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AUSTRALIAN ATOMIC ENERGY COMMISSION
RESEARCH ESTABLISHMENT
LUCAS HEIGHTS

AUS MODULE POW – A GENERAL PURPOSE 0,1 AND 2D, MULTIGROUP
NEUTRON DIFFUSION CODE INCLUDING FEEDBACK-FREE KINETICS

by

J. P. POLLARD

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ABSTRACT

POW is a 'workhorse' module of the AUS system and is used mainly for the following applications:

- (1) 2 region resonance theory data preparation from presently available fast reactor 26- or 16-group libraries,
- (2) 0, 1 and 2D diffusion calculations - eigenvalue or criticality search, source or feedback-free kinetics calculations, and
- (3) perturbation calculations.

Main features of the code include the following:

- (1) it will run under the site AUS system or stand alone (on an IBM360/50),
- (2) the code uses SLOR for inner iterations with region rebalance to enhance convergence, Gauss-Seidel for upscatter iterations with group

rebalance to enhance convergence, Chebyshev source extrapolation for outer iterations and a delayed neutron integrated Crank-Nicholson method for kinetics problems,

- (3) free format style of input is used throughout, and
- (4) output options include 1 and 2D flux or reaction rate plots (on a CALCOMP plotter).

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The following descriptors have been selected from the INIS Thesaurus to describe the subject content of this report for information retrieval purposes. For further details please refer to IAEA-INIS-12 (INIS: Manual for Indexing) and IAEA-INIS-13 (INIS: Thesaurus) published in Vienna by the International Atomic Energy Agency.

COMPUTER CALCULATIONS; CRITICALITY; CROSS SECTIONS; DATA;
DISTURBANCES; EIGENVALUES; IBM COMPUTERS; MOATA REACTOR;
MULTIGROUP THEORY; NEUTRON DIFFUSION EQUATION; NEUTRON FLUX;
NEUTRON LEAKAGE; ONE-DIMENSIONAL CALCULATIONS; P CODES; REACTOR
KINETICS; TWO-DIMENSIONAL CALCULATIONS

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Figure 3 (X,Y) plot of MOATA thermal flux

Appendix A AUS Module Aspects of POW
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1. INTRODUCTION

Vital to any reactor neutronics calculation scheme is a versatile, fast and accurate multidimensional, multigroup neutron diffusion code. On our site IBM360/50 computer we have mainly used CRAM (Hassitt 1962, rewritten in FORTRAN originally for the IBM7040) and GOG (Hopkins and Oakes 1968, somewhat rewritten for the IBM360/50) over the past few years, although a host of other similar codes exist, some of which are not readily made available. Growing out of the use of the site versions of CRAM and GOG were a satisfaction with the versatility of CRAM (but not the speed) and a satisfaction with the speed of GOG (but not the versatility). In addition, obvious shortcomings of both were revealed for some calculations. With the advent of the site AUS modular scheme (Appendix A) a versatile, fast and accurate 2D, multigroup diffusion code was required as the 'workhorse' module and POW was conceived.

POW was a breakaway from the earlier codes in some aspects. One essential difference is that POW makes a better estimate of leakage throughout the reactor compared with the other codes as it uses an edge flux scheme (Wachspress 1966). Other important differences include the ability of POW to obtain extrapolation parameters for successive line over relaxation (SLOR) and Chebyshev extrapolation from detailed analysis of flux calculated using preoptimum estimates of the parameters. In addition both group and region rebalance are carried out to enhance convergence. (Some admittedly non-typical calculations have been speeded up by a factor of 10 since inclusion of these rebalance features.) A brief sketch of the numerical methods is given in Section 3 (and a more detailed presentation is given by Pollard 1973). From the user's point of view, ease of use is extremely important and the DTAV free input routine (Appendix D) helps here considerably.

In addition to the flux calculation requirements for 0, 1 and 2D studies, POW can prepare its own 2-region (equivalent) resonance shielded cross sections from AUS datapools (libraries) - Appendix A. Presently cross sections may be obtained from one of the fast reactor resonance tabular libraries, the 26-group ABBN data (Bondarenko 1964 - Appendix B) or the 16-group Hansen-Roach data (1961 - Appendix C), as well as from an already shielded library possibly prepared from the intermediate and thermal reactor resonance parameter, 127-group GYMEA data (Pollard and Robinson 1969).

The code has reasonably general editing facilities, including a perturbation option. In addition 1 and 2D plots of flux or reaction rate may be produced on a CALCOMP plotter.

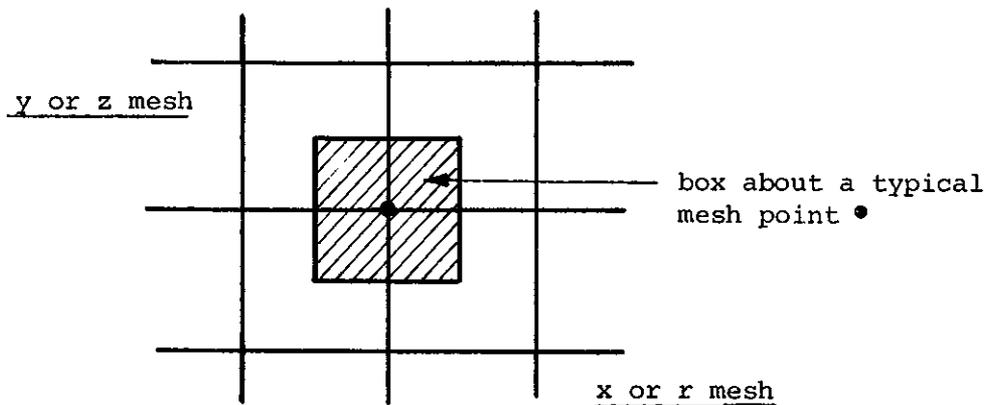
Finally POW can be used for multidimensional kinetic studies for systems perturbed from the steady state with a prescribed pulsed (feedback-free)

variation of some, usually physical, parameter, for example the concentration of a reactor material. (The desirability of including feedback in a later version of the code is being considered.)

The source language of POW is mainly FORTRAN IV for the IBM360/50. The programme, which can run alone as well as under the AUS system, occupies less than 360,000 bytes of core storage and uses several disks for intermediate output. At the time of writing this report, the basic parts of the code have been thoroughly tested and have been running for well over 6 months .

2. THE MULTIGROUP NEUTRON DIFFUSION EQUATION

The general form of the multigroup neutron diffusion equations solved by POW at each mesh point for the flux in a box about each point may be simply obtained from a detailed analysis of neutron events (Stacey 1969). The ultimate method used to solve the equation is a finite difference method generating a numerical solution at the intersection of a selected mesh as illustrated -



We therefore cast the neutron diffusion equations into the form ultimately required, namely

$$\begin{aligned}
 -\frac{1}{v_g} \int_{\text{box}} \frac{\partial \phi_g}{\partial t} dV &= - \int_{\text{box}} \nabla \cdot D_{n,g} \nabla \phi_g dV + \phi_g \int_{\text{box}} \sigma_{\text{rem}g} dV \\
 - \left\{ \sum_{g'} \phi_{g'} \int_{\text{box}} \sigma_{sg' \rightarrow g} dV + \chi_{pg} (1-\beta) \sum_{g'} \phi_{g'} \int_{\text{box}} \frac{v}{k} \sigma_{fg'} dV + \right. \\
 \left. + \sum_i \chi_{ig} \lambda_i C_i + S_g \right\}, \quad g = 1, 2, \dots, NG
 \end{aligned}$$

and in addition we have the precursor concentration equations for delayed neutron groups

$$\frac{\partial c_i}{\partial t} = \beta_i \sum_{g'} \phi_{g'} \int_{\text{box}} \frac{v}{k} \sigma_{fg'} dV - \lambda_i C_i, \quad i = 1, 2, \dots, \text{IGD},$$

where

- k is the effective steady state multiplication,
 $S_g(\underline{r}, t)$ is the energy group g external source in each box,
 χ_{pg} is the prompt fission spectrum (normalised to unit sum),
 χ_{ig} is the delayed fission spectrum (normalised to unit sum), for delayed group i yielding fraction β_i of total emissions, $\beta (= \sum_i \beta_i)$ of which are delayed,
 $\sigma(\underline{r}, t)$ denotes various (macroscopic) cross sections,
 $D_{n,g}(\underline{r}, t)$ denotes possibly directional diffusion coefficients (for direction n or $-n$ parallel to the chosen axes),
 v_g denotes group g average velocity,
 $C_i(\underline{r}, t)$ is the box total concentration of precursor, with decay half life λ_i , of delayed group i ,
 $\phi_g(\underline{r}, t)$ is the group g flux in each box required to be calculated,
 \underline{r} denotes the coordinates of a typical mesh point (or a point in the box),
 t is the time

and sums are taken over all groups (1, 2, ... , NG for energy groups and 1, 2, ... , IGD for delayed groups). The equations are to be solved for ϕ_g subject to:

(i) the outer boundary conditions -

(a) reflective (zero current)

$$\frac{\partial \phi_g}{\partial n} = 0 \quad \text{for each group } g,$$

where n = outward normal,

or (b) reactor (zero flux on extrapolated boundary)

$$D_{n,g} \frac{\partial \phi_g}{\partial n} + \frac{\phi_g}{3d} = 0 \quad \text{for each group } g,$$

where d = extrapolation distance in equivalent transport mean free paths (usually 0.71 is used);

(ii) the internal boundary conditions for boundaries separating different materials say L and R -

(a) continuity of flux

$$\phi_g \Big|_L - \phi_g \Big|_R = 0 \quad \text{for each group } g,$$

and (b) continuity of current

$$n \cdot (D_{n,g} \nabla \phi_g \Big|_L - D_{n,g} \nabla \phi_g \Big|_R) = 0 \text{ for each group } g,$$

where n = boundary normal;

(iii) the initial conditions -

(a) steady state

$$\frac{\partial \phi_g}{\partial t} = 0, \quad \frac{\partial C_i}{\partial t} = 0, \quad S_g = 0, \quad t \leq 0 \text{ for all groups,}$$

$$\sum_{g'} \int_{\text{reactor}} f \sigma_{fg'} \phi_{g'} dV \Big|_{t=0} = P,$$

where f = fission energy release,

P = specified power,

which requires POW to solve an eigenvalue problem (Section 5) for either k

or λ multiplying a physical parameter (perhaps the concentration of a reactor material) to give

$$k \approx 1$$

and in either case for our kinetics study we must retain the steady state value of k in our equations in order that any time dependent variation is purely attributable to a variation from the steady state,

or (b) shut down

$$\phi_g = 0, \quad C_i = 0, \quad S_g = 0, \quad t \leq 0 \text{ for all groups.}$$

The numerical methods used to solve the equations are briefly outlined in the next Section.

3. NUMERICAL METHODS IN OUTLINE

In this Section we will only attempt to provide a brief outline of the numerical methods used by POW which are detailed elsewhere (Pollard 1973).

Central to our time dependent considerations over a small time step from t_{p-1} to t_p , is that we may approximate integrals of the general type

$$\int_{t_{p-1}}^{t_p} f(t) \phi_g(\underline{x}, t) \int_{\text{box}} \sigma_g(\underline{x}', t) dV \quad (\text{with } f(t) = \text{a given function of time})$$

using the assumptions

(i) that the flux ϕ_g varies linearly with time

$$\varphi_g(\underline{x}, t) \approx \left(\frac{t_p - t}{\delta t} \right) \varphi_g(\underline{x}, t_{p-1}) + \left(\frac{t - t_{p-1}}{\delta t} \right) \varphi_g(\underline{x}, t_p) \quad (\text{with } \delta t = t_p - t_{p-1})$$

and (ii) that the cross section σ_g is constant with time

$$\sigma_g(\underline{x}', t) = \sigma_g(\underline{x}', \bar{t}),$$

where \bar{t} is an average time for the step (not necessarily the mean). We incorporate the assumptions into an $e^{\lambda_i t}$ weighted form of precursor concentration equation and a directly integrated form of diffusion equation (Stacey 1969). After some elimination we obtain an equation for the flux at time t_p in terms of the flux and precursor concentrations at time t_{p-1} . In order to eliminate the $-\nabla \cdot D_{n,g} \nabla$ operator we resort to a finite difference method which embodies the required internal boundary conditions (Wachspress 1966). We may then write our equations in a formal way (thereby covering up a multitude of detail)

$$(L + A + a - R - \frac{F}{k}) \varphi(p) = -(L + A - a - R - \frac{F}{k}) \varphi(p-1) + DC(p-1) + S(p, p-1),$$

where

- $\varphi(p)$ is a vector of unknown flux elements (involving space points as well as energy groups) at time t_p ,
- $\varphi(p-1)$ is a vector of known flux elements at time t_{p-1} ,
- $C(p-1)$ is a vector of known precursor concentrations (involving space points as well as delayed groups) at time t_{p-1} ,
- $S(p, p-1)$ is a vector of time integrated external source elements,
- k is the steady state multiplication

and the remaining quantities are matrices derived from the indicated terms:

$$L \sim - \int_{\text{box}} \nabla \cdot D_{n,g} \nabla dV,$$

$$A \sim \int_{\text{box}} \sigma_{\text{remg}} dV,$$

$$a \sim \int_{\text{box}} 2/(v_g \delta t) dV,$$

$$R \sim \int_{\text{box}} \sigma_{sg' \rightarrow g} dV,$$

$$F \sim \chi_g(\delta t) \int_{\text{box}} v \sigma_{fg'} dV,$$

$$F' \sim \chi_g'(\delta t) \int_{\text{box}} v \sigma_{fg}' dv,$$

$$D \sim \chi_g''(\delta t),$$

with $\chi_g(\delta t)$, $\chi_g'(\delta t)$ and $\chi_g''(\delta t)$ being obtained from the fission spectra and delayed neutron data.

In words the method used to calculate $\beta(p)$ consists of the following steps:

- (i) group rebalance (to balance neutron events for all groups),
- (ii) region rebalance (to balance neutron events for the plane) for 1 group,
- (iii) successive line over relaxation (SLOR) inner iterations for solution of 1 group for the entire plane, and
- (iv) Gauss-Siedel upscattering and fission iteration for all groups and all space points,

which is the same approach as is used for a (steady state) source calculation.

However, for a steady state eigenvalue calculation (with perhaps k to be obtained as eigenvalue) step (iv) is replaced by

- (iv) Gauss-Siedel upscattering iteration (fission is not included here),
and

- (v) Chebyshev extrapolated outer iteration fission source calculation.

The brevity of the above leaves much to be desired. Even so, knowledge of the gross details is unnecessary to run a calculation.

4. THE CODE POW

Experience of the author over many years with neutronic codes suggests that no amount of good theory, no matter how good, is enough in a code - it must also be embedded in good coding. This experience is particularly relevant when the code is to be run on a not-so-fast computer such as the site IBM360/50. The author has therefore aimed to achieve a reasonable balance between ease of coding and speed of resulting programme. A compromise was necessary with POW however as its flexibility has tended to make ease of coding a more important consideration than it would have been for a less flexible code. Most of the routines compile with the FORTH compiler, opt=2 which produces reasonable object coding. The most important routine as far as computer time is concerned is the inner loop SLOR scheme for the (x,y) or (r,z) plane and this routine has been written in Assembler.

From the user's point of view perhaps a more important consideration to the above observations, provided the code does the job, is the ease with which the code may be used. A new type of free input routine (DTAV, Appendix D) was therefore written for the job. In addition, easy to follow output is produced

by POW.

The entire programme (using the standard COMMON of 40,000 words - Section 5.5) with the help of numerous overlays fits into less than 360,000 bytes of core storage. Many disk data sets are also involved for both regular and temporary input/output, but these need not reside on more than a few disk drives.

