$r_{\ell_i} = \sum_g \sigma_{\ell_{ig}} \phi_{ig}$$

for the nuclides ℓ which comprise material i.

A material is considered to be burnable if the nuclide composition is an entry in ST1, and if any of its component nuclides is a member of the cross section data pool. The cross section data pool may contain several versions of the one nuclide, since the components of a material are identified by full 20–byte names.

Burnup mechanisms are also obtained from the cross section data pool (Robinson 1975) in which a burnup table includes the decay constant, fission product yields for different fuels, and the simple nuclide name of the product of decay and production reactions. The two possible production reactions are given as cross section entries 7 and 8 and may be any reaction of interest (reaction 7 is usually (n,γ)). Specification of burnup mechanisms, in this way, gives flexibility and is easily transformed for computation.

3.2.2 Solution of the nuclide depletion equations

The previously computed microscopic reaction rates are normalised to the required power or flux level and the following analytic solution of the depletion equations (Pollard & Robinson 1966) is applied to each discrete material in turn.

The equations may be written as a coupled set of first order linear differential equations in the form

$$\dot{\underset{\sim}{N}}(t) = \underset{\approx}{A} \, \underset{\sim}{N}(t) \quad , N(0) \text{ given,} \qquad (4)$$

where
- $\underset{\sim}{N}(t)$ is the vector of nuclide concentrations, $N_\ell(t)$, (ℓ = 1,2...n); and
- $\underset{\approx}{A}$ is an nxn matrix with elements

$$a_{\ell\ell} = -(r_\ell^{(a)} + \lambda_\ell) \quad , \tag{5}$$

$$a_{\ell k} = Y_{k\to\ell}^{(f)} r_k^{(f)} + Y_{k\to\ell}^{(7)} r_k^{(7)} + Y_{k\to\ell}^{(8)} r_k^{(8)} + Y_{k\to\ell}\lambda_k \ , \ k \neq \ell \ ,$$

where
- $r_k^{(f)}, r_k^{(7)}, r_k^{(8)}$ are reaction rates of nuclide k for fission, reaction 7 and reaction 8 respectively;
- λ_k is the decay constant of nuclide k; and
- $Y_{k\to\ell}^{(f)}, Y_{k\to\ell}^{(7)}, Y_{k\to\ell}^{(8)}, Y_{k\to\ell}$ are yields of nuclide ℓ from nuclide k for the various processes.

Advantage is taken of the fact that the main processes to be represented in reactor burnup are fission, (n,γ) and β decay to reorder the equations so that the matrix $\underset{\approx}{A}$ is lower triangular except for a few isolated elements one off the diagonal. This reordering is achieved using the 20th word of the burnup table on the cross section data pool which, for most nuclides, has the fixed point decimal value

PZZAAAI

where
- P = 1 for a fission product, else 0,
- ZZ = nuclide charge number,
- AAA = nuclide mass number, and
- I = 0 for a metastable isomer, else 1.

If this value does not give the requisite order in any nuclide chain, the special values given are

P00000I

where
- P = chain number (> 1), and
- I = number of nuclide in the chain.

The only such chain currently represented in the libraries is

$$Be^9 \to Li^6 \to H^3 \leftrightarrows He^3 \ ,$$

which also provides the only upper triangular matrix element with present libraries.

The almost lower triangular matrix $\underset{\approx}{A}$ is reduced to triangular form by a set of elementary transformations using matrices

$$\underset{\approx}{I}_j(x) = (\delta_{\ell k} + x\,\delta_{\ell,j-1}\,\delta_{jk}) \tag{6}$$

which have the property

$$\underset{\approx}{I}_j^{-1}(x) = \underset{\approx}{I}_j(-x) \quad . \tag{7}$$

Choosing j such that

$$a_{j-1,j} \neq 0 \quad \text{with } a_{j-2,j-1} = a_{j,j+1} = 0 \quad ,$$

the transformation

$$\underset{\approx}{A}' = \underset{\approx}{I}_j(x_j)\ \underset{\approx}{A}\ \underset{\approx}{I}_j(-x_j) \tag{8}$$

gives a transformed matrix $\underset{\approx}{A}'$ which has one less upper triangular non–zero element than $\underset{\approx}{A}$ by a suitable choice of x_j. The equation to be satisfied is

$$a_{j,j-1}\, x_j^2 - (a_{jj} - a_{j-1,j-1})\, x_j - a_{j-1,j} = 0 \tag{9}$$

which has two real roots, either of which will do.