Typical jobs (if these exist) usually take about the following CPU times on the IBM360/50:

O&I	steady state calculations - a few minutes	} these run in the day queue on site,
2D	steady state calculations - about 15 minutes	
2D	fissile source calculations - about 30 minutes,	
2D	kinetics calculations - a few hours,	

although a factor 4 (or thereabouts) increase or decrease is possible with a range of jobs. Jobs other than OD kinetics tend to be CPU bound and so if the jobs were run alone on the machine, rather than in competition with other jobs run under the HASP operating system, the actual times would not be much different. (It is interesting that the same job run under HASP on different occasions may vary in CPU time by as much as 10 per cent. This is attributed to POW being CPU bound with competing jobs stealing machine cycles for input/output.)

5. POW STEADY STATE DATA

5.1 Introduction

In Section 2 we were introduced to the equations solved by POW. Here we detail all of the data needed to carry out a steady state calculation. This calculation may well be carried out (i) as the first stage of a kinetics study or may simply be carried out (ii) as part of routine reactor assessment. The general (REAL) steady state equation solved by POW at each mesh point for the flux in a box about each point may be written as

$$\begin{aligned}
 & - \int_{\text{box}} \nabla \cdot D_{n,g} \nabla \phi_g \, dV + \phi_g \int_{\text{box}} \sigma_{\text{remg}} \, dV \\
 & = \sum_{g'} \phi_{g'} \int_{\text{box}} \sigma_{sg' \rightarrow g} \, dV + \chi_g \sum_{g'} \phi_{g'} \int_{\text{box}} \frac{\nu}{k} \sigma_{fg'} \, dV + S_g, \quad g = 1, 2, \dots, NG,
 \end{aligned}$$

where

k is the effective multiplication (=1 for SOURCE problems),
 $S_g(\vec{r})$ is the group g external source in each box (=0 for EIGENvalue problems),
 χ_g is the group fission spectrum (normalised to unit sum)

$$= \left\{ \begin{array}{l} \chi_{pg}(1-\beta) + \sum_i \chi_{ig} \beta_i \\ \chi_{pg} \end{array} \right.$$

the equilibrium spectrum for (i),
with χ_{pg} the prompt spectrum and χ_{ig} the
delayed fission spectrum for delayed
group i yielding fraction β_i of total
emissions, $\beta (= \sum_i \beta_i)$ of which are delayed;
the (normal) prompt spectrum for (ii),

$\sigma(\underline{r})$ denotes various (macroscopic) cross sections,
 $D_{n,g}(\underline{r})$ denotes possibly directional diffusion coefficients (for direction
n or -n parallel to the chosen axes),
 $\phi_g(\underline{r})$ is the group g flux in each box required to be calculated,
 \underline{r} denotes the coordinates of a typical mesh point (or a point in
the box)

and sums are taken over all groups (1, 2, ..., NG for energy groups and 1, 2, ..., IGD for delayed groups). The equations are to be solved for ϕ_g subject to specified outer boundary conditions

(a) reflective (zero current)

$$\frac{\partial \phi_g}{\partial n} = 0 \text{ for each group } g,$$

where n = outward normal,

or (b) reactor (zero flux on extrapolated boundary)

$$D_{n,g} \frac{\partial \phi_g}{\partial n} + \frac{\phi_g}{3d} = 0 \text{ for each group } g,$$

where d = extrapolation distance in equivalent transport mean free path (usually 0.71 is used).

(The adjoint steady state equation for adjoint flux ϕ_g^* is similarly

$$\begin{aligned} & - \int_{\text{box}} \nabla \cdot D_{n,g} \nabla \phi_g^* \, dV + \phi_g^* \int_{\text{box}} \sigma_{\text{remg}} \, dV \\ & = \sum_{g'} \phi_{g'}^* \int_{\text{box}} \sigma_{sg \rightarrow g'} \, dV + \sum_{g'} \chi_{g'} \phi_{g'}^* \int_{\text{box}} \frac{\nu}{k} \sigma_{fg} \, dV + S_g^*, \quad g = 1, 2, \dots, \text{NG}, \end{aligned}$$

with corresponding boundary conditions.)

The usual calculation undertaken with POW is for EIGENValue problems. For this situation we may (a) calculate k as the eigenvalue of the homogeneous (external source free) equation or we may (b) SEARCH for an eigenvalue, γ , usually multiplying some physical quantity (for example mesh spacing), such that we achieve

$$k = k_{\text{reqd}}, \text{ usually } 1,$$

and \emptyset_g (normalised to a total fission source of unity) is then the corresponding eigenvector (for the REAL case).

Basically data required to run POW can be broken down into 4 main parts:

- (1) IBM360 job control language, JCL,
- (2) occasionally required user supplied additional routines coded in FORTRAN,
- (3) AUS system control language, AUSYS, and
- (4) POW data proper.

Very few applications of POW require other than standard use of (1) and (2) as introduced in Section 5.6. Specialised use of (1) and (2) will not be dealt with further. Data for (3) however, is slightly expanded in Appendix A. The remainder of this Section will be essentially devoted to introducing data required for different types of applications. The presentation is along the lines of description of functional data blocks under headings such as 'card group data' (Section 5.8). An entire run consists of the user logically combining the functional data blocks for his particular application.

We start the main presentation with all the data required of a sample run (Section 5.3) for user familiarisation. Before we do however, we introduce the free format style for all of POW's input.

5.2 Summary of Free Style (DTAV) Input to POW

Input data required by POW is punched in free FORMAT style with keywords indicating the data type, e.g.

```
SP 0.8 0.2 0. 0.
```

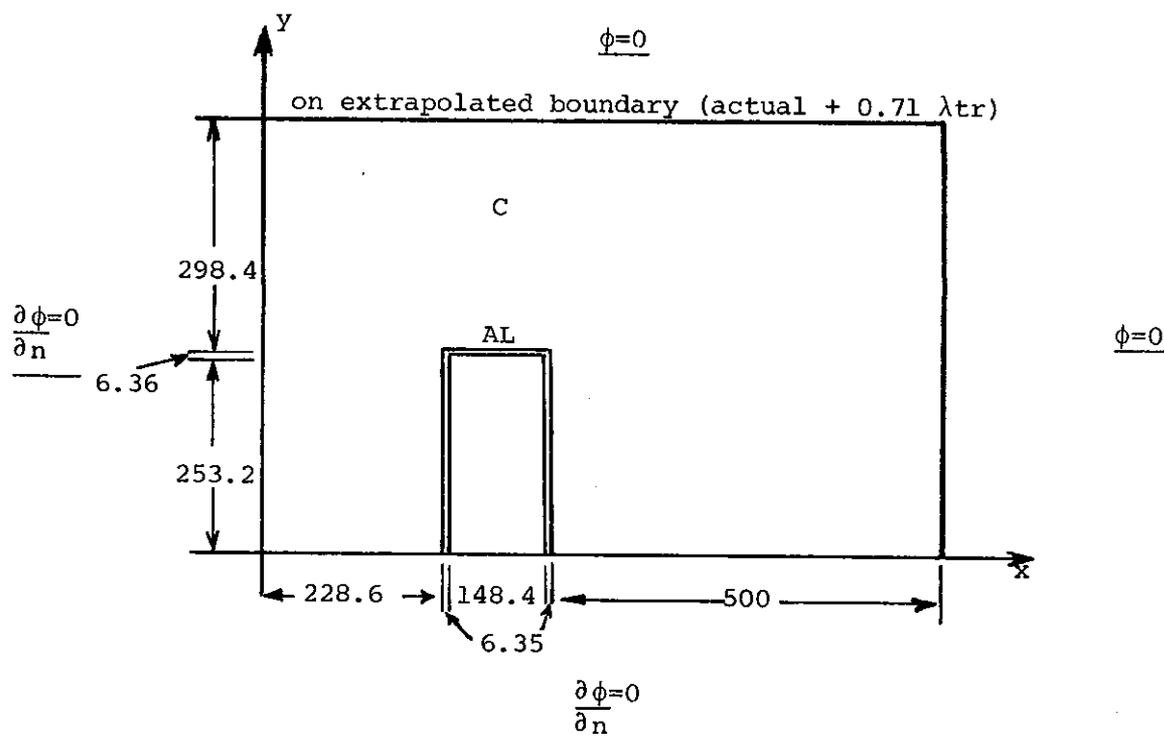
designates data for the fission spectrum (SP). The data is read using the set of subroutines DTAV (Appendix D) which incorporates the subroutine SCAN (Bennett and Pollard 1967). The main features of DTAV and SCAN relevant to running POW are summarised below.

<u>DATA FEATURES</u>	<u>COMMENTS</u>
Card columns	Normally 1 to 72 and each data card is listed when read although \$OPT 1,72,0 \$ in the data turns off the listing option.
Keywords	Normal FORTRAN variable names except that up to 8 characters are permitted and zero is never used, e.g. the last character in ACCFO is the letter O.
Modes	Numeric data may be punched in any mode, e.g. $1, 1., 1.-3 \equiv 1.E-3 \equiv 1.D-3 = 10^{-3}$ and alphanumeric data consists of FORTRAN variable type names which are not keywords.
Extents of Data	Different keywords require different extents of data to trail them, e.g. for a 4-group problem the fission spectrum, SP, would require 4 members to follow.
Repeat, repeats*no.	To save punching we may use, say, $4*0. \equiv 0. 0. 0. 0.$
Increment, from (incr.) to	To save punching we may use say, $1(2)7 \equiv 1 3 5 7$
Readability	Additional special characters may be interspersed throughout the data, e.g. $SP=0.8,0.2,2*0$ and $M(1) 0.07 \equiv M 1 0.07$
Comments	A card punched with an * in column 1 is treated as a comment card and is not scanned for data.

5.3 A Sample Run (MOATA)

MOATA is an enriched uranium light water moderated reactor of Argonaut type used in thermal reactor studies on site. Harrington (1972, unpublished) has undertaken detailed AUS calculations on MOATA as support to an investigation of Connolly (1972, unpublished). A sample run given here is based on data generated under AUS (using our thermal library and module GYMEA, Pollard and Robinson, 1969) for these calculations.

A quarter XY plan of homogenised regions of MOATA is sketched below. All dimensions are in millimetres (although POW uses centimetres).



MOATA REACTOR PLAN

Input data for the calculation follows. Output of a slightly extended version of the run is given in Appendix E.

```
//JPPMOATA JOB (P1B00930,N1),J.P.POLLARD,
// CLASS=J,TIME=10
// EXEC AUS
//GO.SYSIN DD *
*DD1
STEP POW
*DD2
```

JCL
AUSYS

PRELUDE MAXX=23,MAXY=17,MAXG=4,MAXM=3 END

POW MOATA (X,Y) CALCULATION, GYMEA DATA

* NORMALLY AUS DISK GROUP DATA WOULD BE USED

NG=4 ... number of
groups

XSD FUEL M(1) ... cross section
data, FUEL

1.54481-1 3.6863-1 9.02355-1 2.00955 ... σ_{tr}
 9.41612-2 6.02354-2 6.81026-1 1.12777-1 ... σ_{rem} (abs+scat)
 3.73274-4 3.30167-3 3.96448-2 9.77554-2 ... $v\sigma_f$
 0.0 9.37282-2 2*0.0 ... $\sigma_{scat 1}$
 2*0.0 4.88109-2 8.75701-3 ... $\sigma_{scat 2}$
 0.0 5.09412-3 0.0 6.48822-1 ... $\sigma_{scat 3}$
 0.0 1.66342-7 4.77318-2 0.0 ... $\sigma_{scat 4}$

XSD AL M(2)

1.16556-1 1.05169-1 9.05011-2 9.34386-2
 1.64155-2 1.20851-3 1.84524-2 1.34341-2
 4*0.0
 0.0 1.6132-2 2*0.0
 2*0.0 5.06778-4 0.0
 0.0 5.36885-4 0.0 1.28382-2
 2*0.0 1.27736-3 0.0

XSD C M(3)

1.49824-1 3.44423-1 3.74146-1 3.63541-1
 2.24931-2 4.23208-3 9.82699-2 8.3279-3
 4*0.0
 0.0 2.24898-2 2*0.0
 2*0.0 4.22309-3 4.23284-8
 0.0 1.58544-3 0.0 9.65788-2
 2*0.0 8.07923-3 0.0

SP 7.53564-1 2.46436-1 2*0.0

BSQ(0) 1,2,3 1,2,3 3*0.00184

XM=0,5*4.572,0.635,5*2.968,0.635,10*5,0.71

YM=0,5*5.064,0.636,10*2.984,0.71

REG MX=1(1)22 MY=1(1)16 M(3)

REG MX=6(1)12 MY=1(1)6 M(2)

REG MX=7(1)11 MY=1(1)5 M(1)

POW - array sizes
different than
default
Descriptive data
Comment

Group data - simi-
lar to CRAM (Hassitt
1962); in this
example data is
macroscopic (cm^{-1})

Axial $B^2=0.00184$

Geometry data -
region definitions
overlay each other

START		↕	Start calculation
GROUPS	4 1,1(1)4	↕	
MREG	1,2,3,-1=1,2,3	↕	Edit requirement
EDIT	1,1 3	↕	
STOP		↕	Stop run
/*		↕	JCL
//			

5.4 The Functional Data Blocks in Brief

In the sample run of the previous Section we were introduced to the data of POW. Here we briefly look at the functional blocks required to be put together to carry out a steady state calculation. In subsequent Sections we detail the functional blocks one by one. As a further guide the user is reminded that an index is provided (Section 10).

The functional blocks consist of the following-essentially entered in the indicated order to set up data for the actual flux calculation identified thus***

- (5.5) Control languages - JCL, additional FORTRAN coding and AUSYS,
- (5.6) PRELUDE data - to set array sizes for each job of a complete run,
- (5.7) Descriptive data - POW job name and heading,
- (5.8) Card group data - basic cross section data either microscopic or macroscopic (and kinetics data),
- (5.9) Library group data - perhaps from one of the resonance shielded cross section libraries available with the AUS scheme (presently 26-group Russian ABBN library, Appendix B; 16-group Hansen-Roach library, Appendix C),
- (5.10) $P_n(n \neq 0)$ data - Legendre polynomial weighted scattering data for use by other AUS modules,
- (5.11) Cross section modification - changes of selected cross sections,
- (5.12) Mixing rules - data for mixing cross sections,
- (5.13) DB^2 leakage - data for setting up approximate leakage,
- (5.14) Poison absorption - data for setting up poisoning of absorption cross sections,
- (5.15) Geometry data - specification of geometry, mesh spacing, boundary conditions and region layout,
- (5.16) Calculation type - real or adjoint flux; eigenvalue, source (or kinetics problem),
- (5.17) Criticality search data - code adjustment of data to achieve criticality,

- (5.18) Fixed source specification - data for source calculation,
- (5.19) Trial flux specification - normally not required,
- (5.20) Calculation strategy specification - normally not required,
- (5.21) Calculation termination data - accuracy and machine time limits,
- (5.22) Output requirement specification - to set content of output,
- *** (5.23) Calculation START - may use a flux dump (RESTART),
- (5.24) Region EDIT - print and disk (card or AUS) output for regions of materials,
- (5.25) Perturbation EDIT - for small data changes using real and adjoint flux,
- (5.26) Point EDIT - print and plotted edit for reactions about a point,
- (5.27) Possible user written subroutines - for edit before, during or after a flux condition, and
- (5.28) Termination data - END and STOP.

5.5 Control Language

POW may be run on the site IBM360/50 computer using the stand alone catalogue procedure POW or under the AUS scheme called in with the AUS catalogue procedure. For standardisation, and ease of use, the POW catalogue procedure is only used to generate a temporary load module when user supplied routines are to be added. All running is then carried out under AUS.

Below we tabulate the site version of control language cards required for most runs.

Normal Code User	Either User	User Requiring Additional Routines
↑	//XXX JOB NAME, // CLASS=J,TIME=15	// CLASS=K,TIME=30,REGION=480K ...for large core runs only...
If plotting required ...	// EXEC BUFFPROG,PRG=AEPLOT	// EXEC POW,POW='&&POW',GO=0 //FORT.SYSIN DD *
<u>JCL data</u>	<u>FORTTRAN</u> →	<pre> SUBROUTINE CMSIZE(LC) C FOR A USER REQUIRING MORE C CORE THAN MOST JOBS C SETS THE CORE SIZE COMMON C(60000) C LC=LENGTH OF COMMON C STANDARD VALUE LC=40000 LC=60000 RETURN END </pre>
// EXEC AUS	Or if a flux dump data set is required ...	/* // EXEC AUS,POW='&&POW'
// EXEC AUS,...	where ... is FL1='AUS.JPPOWFLX',DISPFL1=OLD	// EXEC AUS,POW='&&POW',... or the users equivalent
↓	//GO.SYSIN DD *	
↑	*DD1	
<u>AUSYS data</u>	STEP POW	
↓	*DD2	
↑	PRELUDE ...	
<u>POW data</u>	to be described in the next Sections	

5.6 PRELUDE Data

PRELUDE data must be given first as the data specifies the sizes of variable dimensional arrays used by POW. The user must supply data between the keywords

PRELUDE END

to set array sizes that are different from default values indicated in the accompanying table. (Should all the default values be satisfactory, then the data

PRELUDE END

suffices.) A normal POW run would require only one assignment of storage and we would supply the data,

PRELUDE data to be described END

remainder of data for a job

STOP (as the terminal card),

however, we change the storage assignment for independent calculations thus

PRELUDE ... END (of prelude)

END (of data associated with preceeding prelude)

PRELUDE data different than standard prelude END

END or STOP

The following table details the basic array sizes. (Other sizes are computed from the basic ones.) The data may be given one word per card as illustrated in the table or may be compacted to fit into as few as possible cards, e.g.

PRELUDE MAXX=23,MAXY=17,MAXG=4,MAXM=3 END

<u>PRELUDE</u>	<u>Standard</u>	<u>Description</u>
MAXX=25	80	Maximum number of x (or r) mesh points - note that the flux is calculated at a mesh point, not in the centre of a mesh cell (MAXX must then be at least 1 plus the number of mesh intervals)
MAXY=27	1	Maximum number of y (or z) mesh points
MAXG=4	26	Maximum number of groups
MAXS=1	3	Maximum number of additional reactions - Section 5.8.2
MAXM=5	15	Maximum number of materials
MAXF=1	0	Maximum number of fixed source or adjoint flux arrays (FSCE) (1 is required for a fixed source problem, for a kinetics problem, or for an adjoint flux problem when the real flux array (FLX) and adjoint flux array are both required for EDIT)
MAXW=0	200	Maximum length of working array WSEA used with SEARCH - Section 5.17
MAXN=10	50	Maximum length of MREG array with EDIT - Section 5.24
MAXC=4	0	Maximum number of groups of coefficient matrix to be held in core - if 0 then the matrix will remain in core if space is available, otherwise supplementary disk storage will be used - if MAXG then the code will only run if all the data will fit in core - if 1 then the use of supplementary disk storage is forced (MAXG≠1)
MIST=30	28	Maximum length of LIST used with printer dump (OUTPUT PDUMP - Section 5.22)
MAXGD=6	0	Maximum number of delayed neutron groups
MAXP=100	50	Maximum data storage associated with description of kinetic PULSES - Section 6.5.1
PRINT		- Causes the printing of actual array sizes used based on the specified PRELUDE data
END		- Terminating word of PRELUDE data

Note: In addition to specifying the above sizes all other common data is set to default values, mostly zero.

The number of 4-byte core storage words required by the programme at the time of writing this report, LCR, is then given very approximately by the expression

$$\text{LCR} = \text{MAXX} * \text{MAXY} * (2 * \max[\text{MAXG} * (1 + \text{MAXF}), \text{MAXG} + \text{MAXGD} - 3] + 5 * \text{MAXC}' + 9)$$

$$+ \text{MAXM} * \text{MAXG} * (\text{MAXG} + \text{MAXS} + 13)$$

+4000 (which includes some allowance for terms not appearing as products) where MAXC' is the actual value used for MAXC (1 or MAXG).

As a rough guide, the above formula suggests the use of standard COMMON (LC-40000-Section 5.5) should enable the following calculations to be undertaken - unspecified data being given by the standard PRELUDE default values (Section 5.6):

MAXG	MAXGD=0		MAXGD=0		MAXF=1	
	MAXM=5		MAXM=15		MAXM=15	
	MAXF=0	MAXF=1	MAXF=0	MAXF=1	MAXGD=1	MAXGD=6
	<u>MAXX*MAXY</u>		<u>MAXX*MAXY</u>		<u>MAXX*MAXY</u>	
1	2000	2000	2000	2000	2000	1600
2	2000	1600	2000	1600	1600	1400
4	1600	1100	1500	1100	1100	1100
8	1100	700	1000	700	700	700
16	700	400	600	350	350	350
26	400	250	300	160	160	160
36	300	150	90	50	50	50
50	170	90	-	-	-	-
69	40	20	-	-	-	-

5.7 Descriptive Data

Descriptive data is given on one card as follows:

<u>POW</u>	JOBNAME	HEADING
where	JOBNAME	is any descriptive job name which needs to be unique to a job when a flux dump is required (OUTPUT FLUX and RESTART, Section 5.23)
and	HEADING	(of no more than 52 characters) is any suitable heading to be used in labelling output.

The data, although normally given as the second functional block, may appear anywhere in a job.

5.8 Card Group Data

Card group data consists of the following:

- (1) NG, the number of energy groups (logically first for this block);

- multigroup data for individual materials,
- (2) XSD, the cross section data (either microscopic, barns, or macroscopic, cm^{-1}),
 - (3) DCX(m) and DCY(m), the x and y directional diffusion coefficients (default values if data not supplied $1/3\sigma_{tr}$);
multigroup data common to all materials,
 - (4) SP, χ_{pg} , the prompt fission spectrum;
along with data which need only be given for kinetics calculations,
 - (5) VEL, v_g , the group velocities (cm sec^{-1}),
 - (6) FER, the fission energy release for all materials (joules/fission),
 - (7) IGD, the number of delayed neutron groups,
 - (8) BETAD, β_i , the delayed neutron fractions per emitted neutron,
 - (9) DLAMDA, λ_i , the decay constants for the precursors (sec^{-1}), and
 - (10) SD(i), χ_{ig} , the delayed neutron fission spectrum.

The data may be read from the normal input stream (unit 1) or we may temporarily switch to

READ CARD LIB ON unit (usually 7), 1 and no more data on card.

(The data on 'unit' is terminated on end of file and need not only consist of cross section data. The second number may be 0 for deletion of print option.)

We will introduce each item in turn.

5.8.1 NG, number of energy groups

The number of groups, NG, is simply set with the data

NG = number of groups, e.g. NG=4

Data to follow must be consistent with the value specified here.

5.8.2 XSD, cross section data

The cross section data, either microscopic, barns, or macroscopic, cm^{-1} , XSD, is entered thus ...

XSD material name M (material number)

then data in CRAM layout (Hassitt 1962)

$(\sigma_{tr,g}, g=1,2,\dots,NG)$... transport
$(\sigma_{rem,g}, g=1,2,\dots,NG)$... removal (absorption + scattering)
$(\nu\sigma_{f,g}, g=1,2,\dots,NG)$... fission emission
$(\sigma_{scat,g' \rightarrow g}, g=1,2,\dots,NG), g'=1,2,\dots,NG)$... scattering given as outscatters from each group

followed by optionally as many as MAXS additional reaction cross sections

$(\sigma_{r1,g}, g=1,2,\dots,NG)$... reaction 1

$(\sigma_{r2,g}, g=1,2,\dots,NG)$... reaction 2

Notes:

- (1) $\sigma_{tr,g}$, $g=1,2,\dots,NG$ must be non-zero.
- (2) $\sigma_{scat,g\rightarrow g}$, $g=1,2,\dots,NG$, the self scatter entries of the scattering matrix, are set to zero by POW.
- (3) The additional reaction cross sections may be for any reactions required by the user for EDIT purposes (Section 5.26). However, the AUS scheme requires the reactions to be
 - reaction 1 = σ_p , the potential scattering cross section (for inclusion of card data in resonance theory calculations),
 - reaction 2 = σ_{tot} , the total cross section,
 - reaction 3 = σ_f , the fission cross section,
 - etc. (Appendix A).

As an example of the data we may have

```

NG=4
XSD FUEL M(1)
1.54481-1 3.6863-1 9.02355-1 2.00955
9.41612-2 6.02354-2 6.81026-1 1.12777-1
3.73274-4 3.30167-3 3.96448-2 9.77554-2
0.0 9.37282-2 2*0.0
2*0.0 4.88109-2 8.75701-3
0.0 5.09412-3 0.0 6.48822-1
0.0 1.66342-7 4.77318-2 0.0

```

Mixing of materials, or conversion of microscopic data to macroscopic data, may be carried out subsequent to this primary input using the DEFN feature described in Section 5.12.

5.8.3 DCX(m) and DCY(m), directional diffusion coefficients

In the absence of user specification of directional diffusion coefficients the code takes the coefficients to be isotropic and given by

$$DCX(m) = DCY(m) = 1/(3 \sigma_{tr,g}), \quad g=1,2,\dots,NG,$$

where DCX(m) denotes the x-direction diffusion coefficients for material m given a group at a time, with a similar meaning for DCY(m). The user may, however, specify anisotropic values

DCX(m) = ($D_{x,g}$, $g=1,2,\dots,NG$), the x-directional diffusion coefficients,

DCY(m) = ($D_{y,g}$, $g=1,2,\dots,NG$), the y-directional diffusion coefficients,
for example

$$DCX(1) = 2.19, 0.9, 0.36, 0.16$$

Almost equivalently we may supply the data for r-z (cylinder) geometry

DCR(m) = ($D_{r,g}$, $g=1,2,\dots,NG$), the r-directional diffusion coefficients (=DCX(m)),

DCZ(m) = (D_{z,g}, g=1,2,...,NG), the z-directional diffusion coefficients (=DCY(m))
 - the only difference compared with the earlier data is that when DCZ is used
 the code also stores a transport cross section consistent with DCZ, namely

$$\sigma_{tr,g} = 1/(3D_{z,g}) .$$

Note: When using x-y (plane) geometry we may have 3 different directional diffusion coefficients for each material

- (1) D_{x,g}
- (2) D_{y,g}
- (3) 1/(3 σ_{tr,g}) which is used in a DB² type approximation for leakage in the z-direction (Section 5.13)

5.8.4 SP, prompt fission spectrum

The prompt fission spectrum, χ_{pg}, taken to be the same for all materials, is supplied as

SP followed by NG numbers of the group integrated fission spectrum χ_{pg}, which is later normalised by the code to unit sum. For example

SP 0.753564,0.246436,2*0

Notes:

- (1) When we are calculating the steady state conditions prior to a kinetics calculation and the delayed fission spectra (Section 5.8.10) are different to the prompt values, the code will use an equilibrium spectrum (Section 5.8.10). It is for this reason that the data to follow is placed in the present functional block.
- (2) Although physically the SP data need not be given after all the cross sections logically it is the last data of this functional block for purely steady state calculations.

5.8.5 VEL (kinetics), group velocities

Kinetics data for the average group velocities in cm sec⁻¹ is supplied trailing the keyword VEL thus ...

VEL = (v_g, g=1,2,...,NG),

for example

VEL 2.5+9,3.5+7,7.5+5,2.25+5

Mainly for use with the AUS system, where the average velocities of the library (in cm/10⁻⁸sec) are stored as the removal cross section of a material with name INV455B (Section 5.9), in the absence of any trailing data,

VEL (and no numeric data),

POW uses v_g = 10⁸/σ_{rem,g} (INV455B).

Note: If prior to a kinetics calculation a steady state calculation is carried out and the number of groups is collapsed (Section 5.24) an

appropriate way to obtain average velocities would be to average the material INV455B over the whole reactor. The short list feature above may then be used subsequently to pick up the reactor-averaged group velocities.

5.8.6 FER (kinetics), fission energy releases

In order to obtain reactor power for a kinetics calculation (Section 6.4) or for specialised EDITing (Section 5.26) the fission energy release (joules/fission) may be supplied for each material given in turn

FER = (f_m, m=1,2,...,MAXM).

For example we may have

FER 3.172-11,2*0

In the absence of any data being provided here the code takes

- (1) fissile materials, FER_m = SFER (default 3.172-11)
- (2) non-fissile materials, FER_m = 0.

Note: The array FER is used during the fission source calculation to bypass unnecessary computation on non-fissile materials (FER_m = 0). This need be of little concern for the user except that he should not set SFER=0.

5.8.7 IGD (kinetics), number of delayed groups

The number of delayed neutron groups, IGD (≤ MAXGD), is given simply as

IGD = number of delayed groups, e.g. IDG=6

Data to follow must be consistent with the value specified here.

Note: Kinetics calculations for prompt excursions may be carried out without delayed neutrons, IGD=0 (the default value).

5.8.8 BETAD (kinetics), delayed neutron fractions

The delayed neutron fractions per emitted neutron, β_i, are supplied thus

BETAD = (β_i, i=1,2,...,IGD),

for example

IGD=1

BETAD=6.4-3

Note: The total delayed neutron fraction

$$\beta = \sum_{i=1}^{IGD} \beta_i$$

is available as a weighting option for reactivity insertion (Section 6.5.2).

5.8.9 DLAMDA (kinetics), precursor decay constants

The decay constants of delayed neutron precursors (sec⁻¹), λ_i are entered

as

DLAMDA = (λ_i , $i=1,2,\dots,IGD$),

for example

DLAMDA=0.08

5.8.10 SD(i) (kinetics), delayed fission spectrum

The delayed neutron fission spectrum for a delayed group i producing neutrons in energy group g , χ_{ig} , is entered as

SD(i) = (χ_{ig} , $g=1,2,\dots,NG$)

and should be supplied for each delayed group, $i=1,2,\dots,IGD$. In order to simplify data presentation the following interpretation of short lists is adopted:

- (1) SD without any further data takes all the spectra to be given by the prompt values (SP)
- (2) SD(i) without any further data uses the last read immediately preceding SD data.

The minimal data here and the usual requirement for few group calculations, is then the lone word

SD

For many group calculations with delayed fission spectrum different from the prompt spectrum the user must select the fission spectrum required for EDITing (Section 5.24). This is because POW always uses an equilibrium spectrum

$$SP_g = \chi_{pg} (1-\beta) + \sum_{i=1}^{IGD} \chi_{ig} \beta_i$$

during the steady state flux calculation (when delayed data is supplied) and normally restores the fission spectrum, SP_g , to the prompt values, χ_{pg} . Management of which fission spectrum is being used is then the responsibility of the user. The required option is indicated to POW thus

NSD n (default value 0), where

	<u>Entry to START</u>	<u>Exit from START</u>	
<u>n</u>	<u>SP</u>	<u>SP</u>	<u>n</u>
0	prompt	prompt	0
1	prompt	equilibrium	3
2	restores	prompt	0
3	prompt from a previous step	equilibrium	3

Notes:

- (1) If available the equilibrium spectrum is used for a steady state

calculation and this is why some of the kinetics data needs to be entered at this stage.

- (2) Normalisation of the supplied data is irrelevant as the code normalises the spectra to unit sum prior to any calculation being carried out.

5.9 Library Group Data

Presently POW may obtain group data from one of the disk libraries:

- (a) a datapool of the AUS scheme already resonance shielded data possible prepared from the 127-group resonance parameter GYMEA library (Pollard and Robinson 1969), Appendix A,
- (b) the 26-group, 3-temperature resonance tabular ABBN library (Bondarenko 1964), Appendix B, and
- (c) the 16-group, 1-temperature resonance tabular Hansen-Roach (1961) library, Appendix C.

Card data and library data (for the same number of groups) may be used together and the potential scattering of data supplied from cards may be used in conjunction with library data to influence resonance absorption. Resonance absorption is calculated for a 2-region fuel-moderator model with the equivalence relation used in GYMEA (Chiarella 1969). The present library data does not include kinetics information - kinetics data must therefore be provided in card form (Section 5.8).