Applying, if necessary, a number of such transformations to Equation (4) gives

$$\dot{\underset{\sim}{N}}'(t) = \underset{\approx}{A}'\ \underset{\sim}{N}'(t) \quad , \tag{10}$$

where
- $\underset{\approx}{A}'$ is of the required lower triangular form,
- $N'_\ell(t) = N_\ell(t) + x_j\, \delta_{\ell,j-1}\, N_j(t) \quad ,$ (11)

for j such that $a_{j-1,j} \neq 0$.

Assuming that the diagonal elements $a'_{\ell\ell}$ are distinct (which is true in practice provided that the nuclides are distinct), the solution of Equation (10) has the form

$$\underset{\sim}{N}'(t) = \underset{\approx}{B}\ \underset{\sim}{e} \quad , \tag{12}$$

where
- $\underset{\approx}{B}$ is the required solution matrix and is lower triangular, and
- $\underset{\sim}{e}$ has elements $e_\ell = \exp(a'_{\ell\ell}\, t)$.

Differentiation of Equation (12) and comparison with Equation (10) gives

$$b_{\ell k} = \sum_{g=k}^{\ell-1} a'_{\ell g}\, b_{gk} / (a'_{kk} - a'_{\ell\ell}) \quad , \quad \ell > k, \quad \text{and} \tag{13}$$

$$b_{\ell\ell} = N'_\ell(0) - \sum_{g=1}^{\ell-1} b_{\ell g} \quad . \tag{14}$$

Equations (13) and (14) express a simple recurrence relation which enables all the required elements $b_{\ell k}$ to be determined provided the indices (ℓ,k) are varied as follows:

(1,1); (2,1),(2,2); (3,1),(3,2),(3,3);...,(n,n).

The nuclide concentrations $\underset{\sim}{N}$ may then be obtained for any time t by applying Equation (12) and the transformation

$$N_\ell(t) = N'_\ell(t) - x_j\, \delta_{\ell,j-1}\, N'_j(t) \quad . \tag{15}$$

Average nuclide concentrations are obtained directly by integrating Equation (12) to give

$$\hat{\underset{\sim}{N}}'(t) = \underset{\approx}{B}\,\hat{\underset{\sim}{e}} \quad , \tag{16}$$

where $\hat{\underset{\sim}{e}}$ has elements $\hat{e}_\ell = (\exp(a'_{\ell\ell}\ t)-1)/a'_{\ell\ell}\ t$.

For small arguments, this exponential is expanded in a power series to avoid round-off error. The solution process as a whole is susceptible to round-off error, but no difficulties have been experienced with double-precision arithmetic used throughout.

The average nuclide concentrations are required to evaluate the average power level for each discrete material using

$$\hat{P} = \sum_{\ell} \hat{N}_\ell\ r^{(f)}_\ell\ E_\ell$$

where
- $\hat{P}$ is the average power level, and
- E_ℓ is the energy release per fission of nuclide ℓ.

This completes the burnup of a discrete material for a time step in which the flux level is held constant. Where a burnup at constant power is required, the time step given should be such that the flux varies only slightly over the time step. Having completed one pass through all the burnable materials, the reaction rates may be renormalised to the required power and the process repeated. If more than one time step is requested for a constant flux normalisation, each material is burnt for the desired number of steps using the original solution matrix for that material.

3.2.3 Cross section remixing

This function has been included in CHAR so that where resonance cross sections and detailed fluxes within a cell remain fairly constant with time, the cell calculation modules may be bypassed for some of the time steps.

A macroscopic material is remixed if all the nuclides comprising the material are in the microscopic cross section library and all the mixing rules are available. Otherwise the material is simply copied, and this fact is noted in the printed output. As for unsmearing, a macroscopic material may have passed through a number of condensing and smearing stages.