Data required to extract information from a library consists of the following:

- (1) XSD, the cross section data selection,
- (2) HOMOVR, the homogeneous volume ratios or homogeneous concentrations,
- (3) ALBAR, the 2-region resonance equivalence relations information, particular \bar{l} , the mean chord length through the fuel region (cm), and
- (4) READ LIB, the particular library required and this data initiates programme action.

The data should be given essentially in the indicated order.

We will introduce each item in turn.

5.9.1 XSD, cross section data selection

Cross sections may be obtained from an AUS XSLIB (Appendix A, B and C) using 2-region equivalent homogeneous resonance shielding. The effective potential scattering cross section for each material (including an allowance for resonance overlap) is calculated and the required cross section is obtained using both potential scattering ($\sqrt{\sigma_p}$) and temperature (\sqrt{T}) interpolation. We specify the required data thus:

XSD material name (optional), data source (optional), mod (optional)
M (material number)
 concentration (default 1.), homogeneous volume ratio (default 0.),
 temperature, K (default 300),

for example

XSD C M(7) 8.291-2

- where
- (1) material name, if given, must correspond to a material in the library, and if not given the material number then selects a library material in the corresponding library position (XSD M(8) selects C from the ABBN library, Appendix B),
 - (2) data source, if given, selects a particular entry for the named material (which may not be unique to the library) and if not given the library recommended data for the material (highest update number) is used,
 - (3) mod, if given, selects a corresponding library entry appropriate to a modification of data from (2) and if not given the library recommended data for the chosen material and data source is used,
 - (4) concentration (default 1.) is the weighting to be applied to the library data on exit from the library retrieval,
 - (5) homogeneous volume ratio (default 0.) is to be provided such that homogeneous concentration = (4)*(5) (that is if (4)=1 then (5)= homogeneous concentration) - see also Section 5.9.2, and
 - (6) temperature K (default 300) is the required material temperature (and a homogeneous average temperature is used if several temperatures are given for the one material using different XSD cards).

As a further example using the Hansen-Roach data (Appendix C) we might use

XSD U238,HANSEN,ORIG M(1) 0.04749,0.1005

XSD U235,HANSEN M(2) 3.425-4,0.1005

XSD D M(3) 0.06655,0.8995

XSD O M(4) 0.03328,0.8995

Note: Data required for a special $1/v$ -absorber (with 2200 msec^{-1} value of $10^8/2.2 \times 10^5$ (≈ 455) barns) obtained from the library entries for group-averaged velocities ($\text{cm}/10^{-8} \text{ sec}$) - mainly for use in kinetics calculations (Section 5.8.5) - is requested thus

XSD INV455B M(5)

5.9.2 HOMOVR, homogeneous volume ratios

The homogeneous volume ratios (or concentrations) are stored in the array

HOMOVR as each XSD card is encountered, so that for the example above we would have

HOMOVR(1)=0.1005, HOMOVR(2)=0.1005, HOMOVR(3)=0.8995 and HOMOVR(4)=0.8995.

We may however use standard type cards (for example

XSD U238 M(1) 0.04749)

and rely on the array HOMOVR to indicate the required quantities set thus, for example

HOMOVR=2*0.1005, 2*0.8995

In general following the XSD cards we may provide data trailing the keyword HOMOVR one word for each material (1,2,...,MAXM), which overwrites the default values set by the XSD data, or 0. if XSD is not provided.

The array HOMOVR is also to be used to specify the homogeneous volume ratios (or concentrations) for previously submitted data from cards or a previous read of a library, when the data influence on resonance absorption is considered to be important. Card data may have the ratio entered into the appropriate element of HOMOVR. We simply provide the same data as for a library material except we immediately trail the data with the cross sections as in the example

XSD C M(3) 1,0.8995 M(3) (note the underlined)

1.5028-1,3.44185-1,3.74146-1,3.63482-1

etc. In addition the cross sections are multiplied by the concentration (1 in the example above) as the data is stored away.

5.9.3 ALBAR, equivalence relation information

POW uses the 2-region resonance equivalence relation for fuel and moderator employed in GYMEA (Chiarella 1969) which is permitted to degenerate to 1 region for normal homogeneous calculations. In the absence of any user provided data here POW returns infinitely dilute cross sections from libraries with resonance tabulations (Appendix B and C) or previously shielded cross sections otherwise (Appendix A).

We provide the required data thus ...

ALBAR g,b,V $\bar{\lambda}_1, \bar{\lambda}_2, \dots, \bar{\lambda}_{\text{maxm}}$ (default values all 0., i.e. a homogeneous system),

where

- g = geometry indicator,
- 0 = slab,
- 1 = cylinder (hexagonal pitch),
- 1.5 = cylinder (square pitch),
- 2 = sphere;

- b = boundary condition indicator,
 0 = fully reflected system (i.e. a cell), otherwise ($\neq 0$) implies a reactor (cf. 0.71 used in geometry data, Section 5.15.1);
 V = homogeneous volume ratio of fuel (resonance absorber) region to total - if V=0 then HOMOVR(k_1) is used instead as indicated below;
 $\bar{l}_k = \begin{cases} \bar{l}(=4V/S), & \text{the mean chord length through the fuel region (cm) if} \\ & \text{M(k) is present in the fuel region,} \\ 0 & \text{, the M(k) is not in the fuel region, i.e. in the moderator.} \end{cases}$

Notes:

- (1) POW, unlike GYMEA, cannot approximately cope with more than 2 regions. Instead POW takes
 (a) $\bar{l} = \bar{l}_{k_1}$, 1st non-zero entry for which HOMOVR(k_1) $\neq 0$ and
 (b) V = HOMOVR(k_1) if V=0 is specified above.
 (2) A material (say ^{16}O) may be present in both fuel and moderator. We simply request data from the library twice as the example ...
 XSD 0 M(4) 0.03328,0.8995 (in moderator)
 XSD 0 M(5) 0.04102,0.1005 (in fuel)
 ALBAR...0,2.53,...

As a simple example we consider natural uranium rods on a regular hexagonal pitch in D_2O . Taking $\bar{l} = 2.53$ cm the data might consist of the following ...

```
XSD U238 M(1) 0.04749
XSD U235 M(2) 3.425-4
XSD D M(3) 0.06655
XSD 0 M(4) 0.03328
HOMOVR 2*0.1005,2*0.8995
ALBAR 1,0,0.1005 2*2.53,2*0
READ LIB ON 8 - as discussed in the next Section.
```

5.9.4 READ LIB, library selection

POW, as run under the AUS scheme (Appendix A), has two main FORTRAN units from which cross section libraries may be read, they are

- (1) 8, for standard resonance tabular libraries (Appendix B and C),
- (2) 10, for a scratch library possibly prepared by GYMEA (Appendix A).

The selection of which standard library is required is made using a feature of the AUS catalogue procedure. We have

```
// EXEC AUS,LIB=HANSEN or simply // EXEC AUS
      for the Hansen-Roach library, and
// EXEC AUS,LIB=ABBN
      for the ABBN library.
```

Cross sections for the previously selected materials (Section 5.9.1) shielded according to the indicated resonance equivalence data (Section 5.9.2 and .3) are then sought when the following data is encountered

READ named LIB ON unit, sop

where

named (say HANSEN) is an optional name for user information (otherwise ignored by POW unless CARD see Section 5.8),
 unit (8 or 10) selects the required FORTRAN unit, and
 sop (default value 1) selects the fission spectrum weighting as discussed below (note 2).

Notes:

(1) Data for at most MAXS additional reactions of the AUS XSLIB set (Appendix A), ignoring anisotropic diffusion coefficients, are returned in the order ...

- (i) σ_p , potential scattering,
- (ii) σ_{tot} , total
- (iii) σ_f , fission,

If anisotropic diffusion coefficients are available they are stored in the appropriate elements of DCX(m) and DCY(m) - Section 5.8.3.

(2) POW only permits one prompt fission spectrum (SP) which is taken to be an average for all fissile materials of importance. With the Hansen-Roach library the particular weighting required for each material is irrelevant since all materials have the same fission spectrum. However, the ABBN library has different spectra for different materials. The data item sop above selects an approximate weighting thus

- (i) sop=0, SP data not entered into core,
- (ii) sop=+G (default 1)

$$SP_g = \sum_{m=1}^{\text{maxm}} v\sigma_{f,G}^{(m)} \text{HOMOVR}^{(m)} \chi_{p,g}^{(m)},$$

that is each spectrum is weighted by a particular group (G) homogeneous fission emission cross section for each material (say 1 for fast reactor studies, NG for thermal reactor studies)

- (iii) sop= - G

as above except that the sum is added to the already existing SP data (presumably set up from a previous read of the library). Here we should note that normalisation of SP_g to unit sum is not carried out until

- (a) just prior to a flux calculation START (Section 5.23), or
 - (b) just prior to an EDIT calculation (Section 5.24).
- (3) When reading two different libraries the influence of materials of the first library on resonance materials in the second library is correctly maintained through in-core cross sections provided the same resonance material is not in both libraries.
- (4) POW may also write AUS-type libraries (Section 5.24.5).

5.10 P_n ($n \neq 0$) Data

Although POW makes no allowance for scattering matrices other than P_0 we may include P_1 weighted matrices, etc., as data for separate 'materials'. These 'materials' may not appear in a POW calculation, however, they may be group collapsed for use by other AUS modules.

P_n ($n \neq 0$) data is given in either (1) card form or (2) as a request for library data. In either case we follow the data requirements of the appropriate Section ((1) = Section 5.8.2 and (2) = Section 5.9.1) for a normal material except P_n ($n \neq 0$) data is indicated with the name DITTO and must be for consecutive materials. For example

XSD HPOL,HANSEN M(1) 0.066

XSD DITTO,P₁ M(2) 0.066

and if P_2 data were available, and is required, we would supply further

XSD DITTO,P₂ M(3) 0.066

Note: When using AUS XSLIB data with P_n ($n \neq 0$) data effectively we must address each material by name, that is, we cannot use the purely positional type request (Section 5.9.1)

XSD M(1) 0.066 XSD M(2) 0.066

since P_1 data does not exist in the library as a separate material.

5.11 Cross Section Modification

A feature is available to MODIFY cross sections (either previously read from cards or obtained from disk). We use the data

XSD MODIFY M (material number) and optionally {f M (same material number)
when the default value f=1 is
not satisfactory}

then numbers, one corresponding to each cross section,

($x_{tr,g,g=1,2,\dots,NG}$), ($x_{abs,g,g=1,2,\dots,NG}$), ($\forall x_{f,g,g=1,2,\dots,NG}$),

(($x_{scat,g' \rightarrow g,g=1,2,\dots,NG}$), $g'=1,2,\dots,NG$), followed by as many as MAXS optional additional reactions with corresponding numbers

($x_{reac1,g,g=1,2,\dots,NG}$), ($x_{reac2,g,g=1,2,\dots,NG}$), etc.

We note that the second group of numbers, $x_{abs,g}$, relates to absorption rather

than removals. The procedure adopted is the following, where a prime denotes the modified data.

$$(1) \quad \sigma'_{\text{abs},g} = \sigma_{\text{rem},g} - \sum_{g \neq g'} \sigma_{\text{scat},g' \rightarrow g}, \text{ and this becomes reaction 2}$$

(2) If $x=0$ then $\sigma' = \sigma$, i.e. the cross section is unaltered;

$$\text{otherwise } x' = \begin{cases} x & \text{if } |x| > 10^{-40} \\ 0 & \text{if } |x| \leq 10^{-40} \end{cases}$$

and the data modification carried out is

$$f \begin{cases} \leq 0 & , \quad \sigma' = |f| \sigma + x' \\ > 0 & , \quad \sigma' = f \sigma x'; \end{cases}$$

($\text{DCX}'_g = \text{DCY}'_g = 1/3 \sigma'_{\text{tr},g}$ if a transport cross section is modified).

$$(3) \quad \sigma'_{\text{rem},g} = \sigma'_{\text{abs},g} + \sum_{g \neq g'} \sigma'_{\text{scat},g' \rightarrow g}, \text{ restoring reaction 2 to removals.}$$

The main purpose of the feature is to enable the effect of data perturbations to be studied and this becomes particularly simple using the option $f=1$ whereby we multiply the data by selected factors x (e.g. 1.01 for a 1% increase).

As an example say we require to increase absorption for material M(2) in group 1 (of 16-group data) by 1% we could use the data

```
XSD MODIFY M(2) 16*0,1.01,15*0,272*0
```

5.12 Mixing Rules

Mixing of cross section data may be required for example to form data for mixtures (and components) both microscopic and macroscopic. The data is of the form

DEFN material name M (material number for material being defined) =

M (material number 1), material 1 concentration

M (material number 2), material 2 concentration, etc.

For example, say we have microscopic cross section data available for M(1) and M(2) as illustrated

```
XSD H M(1), etc.,
```

```
XSD O M(2), etc.,
```

then we might define

```
DEFN H2O M(3) = M(1) 2 M(2) 1
```

```
DEFN WATER M(4) = M(3) 0.033
```

Let I_d denote the material number for the material being defined

I_1 denote the material number 1, etc.,

then the cross sections are built up in the following way.

(i) If $I_d \neq I_1$

then the cross sections are initially cleared and the cross sections of material 1 (including any additional reactions) multiplied by the

concentration of material 1 are added to the cross sections required. Otherwise the existing cross sections are multiplied by the concentration of material I_1 .

- (ii) Similarly for the 2nd material, except that the cross sections are no longer cleared, and so on.

The mixture diffusion coefficients for both x (or r) and y (or z) directions, $D_{x,g}$ and $D_{y,g}$ are obtained from the constituent diffusion coefficients using $1/D_{x,g}$ and $1/D_{y,g}$ in place of cross sections in the rules given above.

Using the above rules we may abbreviate our examples to

```
DEFN H2O      M(3) = M(1) 2 M(2) 1
```

```
DEFN WATER   M(3) = M(3) 0.033
```

or even

```
DEFN WATER   M(3) = M(1) 2 M(2) 1 M(3) 0.033
```

Later when we come to provide layout data for the materials that constitute the reactor (Section 5.15.4) we will obviously only be concerned with those materials that have macroscopic data available. Microscopic data may however, be required for EDIT purposes (Section 5.24). We shall note that the mixing process is normally carried out immediately the DEFN data is encountered, however, the process may be carried out as part of a criticality SEARCH - Section 5.17.1.

5.13 DB² Leakage

Inclusion of DB² leakage in the removal cross section for each material

$$\sigma'_{rem,g} = \sigma_{rem,g} + B^2 / (3\sigma_{tr,g})$$

is a standard way of making at least approximate allowance for leakage of neutrons in directions not otherwise accounted for in the calculation to be undertaken. (For zero dimensional calculations all leakage is included this way.) Considering we may require B² to be such that the reactor multiplication k=1 (a criticality SEARCH Section 5.17) we first introduce DB² leakage data required for this type of calculation.

We specify DB² leakage data to POW thus ...

```
BSQ (additional reaction number) = {set L of material numbers to have leakage
                                     added},
```

```
{set M of material numbers for required transport cross sections},
```

```
{set N of required bucklings, B2},
```

where the selected additional reaction of the 1st material of set L has stored in it the 1st B² of set N divided by 3 times the transport cross section of the 1st material of set M and so on. For example, we may use the data (provided MAXS (Section 5.6) ≥ 3)

$$\text{BSQ}(3) = \underbrace{1,2,3,4}_L \quad \underbrace{1,2,3,4}_M \quad \underbrace{1.-3,1.-3,1.-3,1.-3}_N$$

Correspondence of 1st Items of Data

which may be punched more compactly

$$\text{BSQ}(3) = 1(1)4 \quad 1(1)4 \quad 4*1.-3$$

Further we may add the leakage cross section to data already given for the selected additional reaction by specifying data as above except with the additional reaction number set negative, e.g.

$$\text{BSQ}(-3) = 1(1)4 \quad 1(1)4 \quad 4*1.-3$$

When we simply require the leakage cross section to be added to the removal cross section, probably the most usual requirement, we indicate this requirement by specifying zero for the additional reaction number, e.g.

$$\text{BSQ}(0) = 1(1)4 \quad 1(1)4 \quad 4*1.-3$$

Notes:

- (1) The additional reaction number \leq MAXS set in the PRELUDE (Section 5.6).
- (2) We may also specify group dependent bucklings for each material. These bucklings may also be calculated by POW. We defer further consideration of this feature until Section 5.25.1.
- (3) After a criticality SEARCH (Section 5.17) we may require the critical leakage to be permanently associated with the removal cross section rather than simply as an additional reaction added only during the critical SEARCH. We achieve this using short data, BSQ(-additional reaction number) and no other trailing data. The removal cross section of each material in the previously specified set L then has added the cross section corresponding to the additional reaction number. Sets M and N are ignored. For example, we may use
BSQ(-3)

5.14 Poison Absorption

Inclusion of poison absorption in the removal cross section of each material

$$\sigma'_{\text{rem},g} = \sigma_{\text{rem},g} + \sigma_{a,g} \text{ (poison)}$$

is a possible way of making a reactor just critical (Section 5.17.1). The feature is exactly analogous to DB^2 leakage of the previous Section and data is specified in a similar way except that the keyword ABS is used instead of BSQ. For example we may use the data

$$\text{ABS}(3) = 1(1)4 \quad 4*5 \quad 4*1.-3$$

where M(5) is the poison material and 1.-3 is the concentration.

5.15 Geometry Data

Geometry data is required to specify:

- (i) type of geometry -
 - 2D - (a) slab (x,y)
 - (b) cylinder (r,z);
 - 1D - (a) slab x (y degenerated to 1 point),
 - (b) cylinder r (z degenerated to 1 point),
 - (c) sphere r;
 - 0D - (a) slab (z reduced to 2 points),
 - (b) cylinder (r reduced to 2 points),
 - (c) sphere (r reduced to 2 points);
- (ii) width of mesh spacing (cm);
- (iii) boundary conditions on the flux, ϕ_g -
 - (a) reflective (zero current),

$$\frac{\partial \phi_g}{\partial n} = 0 \text{ for each group } g,$$

where n = outward normal;

- or (b) reactor (zero flux on extrapolated boundary)

$$D_{n,g} \frac{\partial \phi_g}{\partial n} + \frac{\phi_g}{3d} = 0 \text{ for each group } g,$$

where d = extrapolation distance in equivalent transport mean free paths (usually 0.71 is used), and

- (iv) region layout.

Card data may be provided using the following -

- (1) XM or RM, x or r mesh spacing,
- (2) YM or ZM, y or z mesh spacing,
- (3) RM(SPHERE), spherical mesh spacing,
- (4) REG, region layout;

disk data from an AUS GEOM library is entered with the words

- (5) READ REG, for complete geometry data,

and is written with the words

- (6) WRITE REG of complete geometry data.

5.15.1 XM or RM, x or r mesh spacing

The x mesh data is specified thus

XM d_L, δx_1 , $\delta x_2, \dots, \delta x_{NXMI}$, d_R

where the keyword XM sets the (x,y) geometry option,

- d_L denotes the left hand extrapolation length in transport mean free paths except that ∞ is replaced by 0 for a zero current boundary condition,
- δx_1 denotes the width of the 1st mesh interval in cm,
- δx_2 denotes the width of the 2nd mesh interval in cm,
- \vdots
- δx_{NXMI} denotes the width of the NXMI and last mesh interval in cm, and
- d_R denotes the right hand extrapolation length in transport mean free paths where again ∞ is replaced by 0.

The edge flux is calculated by POW for reactions about a mesh point (rather than at the centre of a mesh interval) and therefore the number of x mesh points is

$NXM = NXMI + 1$ (note the extra one).

Data for (r,z) geometry is supplied in the same style as above, namely

RM 0, δr_1 , $\delta r_2, \dots, \delta r_{NXMI}$, d_R

where the notation is obvious.

An example of the data follows from the MOATA run of Section 5.3 -

$XM = 0, 5 * 4.572, 0.635, 5 * 2.968, 0.635, 10 * 5, 0.71$

Notes:

- (1) Reflective (zero current) conditions require d_L or $d_R = 0$.
- (2) Reactor (zero flux on extrapolated boundary) conditions usually require d_L or $d_R = 0.71$, although 1.-4 may be used to force the condition $\phi_g = 0$ on the actual boundary.
- (3) The choice of mesh spacing is somewhat ill defined although the following ideas provide some very rough guidelines:
 - (a) physical regions, unless homogenised with neighbouring regions, need to have their boundaries along mesh intervals;
 - (b) large mesh spacing (2 or 3 transport mean free paths for 'important' neutrons) should be avoided as estimation of spatial variation becomes inadequate,
 - (c) small mesh spacing (1/10 transport mean free path for 'important' neutrons) should be avoided as convergence of the iterative solution is needlessly slowed down.
- (4) OD problems are tackled by reducing the solution to 2 points for a fully reflected system using the data

$XM = 0, 1, 0$, or

$RM = 0, 1, 0$

along with corresponding YM or ZM data (next Section).

5.15.2 YM or ZM, y or z mesh spacing

The y or z mesh data are specified in much the same way as the x mesh data.

We have

YM $d_B, \delta y_1, \delta y_2, \dots, \delta y_{NYMI}, d_T$

where the keywords YM and ZM are equivalent

d_B denotes the bottom extrapolation length in transport mean free paths except that ∞ is replaced by 0,

$\delta y_1, \delta y_2, \dots, \delta y_{NYMI}$ are mesh interval widths in cm, and

d_T denotes the top extrapolation length in transport mean free paths where again ∞ is replaced by 0.

The number of y mesh points NYM is then

$$NYM = NYMI + 1$$

and the (x,y) or (r,z) plane, is divided into cells by extending lines perpendicular to the axes from the given mesh points. The corners of all cells (the intersection of all mesh lines) then become the mesh points at which the flux is to be calculated. The total number of mesh points NXY is then $NXY = NXM * NYM$.

The MOATA run of Section 5.3 again provides us with an example of the type of data we use -

YM = 0,5*5.064,0.636,10*2.984,0.71

Notes:

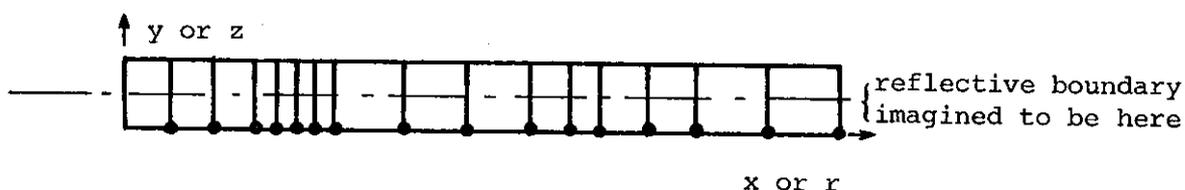
- (1) 1D problems are degenerated to y or z point with the fully reflective data

YM = 0,2,0, or

ZM = 0,2,0 (anything other than 2 will do if the volume is not important).

In the absence of special coding the above data would specify 2 points, however the degeneracy to 1 point is particularly important as the inner line solution is thereby exact without any line relaxation.

The 1D solution points are as sketched ...



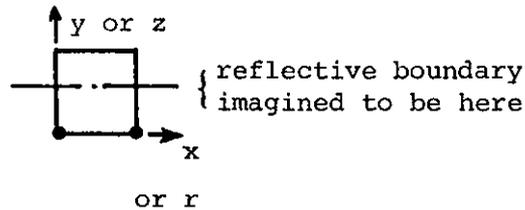
- (2) OD problems are 1D problems reduced to 2 x or r points with the fully reflective data

$XM=0,1,0$ or $RM=0,1,0$, and

$YM=0,2,0$ or $ZM=0,2,0$.

No special coding is introduced to degenerate the problem to 1 point.

The OD solution points are as sketched ...



5.15.3 RM(SPHERE), spherical mesh spacing

The r(spherical) mesh data is given with a single specification

$RM(SPHERE) \ 0, \delta r_1, \delta r_2, \dots, \delta r_{NXMI}, d_R,$

where

δr_1 denotes the radius of the 1st mesh interval in cm,

δr_2 denotes the thickness of the 2nd mesh interval in cm,

δr_{NXMI} denotes the thickness of the NXMIth and last mesh interval in cm
and,

d_R denotes the right hand extrapolation length in transport mean free paths, where again ∞ is replaced by 0.

An example of the data is afforded by GODIVA, a critical ^{235}U sphere of radius 8.71 cm (Argonne National Library 1963). We might use the data

$RM(SPHERE)=0,10*0.871,0.8$

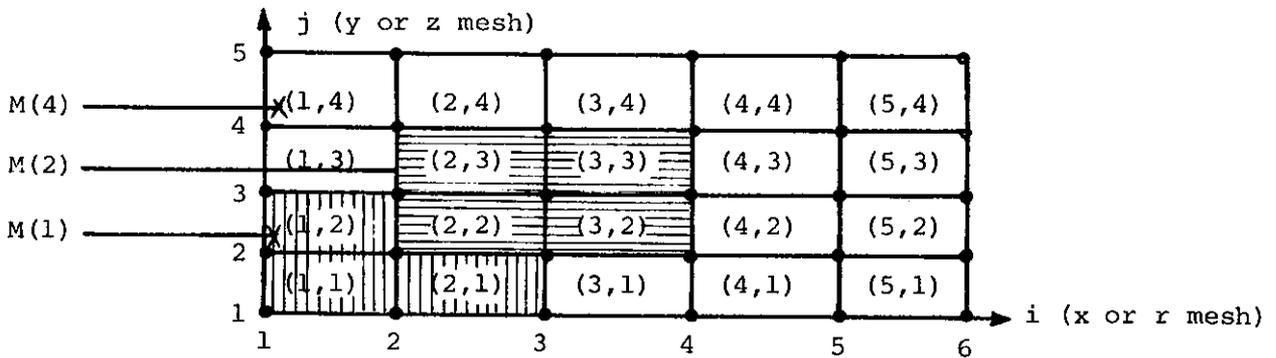
where here the extrapolation distance of 0.8 (instead of the usual 0.71) transport mean free paths is found to give better agreement with an equivalent transport calculation.

Note: OD calculations may be specified simply as a reflective sphere with the data

$RM(SPHERE)=0,1,0.$

5.15.4 REG, region layout

The layout of constituent materials of the reactor in mesh cells is specified as follows. We number the cells as illustrated in the sketch (as for a transposed upside down matrix)...



$$\text{cf. } \Gamma^T = \begin{pmatrix} l_{14} & l_{24} & l_{34} & l_{44} & l_{54} \\ l_{13} & l_{23} & l_{33} & l_{43} & l_{53} \\ l_{12} & l_{22} & l_{32} & l_{42} & l_{52} \\ l_{11} & l_{21} & l_{31} & l_{41} & l_{51} \end{pmatrix}$$

where L is the layout matrix with elements l_{ij} stored in the usual way. We then use a succession of items of data of the type

REG MX i_1, i_2, \dots, i_I MY j_1, j_2, \dots, j_J M(m)
 or... MR... MZ...

which fill up elements of a layout matrix L

such that $l_{ij} = m$ if $i \in \{i_1, i_2, \dots, i_I\}$ and $j \in \{j_1, j_2, \dots, j_J\}$.

The keyword REG need not be repeated for each such data item when given one after the other and MX and MY data need not be supplied unless the data is changed.

As an example, say we require the layout to be specified for the reactor illustrated earlier. We could start this layout using

REG MX 1(1)5 MY 1(1)4 M(4)

and we would have

$$\Gamma^T = \begin{pmatrix} 4 & 4 & 4 & 4 & 4 \\ 4 & 4 & 4 & 4 & 4 \\ 4 & 4 & 4 & 4 & 4 \\ 4 & 4 & 4 & 4 & 4 \end{pmatrix}$$

If the above data were followed by

(REG)-optional MX 1,2 MY 1,2 M(1)

we would then have

$$\Gamma^T = \begin{pmatrix} 4 & 4 & 4 & 4 & 4 \\ 4 & 4 & 4 & 4 & 4 \\ 1 & 1 & 4 & 4 & 4 \\ 1 & 1 & 4 & 4 & 4 \end{pmatrix}$$

and finally

(REG)-optional MX 2 3 MY 2 3 M(2)

would give the required layout

$$\Gamma^T = \begin{pmatrix} 4 & 4 & 4 & 4 & 4 \\ 4 & 2 & 2 & 4 & 4 \\ 1 & 2 & 2 & 4 & 4 \\ 1 & 1 & 4 & 4 & 4 \end{pmatrix}$$

Notes:

- (1) Clearly no part of the reactor should remain unfilled with material.
- (2) 1D data specifications do not require MY (or MZ) information, for example
REG MX=1(1)5 M(1) MX=6(1)10 M(2)
- (3) OD data specifications require only the material number, for example
REG M(3)

5.15.5 READ REG, for complete geometry data

Geometry data of the AUS scheme (Appendix A) is read in POW with the data
READ REG ON 6

All geometry information (Sections 5.15.1 to 5.15.4) is thereby made available to POW from another module of AUS on POW's FORTRAN unit 6.

As an extension of the AUS GEOM library, POW can have several different geometries for different jobs held in the one library. We recall named entries with the data

READ NAME REG ON 6,1,

where the trailing 1 selects the option that reads through the entire library and the last appearing data identified by NAME is used. If on the other hand the trailing number is -1 then only the layout matrix is read. (This latter feature is mainly for use with complicated EDITS, Section 5.24, where elements of the layout matrix are changed as part of the EDIT requirement.)

5.15.6 WRITE REG of complete geometry data

Geometry data of the AUS scheme (Appendix A) is written in POW with the data

WRITE REG ON 6

which writes the data on FORTRAN unit 6.

As an extension of the AUS GEOM library, POW can have several different geometries for different jobs held in the one library. We write named entries with the data

```
WRITE NAME REG ON 6,1,
```

where the trailing 1 selects the option that writes the NAMED data at the end of the library.

Note: The first NAMED data required in the library must be forced to be written at the beginning of the library with the data

```
WRITE NAME REG ON 6
```

5.16 Calculation Type

We indicate the type of calculation to be pursued later using the data

$$\underline{\text{CALC}} = \left\{ \begin{array}{l} \text{REAL} \quad \text{EIGENV} \\ \text{ADJOINT} , \text{SOURCE} , \text{PROBLEM} \\ \quad \quad \text{KINETICS} \end{array} \right\} ,$$

where we select the required options (except ADJOINT, KINETICS) from the above set. The default values correspond to the normal code requirement

```
CALC=REAL,EIGENV,PROBLEM
```

and need therefore not be specified further. The third word is provided to enable a user to give two unique job identifying names (POW jobname and CALC, this) to a flux dump (Section 5.23), particularly one shared with other users and may well be omitted.

Notes:

(1) If storage is made available for the fixed source array FSCE during an adjoint eigenvalue calculation (MAXF=1 in the PRELUDE-Section 5.6) then the adjoint solution is stored in the fixed source array. We may then use both the real and adjoint flux concurrently for EDIT purposes (Section 5.24).

(2) Even if we are intending to pursue a kinetics calculation we would normally require a steady state calculation

```
CALC=REAL,EIGENV
```

to be carried out first. The calculation type

```
CALC=REAL,KINETICS
```

would then be specified as data after the steady state calculation (i.e. after the START card, Section 5.23).