After forming macroscopic cross sections Σ_{ig} for a discrete material i with the nuclide library group structure g, the following equations are used to form a material I with groups G:

$$\Sigma'_{IG} = \sum_{g\in G}\ \sum_{i\in I}\ f_i\ d_{ig}\,\Sigma_{ig} \tag{17}$$

$$\Sigma'_{IG} = 1/\left(\sum_{g\in G}\left(\left(\sum_{i\in I} f_i\ d_{ig}\right)^2 / \sum_{i\in I} f_i\ d_{ig}\ \Sigma_{ig}\right)\right) \tag{18}$$

$$\Sigma'_{I,G\to G'} = \sum_{g\in G}\ \sum_{g\in G'}\ \sum_{i\in I}\ f_i\ d_{ig}\ \Sigma_{i,g\to g'} \quad . \tag{19}$$

Equation (17) is applied to all cross sections apart from the transport cross section and the total (or transport) component of the self-scatter term of the P_0 scatter matrix for which Equation (18) is used. Equation (19) is applied to all orders of P_n scatter matrices apart from the P_0 self-scatter term. This flux weighting of all P_n matrices can only be improved by including additional mixing rules; this is not considered to be worthwhile.

3.3 Input Data Specification

3.3.1 Data layout

Input data is punched in free format using keywords to indicate the data type. Each keyword must begin on a new card and all data must be punched between columns 1 and 72. The module uses the input subroutine SCAN (Bennett & Pollard 1967) to process the data. Default values have been set for most variables. Data to be reproduced exactly has been underlined.

3.3.2 Flux normalisation

The flux level at which the system is to be burnt may be specified as a volume integrated flux, flux, power, or power density for the whole or a part of the system. The format of the card is

FLUX (DENSITY) flux FOR name GRPS m TO n, or

POWER (DENSITY) power FOR name,

where

- DENSITY is given only if a flux or power density is to be specified,
- flux is the volume integrated flux (neutrons cm sec^{-1}) or flux (neutrons cm^{-2} sec^{-1});
- power is the fission power (W) or power density (W cm^{-3});
- name is $ALL, $FUEL or a fully qualified name of a discrete material in the system. $ALL means the normalisation is for the whole system; $FUEL means the fuel materials; and a material name means the normalisation is for the named material only. $ALL is the default value;
- m,n are the first and last energy groups of the isotope group structure to be included in the flux normalisation. The default is all groups.

For example

POWER 1.E+9

specifies a total power of 1000 MW.

FLUX DENSITY 1.E+14 FOR FUEL,CELLA,ORIG GRPS 5 TO 5

specifies a flux level of 1.E+14 neutrons cm^{-2} sec^{-1} in group 5 for the named material.

3.3.3 Time Step

The time step interval is given by

STEP t n

where

- t is the time interval in days,
- n is the number of steps to be taken (default 1).

As the solution of the depletion equations is analytic, the time step is that at which power renormalisation is carried out. That is, the time step is limited only by the requirement that the flux changes fractionally over the step. For burnup at constant flux (FLUX normalisation card), one step only is required unless intermediate printed output is desired.

3.3.4 Flux data pool

The flux distribution may be obtained either from an AUS FLUXA data pool (POW dump) on FORTRAN unit 5 or an AUS FLUXB data pool (WDSN dump) on FORTRAN unit 6. The choice between them is made by

FLUXLIB FL n

where n is { 1 for FLUXA, 2 for FLUXB.

If n is zero, a one point burnup is performed, in which case the XS library must be one energy group. The default value is n equals 2, a FLUXB data pool.

3.3.5 Cross section data pools

Macroscopic cross sections are obtained from FORTRAN unit 7. The default option is for microscopic data to follow the macroscopic data on this unit. Otherwise the data

XSLIB n

is given and the microscopic data is obtained from unit n, where n would normally be 8. The microscopic data must be on a separate unit if the macroscopic data is to be remixed. Remixing is requested by including the control card

REMIX .

3.3.6 Prelude data

The only prelude data required is the maximum number of burnable materials, as other data is obtained from the various data pools. The control card is

MAXM m

where 100 is the default value.

3.3.7 Print options

The print options are controlled by a single number n, which is specified by

PRINT n .

If n $\geq$ m printout of type m is produced where the print types are:

0 a minimal print of materials and irradiations for each time step,

1 print concentrations and time average concentrations at the end of each time step for each nuclide for each material,

2 print group fluxes for each material, and

4 print one group microscopic reaction rates for each nuclide for each material.

The default value of n is 1.

3.3.8 START

The control card

START

causes calculation to begin.

4. REFERENCES

Bennett, N.W. & Pollard, J.P. (1967) – SCAN – a free input subroutine for the IBM360. AAEC/TM399.

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