5.17 Criticality Search Data

Presently three types of criticality SEARCH are available. (These vary an eigenvalue λ , which normally multiplies some physical quantity, to achieve a required effective multiplication $k=k_{\text{reqd}}$, usually 1.) The searches are

controlled by the routines SUB n , $n=1,2,\dots,9$, where only the first three have so far been dedicated to specific tasks. (An independently informed user may write his own routines in FORTRAN and load them with the temporary update feature briefly introduced in Section 5.5.) We have

- (1) SUB1 - a general concentration adjustment routine which may make simple data changes associated with a poison search to more complicated data changes associated with materials forming part of mixtures,
- (2) SUB2 - a general mesh width adjustment routine which may make simple changes of scale of all mesh intervals to more complicated data changes associated with differential and coupled adjustment,
- (3) SUB3 - a general region adjustment routine which may move material in or out of regions of the reactor either in single channels or coupled channels according to a specified schedule.

Before we detail the way we use each of these subroutines we first introduce

- (i) data to select the required SEARCH option, and
- (ii) additional data required by the search subroutines.

(i) The main data item is associated with effective multiplication parameters -

$$\text{SEARCH}(x) = k_{\text{reqd}}, k_{\text{acc}}, k'_{\text{acc}}, h$$

where

- x is the option parameter that sets the required search (default value 0.) and is detailed below,
- k_{reqd} is the required effective multiplication (default value 1.),
- k_{acc} is the required accuracy in k_{reqd} such that for convergence $|k - k_{\text{reqd}}| \leq k_{\text{acc}}$ (default value 2.-3),
- k'_{acc} is the required accuracy in k_{reqd} before source extrapolation is permitted (default value 1.-2) - not used with all options, and
- h is an exponent used in the interpolation - extrapolation process such that chord approximation of k^h as a function of critical eigenvalue λ is as reasonable as possible ($h=-1$. is best for variation of purely absorbing materials (poison search): default value 1.).

The option parameter x is of the form

$$x = \text{SI.D}_1\text{D}_2$$

where

- S = sign
 I = integer part of x ,
 D_1 = 1st fractional digit

and D_2 = 2nd fractional digit

Let

$d = D_2$ if $D_1=0$, otherwise $d=D_1$

then provided $x \neq 0$ the SEARCH subroutine called is SUB d . For example SEARCH (-0.02) sets a call to be made to SUB2 at convenient stages of the calculation. If we use an option parameter of $x=0$ then no SEARCH is carried out (the default option).

The sign of x is used to specify the required strategy to be used in updating λ :

S=+ve -

λ updating occurs every fixed number of outer iterations regardless of the source convergence (set with ℓ_1 - Section 5.17.0)

S=-ve -

λ updating occurs after a minimum source convergence (set with ACCFO - Section 5.20.1).

If S=+ve, extrapolation of the fission source occurs concurrently with λ changes and hence this strategy should only be used when the data changes are minimal - for example with a poison search (Section 5.17.1). If S=-ve, extrapolation of the fission source does not occur unless $|k - k_{\text{reqd}}| < k'_{\text{acc}}$ and hence this strategy is suitable when data changes are drastic - for example with a critical size search (Section 5.17.2).

The 1st fractional digit of x is given the meaning:

$D_1 = 0$ - λ_{n+1} or λ_{n+1}^* (AEIGEN) is calculated for use in SUB d

$D_1 \neq 0$ - no adjustment is made to λ and presumably the user is adopting his own computational strategy for λ .

The integer part of x, I , is available for use by some of the SEARCH subroutines.

For most uses we find that the simple specification, for example, SEARCH(-0.02)

is all we need enter for this keyword as the default values are otherwise usually satisfactory.

(ii) In addition to SEARCH data all the presently available routines require extra data to be entered in the user's work area array (as detailed for each routine later)

WSEA (w_k , $k=1,2,\dots$ to a maximum of MAXW)

and we must remember to assign sufficient storage for this array in the PRELUDE, Section 5.6 (MAXW=200 is the default value). (A fixed point array sharing the same storage, MSEA, is also available, but POW itself makes no reference to the array.)

Note: If we intend to pursue a normal effective multiplication calculation after a search calculation we must later turn off the search with the data SEARCH(0)

5.17.1 Additional infrequently required search data

The data item associated with eigenvalue parameters is

FSEA $\lambda_L, \lambda_1, \lambda_2, \lambda_U, d$

where

λ_L is a lower limit to λ such that $\lambda < \lambda_L$ will cause programme termination (default value 1.-2)

λ_1 is a 1st estimate of λ (default value 1.)

λ_2 is a 2nd estimate of λ (default value 1.1)

λ_U is an upper limit to λ such that λ_U will cause programme termination (default value 1.+2), and

d is an extrapolation limit parameter (default value 3.) such that if λ_n and λ_{n-1} are consecutive estimates of λ , λ_{n+1} is the next estimate and m is the index such that

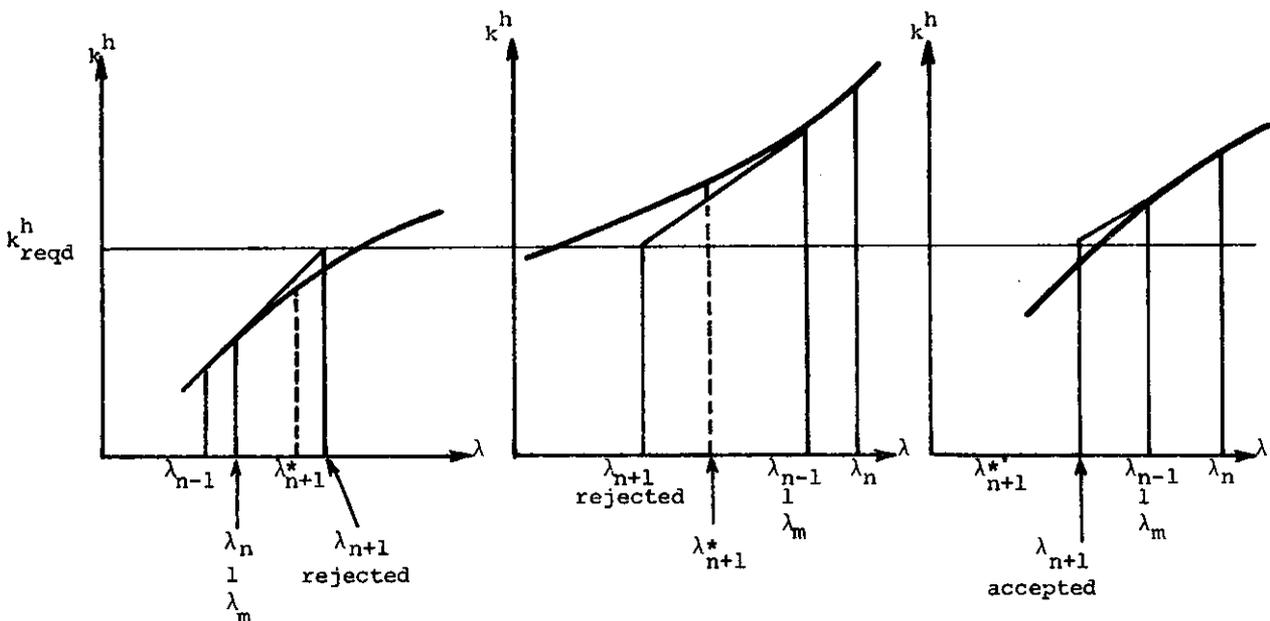
$$|\lambda_{n+1} - \lambda_m| = \min (|\lambda_{n+1} - \lambda_n|, |\lambda_{n+1} - \lambda_{n-1}|)$$

then if $|\lambda_{n+1} - \lambda_m| < d|\lambda_n - \lambda_{n-1}|$

we accept λ_{n+1} , otherwise we take

$$\lambda_{n+1}^* = \lambda_m + d \text{ sign} (\lambda_{n+1} - \lambda_m) |\lambda_n - \lambda_{n-1}| .$$

An illustration (with $d=2.$) best shows the idea here.



The reason for using the simple chord method to estimate a critical value of λ is that during early stages of the calculation we are working with inaccurate values of k resulting from only partially converged fluxes and hence more complicated interpolation or extrapolation is unlikely to be better (and may well be worse). The hesitant extrapolation process described earlier would be desirable no matter what process we use for estimating λ_{n+1} . The process does permit extensive extrapolations after several goes, however, since we could have, for example,

$$\lambda_{n+1}^* = \lambda_2 + d (1+d+d^2+\dots+d^{n-2}) |\lambda_1 - \lambda_2|$$

$$(\lambda_5^* = \lambda_2 + 39|\lambda_1 - \lambda_2| \text{ when } d = 3) \quad .$$

(We see here the desirability of not using λ_1 and λ_2 too close together unless they are good estimates for the critical value of λ .)

Finally the last additional data for use with SEARCH is

LSEA ℓ_1, ℓ_2

where

ℓ_1 is the minimum number of outer iterations between consecutive estimates of λ (default value 3), and

ℓ_2 is the number of estimations of λ before fresh inner relaxation factors ($\omega_g, g 1, 2, \dots, NG$) are sought (default value 3).

5.17.2 SUB1 - a general concentration adjustment routine

The search subroutine SUB1 is used to adjust concentration of materials in selected parts of the reactor, either

(i) poison materials (materials with absorption only and set with ABS feature - Section 5.14), or

(ii) general materials.

(i) A poison search is set using the data

SEARCH (I.01) (other data supplied if any non-default values required)

where I is an additional reaction number, and a +ve search strategy is satisfactory (Section 5.17).

For example we may have

XSD FUEL M(1) ...

XSD MOD1 M(2) ...

XSD MOD2 M(3) ...

XSD POISON M(4) ...

and we may require MOD1 to be poisoned to achieve criticality ($k_{\text{reqd}}=1$).

We would use the data, say,

ABS(3) = 2 4 1.-3 (Section 5.14 and we note that MAXS must be set to at least 3 in the PRELUDE - Section 5.6)

SEARCH(3.01) 1. 2.-3 1.-2 -1.

All poison concentrations are initially set as given with the ABS data (1.-3 in the example) however the concentrations need not all be adjusted at the same rate in order for criticality to be achieved. Associated with each material we must supply a weight w_k thus

WSEA $w_1, w_2, \dots, w_{MAXM}$

then if c_k denotes the initial concentration of poison associated with $M(k)$ and $c_k(\lambda)$ denotes the adjusted concentration of poison associated with $M(k)$ corresponding to an eigenvalue λ ,

we have

$$c_k(\lambda) = c_k \{1 + (\lambda - 1)w_k\}, \quad k=1, 2, \dots, MAXM .$$

For example we would therefore also need the data

WSEA 0,1,2*0

Note: After the SEARCH is carried out (following a START or RESTART card - Section 5.23) the concentration of poison corresponding to additional reaction I is built into the cross section corresponding to additional reaction I. If we require the poison to be permanently associated with the material (that is associated with σ_{rem}) we should follow the START (or RESTART) card with the data

ABS(-I)

as described in Section 5.13. We need to be aware of this point when interpreting output from the EDIT subroutines (Section 5.24).

(ii) A general search on material concentration (including fissionable materials) is set using the data

SEARCH(-0.01)

WSEA $w_1, w_2, \dots, w_{MAXM}$

where here the concentration of materials (not just a particular reaction as for (i)) are adjusted using the same rules as for (i) with $c_k = 1$, that is

$$c_k(\lambda) = \{1 + (\lambda - 1)w_k\}, \quad k = 1, 2, \dots, MAXM$$

For example if we use the data

SEARCH(-0.01)

WSEA 0,1,2*0, say, for 4 materials

and the critical eigenvalue is, say, λ_c then all cross sections of material 2 would be multiplied by λ_c and all diffusion coefficients of material 2 would

be divided by λ_c at the termination of the calculation.

In addition to the above we may adjust the concentration of materials that are subsequently mixed to form material constituting the reactor. We do this by trailing the WSEA card with special DEFN cards (Section 5.12) which rather than produce the mixtures immediately, add data to the WSEA array (elements W_{MAXM+1} , W_{MAXM+2} , ..., to a maximum of W_{MAXW} , one element for each number given with DEFN) for mixing to be carried out during the SEARCH calculation. The cards take the form

```
DEFN MIX WSEA M(k)= ...
```

where the underlined is the only difference from a 'normal' definition.

For example, say we require the critical ^{235}U enrichment of an essentially natural uranium reactor. (The microscopic cross section changes resulting from different resonance shielding, for example, are ignored.)

We could use the data

```
XSD U235 M(1) ... (microscopic data)
```

```
XSD U238 M(2) ... (microscopic data)
```

```
XSD MOD M(3) ... (microscopic data)
```

```
DEFN URANIUM M(4) and no more data (this simply enables M(4) to be used with
the REG layout card to follow)
```

```
DEFN ADDU M(5) = M(1) 1 M(2) -1
```

```
XM... YM... REG MX... MY... M(4), etc.
```

```
SEARCH(-0.01)
```

```
WSEA 4*0,1,0,...(MAXM elements must be supplied)
```

```
DEFN URANIUM WSEA M(4) = M(2) 1 M(5) 0.007 M(4) 4.78-2
```

The composition of uranium during the actual critical search calculation is then

$$c_4(\lambda) = \{(1-0.007\lambda) ^{238}\text{U} + 0.007 \lambda ^{235}\text{U}\} 0.0478$$

(We note that the DEFN adds 7 numbers to the array WSEA and so we must have $MAXW \geq MAXM+7$ in the PRELUDE.)

Note: At the termination of the critical search (after START or RESTART - Section 5.23) the critical value of λ is built into the corresponding cross sections.

5.17.3 SUB2 - a general mesh width adjustment routine

The search subroutine SUB2 is used to adjust mesh widths for selected parts of the reactor. A call to the subroutine is set with the data, for example,

```
SEARCH(-0.02)
```

In addition we must supply additional data in the array WSEA which is used to

give the mesh adjustment required with each mesh interval (including boundary conditions). Given

XM (or RM) $d_L, \delta x_1, \delta x_2, \dots, \delta x_{NXMI}, d_R$ (NXMI = number of x mesh intervals)

YM (or ZM) $d_B, \delta y_1, \delta y_2, \dots, \delta y_{NYMI}, d_T$ (NYMI = number of y mesh intervals)

we must supply the additional data

WSEA $w_L, w_1, w_2, \dots, w_{NXMI}, w_R, \dots$ (MAXX+1 elements must be supplied)

$w'_B, w'_1, w'_2, \dots, w'_{NYMI}, w'_T$ (NYMI+2 elements must be supplied)

then the mesh spacing corresponding to an eigenvalue λ is

$$d_L(\lambda) = d_L(1 + (\lambda-1)w_L)$$

$$\delta x_1(\lambda) = \delta x_1(1 + (\lambda-1)w_1)$$

$$\vdots$$

$$\delta x_{NXMI}(\lambda) = \delta x_{NXMI}(1 + (\lambda-1)w_{NXMI})$$

$$d_R(\lambda) = d_R(1 + (\lambda-1)w_R)$$

$$d_B(\lambda) = d_B(1 + (\lambda-1)w'_B)$$

$$\delta y_1(\lambda) = \delta y_1(1 + (\lambda-1)w'_1)$$

$$\vdots$$

$$\delta y_{NYMI}(\lambda) = \delta y_{NYMI}(1 + (\lambda-1)w'_{NYMI})$$

$$d_T(\lambda) = d_T(1 + (\lambda-1)w'_T) \quad .$$

For example, say we have the data

MAXX=20 ...

RM 0., 5*1.3, 10*1.1, 0.71

ZM 0., 4*1.3, 8*1.1, 0.71

and we require the height of the core (underlined data) to be adjusted to achieve criticality with the reflector (the remaining data) adjusted so that the overall height does not change. We would use the data

WSEA 21*0., (since MAXX=20, although MAXX=16 would be satisfactory)

0., 4*1., 8*-0.590909, 0.

which would set

$$\delta z_1(\lambda) = \dots = \delta z_4(\lambda) = 1.3 + 1.3(\lambda-1)$$

$$\delta z_5(\lambda) = \dots = \delta z_{12}(\lambda) = 1.1 - 0.65(\lambda-1)$$

since then the core height = $\delta z_1(\lambda) + \delta z_2(\lambda) + \dots + \delta z_4(\lambda) = 5.2 + 5.2(\lambda-1)$

and the reflector height = $\delta z_5(\lambda) + \delta z_6(\lambda) + \dots + \delta z_{12}(\lambda) = 8.8 - 5.2(\lambda-1)$.

Here we would be recommended to set an upper limit to λ corresponding to the vanishing of the reflector. (POW sets any non-boundary mesh spacing less than 10^{-4} to 10^{-4} .) We would then supply the additional data

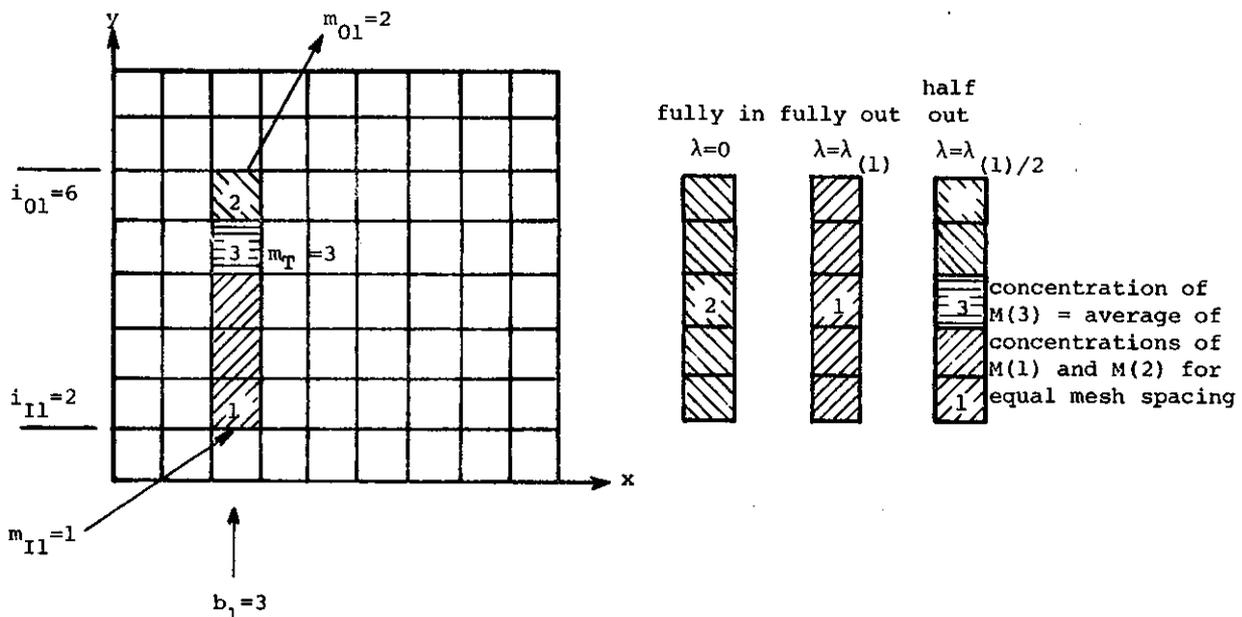
FSEA 1.-2,1.,1.1,2.69,3.

Note: At the termination of the critical search (after START or RESTART - Section 5.23) the critical value of λ is built into the corresponding mesh widths.

5.17.4 SUB3 - a general region adjustment routine

The search subroutine SUB3 is used to adjust the movement of control materials along directions (channels) parallel to the axis. A collection of channels with materials moved together we will call a bank, b_ℓ . Then a bank b_ℓ may be moved from a fully in position corresponding to mesh interval $i_{I\ell}$ to a fully out position corresponding to mesh interval $i_{O\ell}$. All banks start fully in. When one bank b_ℓ is moved to the fully out position, the next bank $b_{\ell+1}$ may be moved. The movement of banks forms the basis of the criticality search available here. As adjustment is made to a bank, if the bank is to be moved out then material $m_{I\ell}$ comes into the channels at mesh interval $i_{I\ell}$ and material $m_{O\ell}$ goes out of the channels at mesh interval $i_{O\ell}$. Fine adjustment is carried out by providing a 'tip' material m_T , between the materials $m_{O\ell}$ and $m_{I\ell}$. The concentration of the tip is varied so that we obtain the equivalent of homogenisation of materials $m_{O\ell}$ and $m_{I\ell}$ corresponding to a bank position partway between mesh intervals. Here we will be content to present the data requirement using simple examples.

As a first example we will consider only one bank and that of only one channel. Say we have the following reactor layout.



permitted with POW we must simulate the conditions using modified data for the control absorber, C,

$$D_C = 0 \text{ (} 10^{-4} \text{ is used instead to prevent code foul up)}$$

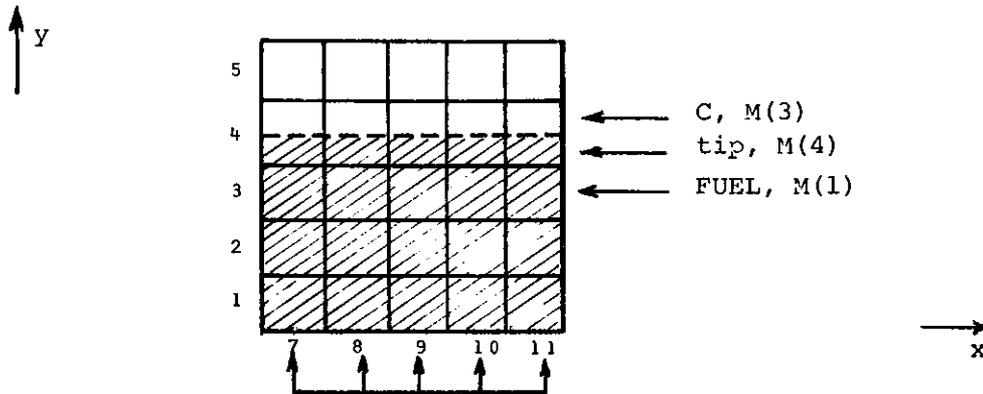
and

$$\sigma_{\text{remC}} = \frac{2}{\ell} \left(\frac{1}{d_L} + \frac{1}{d_R} \right) ,$$

where $\bar{\ell}$ = mean chord length for C (=4V/S).

The adjustment may be made to the data of C for some, or all, of the groups.

As an example of an application of SUB3 we consider the MOATA calculation of Section 5.3. Say we require the fuel loading to give $k_{\text{eff}}=0.9$. We set up 5 fuel channels to be moved together as 1 bank



We would need the additional data to that given earlier.

```
PRELUDE ... MAXM=4 END
SEARCH(-0.03) 0.9
WSEA 4 -1=1.25 2 1,5 1,3 7(1)11
```

5.18 Fixed External Source Specification

A fixed external source (in boxes around the intersection of mesh lines for all groups) is specified using

FSCE followed by data to sensibly fill the array DIMENSIONED as indicated

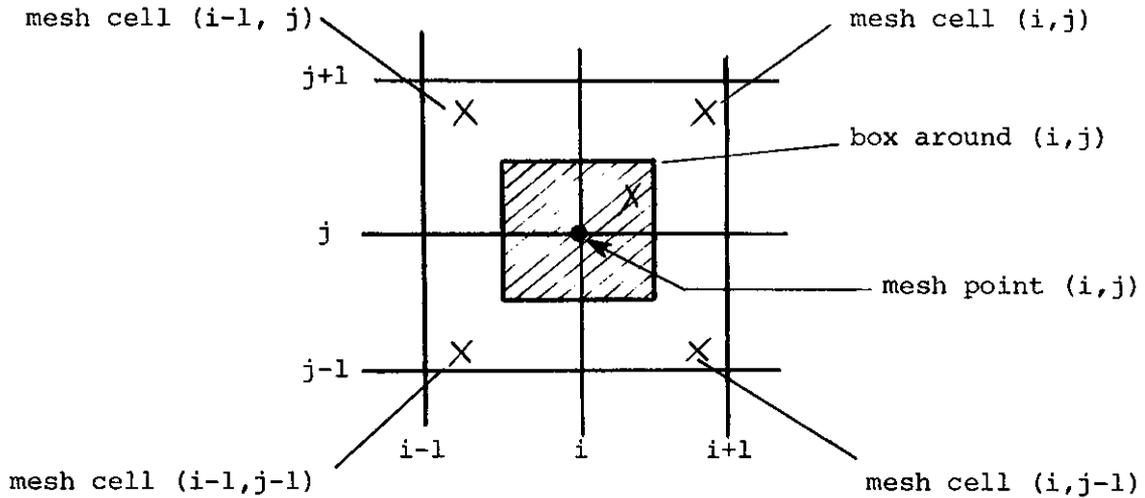
```
REAL*8 FSCE(MAXX,MAXY,MAXG,MAXF)
```

that is

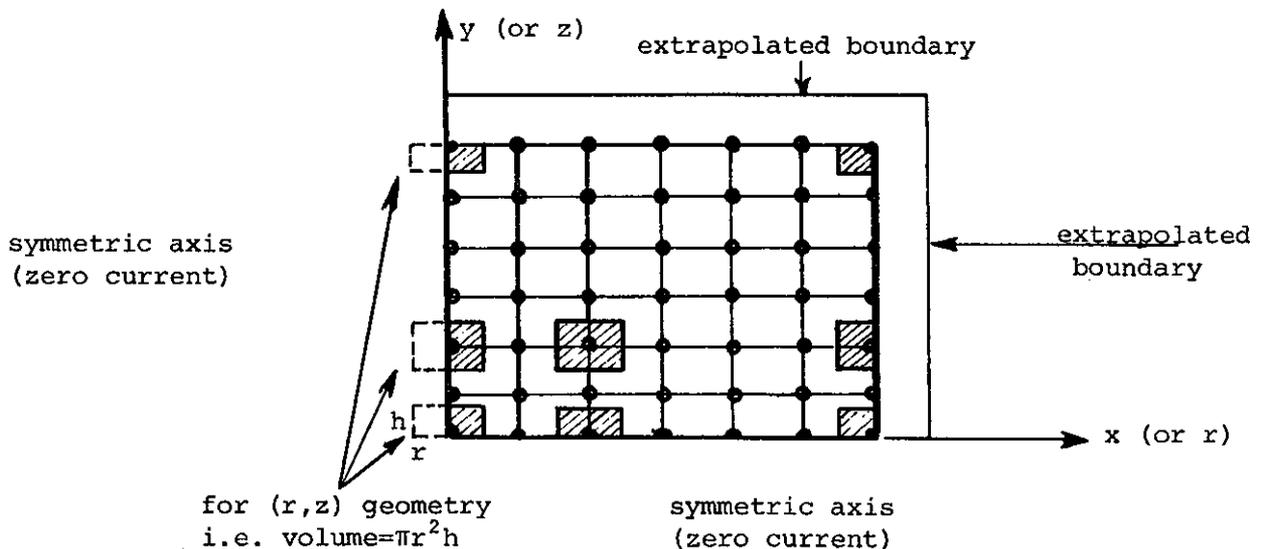
```
s(1,1,1,1), s(2,1,1,1), ..., s(MAXX,1,1,1),
s(1,2,1,1), s(2,2,1,1), ..., s(MAXX,2,1,1), ...,
s(1,MAXY,1,1), s(2,MAXY,1,1), ..., s(MAXX,MAXY,1,1),
s(1,1,2,1), s(2,1,2,1), ..., s(MAXX,1,2,1), ...,
```

$s(1,MAXY,MAXG,1), s(2,MAXY,MAXG,1), \dots, s(MAXX,MAXY,MAXG,1)$.

(In order that storage be available to contain the above data we must set $MAXF=1$ in the PRELUDE - Section 5.6.) The source $s(i,j,g,1)$, in units of n/sec (appropriately scaled for ease of presentation), is the total fixed source entering a box around the mesh point (i,j) for group g as illustrated...



We must note that the code uses fractions of boxes along boundaries as illustrated...



For spherical geometry the central box has the volume $\frac{4}{3} \pi r^3$.

In order to simplify data presentation for sources normally encountered in practice the following feature is available.

For the x-direction we would use, say,

FSCEL(1-3,1,1)=s(1,1,1,1) s(2,1,1,1), s(3,1,1,1)

for the y-direction we would use, say,

FSCEL(1,1-3,1)=s(1,1,1,1), s(1,2,1,1), s(1,3,1,1)

and for groups we would use, say,

FSCEL(1,1,1-3)=s(1,1,1,1), s(1,1,2,1), s(1,1,3,1)

Only one multiple argument may appear in the one specification.

As an example, say we require a unit line source ($1 \text{ n cm}^{-1} \text{ sec}^{-1}$) in the fastest group and centred at the origin of a symmetric xy system. We would use the data FSCE 0.25 (because of the 1/4 box) 100000*0 (too much data is of no consequence). Or if this is the first calculation to use the FSCE array (since storage is mostly set to zero)

FSCE 0.25 would suffice.

As a further example say we require a unit centre point source (1 n sec^{-1}) in a symmetric rz system but with a strength of 0.7 in group 1, 0.2 in group 2, 0.1 in group 3 and 0. in group 4 then with MAXX=25,MAXY=27,MAXG=4,MAXF=1 in the PRELUDE (Section 5.6) we would use the data

FSCE 0.35, 674*0., 0.1, 674.0., 0.05,100000*0

or more simply

FSCE 100000*0 (if the array needs to be cleared) FSCEL(1,1,1-3)=0.35, 0.1, 0.05

For a full spatial source the extent of data would be prohibitive, however this type of job is not often required.

Note: If no fissionable material is present in the reactor we may set

NOFISS = n,

where n is a reaction index

1 ~ σ_{tr}

2 ~ σ_{rem} - default option

3 ~ $\nu\sigma_f$ - normal option with fission

and with NG = number of groups

4+NG ~ $\sigma_{\text{reac 1}}$ (1st additional reaction)

5+NG ~ $\sigma_{\text{reac 2}}$ (2nd additional reaction)

6+NG ~ $\sigma_{\text{reac 3}}$ (3rd additional reaction)

⋮

then the normal source convergence (Section 5.21.1) is carried out but based on the group collapsed reaction n instead of fission emission. For example with 4 groups (NG=4) and the 1st additional reaction set to ABSorption (Section 5.14) we would use the data

NOFISS=8 to obtain convergence criteria based on the total absorption.

5.19 Trial Flux Specification

For most runs a user would not be particularly concerned with the default trail flux generated by POW, except to note that it is always adequate. (POW uses a flux appropriate to a bare homogeneous system as a trail solution.) However he should at least be aware of a few points.

Notes:

- (1) A trial flux may be used from a flux dump of a similar job (RESTART - Section 5.23).
- (2) For other than the first calculation of a run the flux solution of the previous calculation is used unless an element of flux is zero (as it would be if now we had more mesh points than before).
- (3) We may force a POW generated trial solution to be used simply by entering the data
 FLX=0 usually, although we need instead
 FSCE=0 if CALC=ADJOINT and MAXF=1
 since the adjoint flux is stored in the array FSCE when storage is made available (MAXF=1).

5.20 Calculation Strategy Specification

Much of the calculation strategy employed by POW is set with data read from disk (unit 4) as part of the normal use of DTAV routines (Appendix D). The strategy is briefly discussed in Section 3 and although we may vary the strategy the user would infrequently, if ever, need to make changes. Over the past few months the strategy data has been 'tuned' for a variety of calculations and this 'tuning' is likely to continue. The only data the user may wish to use (although this is unlikely) is to set the supermesh associated with region rebalance.

For region rebalance we supply data to specify supermesh segments of the solution plane. The minimum additional data consists of specifying MAXR (default $\sqrt{\text{MAXX}}$ $\sqrt{\text{MAXY}}$) in the PRELUDE for assigning storage to the solution array of MAXR*(MAXR+1) elements, then if

M_x = the number of supermesh segments in the x (or r) direction

M_y = the number of supermesh segments in the y (or z) direction

we require $M_x M_y \leq \text{MAXR}$.

Should no further data be specified a simple (but usually effective) procedure is adopted by the code to generate M_x , M_y and the segmenting boundary lines.

User specification of segmenting boundary lines, if required, must be carried out prior to each START (or RESTART) thus

$$\underline{\text{LX}} \quad M_x, I_1, I_2, \dots, I_{M_x+1}$$

$$\underline{\text{LY}} \quad M_y, J_1, J_2, \dots, J_{M_y+1}$$

where $I_1 (=1) < I_2 < \dots < I_{M_x+1}$ ($=NXM$, the number of x mesh solution lines)

and $I_\ell \leq i \leq I_{\ell+1}$ identifies the lines i forming the ℓ^{th} supermesh segment for the n direction, with a similar meaning for the Js,

$$J_1 (=1) < J_2 < \dots < J_{M_y+1} \quad (=NYM, \text{ the number of y mesh solution lines}).$$

The choice of plane segmentation is not always clear but a good rule (in the absence of specific experience) is to attempt to isolate regions which may be slow to converge (for example fuel regions or strongly diffusing regions in the vicinity of fuel regions).

As a simple example we consider the MOATA calculation of Section 5.3.

Say we require segments to isolate the FUEL region (the default procedure would do this anyway). We might use the data

```
PRELUDE ..., MAXR=6 END
```

```
⋮
LX=3 1,7,12,23
```

```
LY=2 1,6,17
```

```
START
```

5.21 Calculation Termination Data

Termination data for a calculation is initialised to a default set of values by POW and for the usual job these values should be adequate. Except for error termination (when POW simply 'browses' through the remaining data) a calculation ceases when one or more of the following termination conditions is met.

- (1) If,
 - (i) overall neutron balance accuracy \leq ACCLAM(1), default 1.-4,
 - (ii) local fission source accuracy \leq ACCFO(1), default 1.-4, and
 - (iii) critical k accuracy \leq k_{acc} if a SEARCH is requested (Section 5.17).
- (2) If machine time exceeds a specified limit (default 90% of the time remaining for the current job step).
- (3) If number of outer iterations, $n \geq$ NOL, a set limit (default 100);
- (4) If NIL, the set limit to the number of inner iterations = 0.

As a user you would probably only be interested in the above under the following circumstances:

- (1) to reduce (the already tight) accuracy for a lengthy calculation,
- (2) if the anticipated run time is uncertain,
- (3) if a calculation is not physically meaningful, and
- (4) if a previous flux dump is to be entered for EDIT purposes.

For the user requiring more than a brief run through the termination conditions we provided further details in the next Sections.

5.21.1 Accuracy termination (ACCLAM and ACCFO)

POW uses two main quantities to assess convergency of a calculation -

- (i) overall neutron balance, $b^{(n)}$, and
- (ii) local reaction (usually fission source) error, $S_{err}^{(n)}$,

both of which change with each outer iteration n . (In addition for a criticality SEARCH we need consider a further quantity.

- (iii) effective multiplication error, $|k^{(n)} - k_{reqd}|$.

Let $S_{ij}^{(n)}$ be the total reaction of indicated type for outer iteration number n in a box about the mesh point (i,j) , then we have the following meanings:

$$\text{CALC=REAL,EIGENV, } S_{ij}^{(n)} = \sum_g \phi_{ijg}^{(n)} \int_{(i,j)} v \sigma_{fg} dV ;$$

CALC=REAL,SOURCE, as above if any reactor material is fissile,

$$\text{otherwise } S_{ij}^{(n)} = \sum_g \phi_{ijg}^{(n)} \int_{(i,j)} \sigma_{\text{NOFISS},g} dV ,$$

and NOFISS is usually 2 (removals) as indicated in Section 5.18;

$$\text{CALC=ADJOINT, } S_{ij}^{(n)} = \sum_g \phi_{ijg}^{(n)*} \chi_{pg} .$$

We then have

$$(i) \quad b^{(n)} = \frac{\sum_i \sum_j S_{ij}^{(n)}}{\sum_i \sum_j S_{ij}^{(n-1)}}$$

$$(ii) \quad S_{err}^{(n)} = \max_{i,j} \left[S_{ij}^{(n)} / S_{ij}^{(n-1)} \right] - \min_{i,j} \left[S_{ij}^{(n)} / S_{ij}^{(n-1)} \right]$$

with i and j taken over the whole reactor for which $S_{ij}^{(n-1)} \neq 0$.

POW utilises a convergence count down scheme from trial solution stage (MOP=3) to ultimate convergence stage (MOP=0). Briefly for the usual problem we have ...

<u>Stage</u>	<u>Type</u>	<u>Mode of Change</u>
3	Power iteration	$b^{(n)} \leq \text{ACCLAM}(3)$
2	Chebyshev extrapolation	$b^{(n)} \leq \text{ACCLAM}(2)$ and $S_{err}^{(n)} \leq \text{ACCFO}(2)$
	$4 \leq \text{order} \leq 6$	

<u>Stage</u>	<u>Type</u>	<u>Mode of Change</u>
1	As above but more confident use $6 \leq \text{order} \leq 10$	$b^{(n)} \leq \text{ACCLAM}(1)$ and $S_{\text{err}}^{(n)} \leq \text{ACCFO}(1)$
0		CONVERGED (provided $ k^{(n)} - k_{\text{reqd}} \leq k_{\text{acc}}$ for a SEARCH calculation - Section 5.17)

We may change the default values for the accuracy limits,

(ACCLAM(1)=1.-4, ACCLAM(2)=1.-3, ACCLAM(3)=1.-2,
ACCFO(1)=1.-4, ACCFO(2)=1.-3, ACCFO(3)=1.-2)

using the data, for example,

ACCLAM = 1.-3

ACCFO = 1.-3

where here and normally we would be interested in changing only the final accuracy.

Note: The tight limits ACCLAM=1.-5, ACCFO=1.-5 are seldom, if ever, required.

5.21.2 Machine time limit (TLIM)

The time limit parameter may need to be set by the user, since if time is exceeded the calculation is thereby terminated with output rather than abruptly by the operating system. We use the data

TLIM = f

where f is the fraction of remaining time for the job step (set using JCL-Section 5.5) beyond which termination of the calculation (and output) is forced. The job does not terminate completely but following the START (or RESTART) data (Section 5.23) the Keyword TLIM is sought. (The job will terminate however, with the keywords END or STOP.) After resetting the time limit we may then proceed with our EDITING requirement before programme termination. For example we may have

TLIM = 0.9

⋮

START

TLIM = 0.9

If no TLIM data is given

TLIM = 0.9

is the default value.

5.21.3 Outer iteration count limit (NOL)

The current calculation being pursued terminates (successfully but with an appropriate note) if

$n \geq \text{NOL}$ (default value 100).

We may change the limit simply however with the data, for example,

NOL = 10

One reason for setting a small limit may be that only a few iterations of a criticality SEARCH are to be followed.

5.21.4 Inner iteration count limit (NIL)

POW uses an inner iteration count limit of NIL=100. If the limit is exceeded for one energy group the next group is started as in the normal solution process. If however we specify

NIL = 0

the code uses this cue to bypass all calculation. We may thus RESTART a flux dump (Section 5.23) and not carry out any further computation on the flux. Instead we may proceed with EDITING operations using the flux (Section 5.24). When we have finished with this feature we must remember to restore the usual limit

NIL = 100

5.22 Output Requirement Specification

The OUTPUT requirement is set with the following data

OUTPUT CRAM GOG DATA SOURCE FLUX PRINT DATAFT UEDIT PDUMP PRINTE

where any of the above descriptive words may follow OUTPUT in any order (although the code will produce OUTPUT in the given order). The descriptive words have the meaning

- GOG - produce data for GOG (Hopkins and Oakes 1968) on unit 2 (for a 2D eigenvalue problem only),
- CRAM - produce data for CRAM (Hassitt 1962) on unit 2 (for a 2D eigenvalue problem only),
- the above options which are carried out before the calculation is started, were mainly set up for comparison tests of POW with other codes,
- DATA - print cross section data (before the calculation is started),
- SOURCE - print (edge) source if CALC=REAL (or ADJOINT) SOURCE (Section 5.18),
- FLUX - at the termination of a calculation (Section 5.21) produce a flux dump at the end of the data set on unit 9 (consisting of possibly many flux dumps from different jobs),
- see also Section 5.23,
- PRINT - print (edge) flux ($\phi \times 1.E+08 = 1.102877$ means $\phi = 1.102877 \times 10^{-2}$)
- DATAFT - print cross section data layout and mesh spacing after a SEARCH calculation,
- UEEDIT - calls a subroutine provided by the user as briefly detailed in Section 5.27.

PDUMP - produce a printer dump of all POW variables referenced in LIST
(Appendix D4)
- the above option was mainly set up to assist programme implementation, and

PRINTE - as for PRINT except with exponents printed ($\emptyset \times 1.E+03 = 1103-02$ means $\emptyset = 1.103 \times 10^{-2}$).

OUTPUT DATA SOURCE PRINT DATAFT is the default option.

If no OUTPUT is required we would use

OUTPUT with no data following.

It is possible to produce OUTPUT at intermediate stages of the calculation for items normally only produced on termination of the calculation. Say we have

OUTPUT DATA FLUX PRINT

then we supply the data (one number for each item above and taken in the same order)

IOUT 0 0 5

which will result in the following OUTPUT:

DATA - at the start of the calculation,

FLUX - at the termination of the calculation (created at the end of the data set), and

PRINT - every 5 outer iterations and also at the termination of the calculation.

IOUT 0 0 0...are the default values.

***5.23 Calculation START

A calculation is started when the following data is encountered:

START

or if a flux dump is to be used as a trial flux

RESTART etc.

With the RESTART option we may supply additional data

RESTART JOBNAME PRINT

where

JOBNAME is normally the name of a job in which an acceptable flux dump was created on disk (or tape) unit 9 and may be the same as the current job, and

PRINT causes all flux dump headings to be printed.

Even though specified, the flux dump JOBNAME is only used if several important variables, including CALC (Section 5.16), match for both core (current job) and disk (previous job). When several acceptable dumps are available they are all

read, which results in the last one read (and the last one created) being used in subsequent calculation. In addition we have the following interpretations.

- (i) If JOBNAME and PRINT are not given (that is RESTART only) then
JOBNAME = current jobname (given with POW data - Section 5.7).
- (ii) If JOBNAME = current jobname then k, critical eigenvalue, etc., including calculation accuracy data, relaxation coefficients and dominance ratio are used along with the flux, otherwise standard values are taken. (When the current job is not closely similar to the previous job we should use a different JOBNAME.)
- (iii) If JOBNAME = SCRATCH (for use under AUS scheme) then
 - (a) names are ignored in the search for an acceptable dump,
 - (b) the data is completely scratched after the search so that any new flux dump will start at the beginning of the library,
 - (c) k and critical eigenvalue are used along with the flux, but the relaxation coefficients and dominance ratio are set to be recalculated, and
 - (d) if no acceptable dump is found no computation is carried out.
- (iv) If JOBNAME \neq SCRATCH and no acceptable dump is located, data appropriate to a normal START is set up.
- (v) If a flux dump is to be created for the first time (or all previous data is to be scratched) we must supply the data
RESTART DISP=NEW
which otherwise is equivalent to START. A file mark is written at the beginning of the flux dump, unit 9.

Notes:

- (1) The following restatement enlarging (ii) and (iv) is most important. The code considers that if JOBNAME=current jobname, e.g.

```
POW MOATA (X,Y) CALCULATION, GYMEA DATA
```

```
RESTART MOATA (or simply RESTART)
```

then the same, or almost the same, calculation is being pursued and the previously estimated relaxation coefficients and dominance ratio should suffice. When the jobs differ substantially we should use different jobnames, e.g.

```
POW MOATA1 (X,Y) CALCULATION, GYMEA DATA (MOD1)
```

```
RESTART MOATA (but not RESTART)
```

as then only the flux shape is employed.

- (2) When a normal START is initiated, k, critical eigenvalue, etc. are reset to standard values although a trial flux is only created if any FLX element is zero as discussed in Section 5.19. When we follow

one calculation with another (i) we may want the previous data for k and critical eigenvalue to be used although calculation accuracy data relaxation coefficients and dominance ratio are to be taken as standard default values, (ii) we may want only the previous FLX to be used or (iii) we may not want any of the previous data to be used. We supply the following data for each case cited...

- (i) some data from previous calculation (similar to current calculation)
RESTART CONTINUE
- (ii) FLX only from previous calculation (vaguely similar to current calculation)
START
- (iii) no data from previous calculation (an independent calculation)
FLX=0. START

An additional, infrequently required, option is also available in conjunction with the RESTART feature. Consider the set of acceptable dumps (jobname, CALC, etc. the same). The last read in the set (the most up-to-date dump) is normally required. We may however select the n^{th} member of the set with the data

AFTER n RESTART ...

When we use this option we must remember to restore n to a large number for any future RESTART in the current job if the last read dump is required. The option is mainly made available to enable later EDITING (Section 5.24) to be carried out, for example we may want to plot out the flux after each outer iteration (or more usefully after each time step of a kinetics calculation).

5.24 Region EDIT (1st word + ve)

Basically POW region edit produces output for regions of materials constituting the reactor system or mixtures of these materials. Cross sections may be collapsed with simply flux (the usual requirement) or flux-adjoint (mainly for perturbation calculations, Section 5.25). Card output may be directed to the printer (unit 3), punch (unit 2) or disk (unit 7) and cross sections may be stored in core for later use or creation of an AUS library. The user is required to specify the following items

- (1) GROUPS, collapsed group structure,
- (2) MREG, material regions,
- (3) MXS, cross section correspondence,
- (4) EDIT, initiates the edit calculation, and
- (5) WRITE LIB, if an AUS XSLIB (Appendix A) is to be produced.

We introduce each keyword and associated data in turn.

5.24.1 GROUPS, collapsed group structure

The required collapsed group structure is defined using the data, for example,

GROUPS 4 1,2,4,6,8

where the 1st number is the required number of collapsed groups

the 2nd number is the starting group for the collapsed group 1

the 3rd number is the finishing group for the collapsed group 1

and 1 more than the number is the starting group for the next collapsed group, if one is given,

etc.

Note: Should we require all of the original groups of, say, a 26-group set we would use the data

GROUPS 26,1,1(1)26

5.24.2 MREG, material regions

The required materials for output, except as described in the next Section (5.24.3), consist of union of the regions of the reactor filled by particular materials as described by REG data (Section 5.15.4). For example

MREG 1,2

will produce output for 2 materials - the 1st consisting of material M(1)

averaged over each region of the reactor containing M(1), and the 2nd consisting

of material M(2) averaged over each region of the reactor containing M(2).

We identify union of materials, thus

MREG -3=1,2

which identifies a material, designated with a negative number, which is the union of all of the materials following the negative number up to either the end of the list or a non-positive number (0 is otherwise ignored). For the example we then produce output for 1 material which is averaged over all the reactor regions containing either M(1) or M(2) and with the cross section appropriate to each region.

As a further example we may use the data

MREG 1,2, -3=1,2,3,4, -4=1,3,0,4

which will produce output for the 5 materials underlined.

Notes:

- (1) Any material not present in the reactor is ignored in the edit routine so that to obtain data for 1 material appropriate to the whole reactor we could just as well use say,

MREG -1=1(1)30,

to actually select out the correct individual materials.

- (2) We may need to modify the REG data (Section 5.15.4) in order to select out isolated regions of the reactor. Should this be so we may save the original layout on disk and readily restore when required (Section 5.15.5).
- (3) The array used to store MREG data (MATS, an equivalent keyword) is DIMENSIONED MATS (MAXN). The PRELUDE default value for MAXN is 50 (Section 5.6) and this should be increased for excessively long MREG lists.

5.24.3 MXS, cross section correspondence

For some applications we may need to use the data $MXS = I_1, I_2, \dots, I_J$ ($J = \max i$ for materials $M(i)$ of MREG data) to give a correspondence of actual materials $M(i)$ filling the reactor with materials $M(I_i)$ giving cross sections to be used. For example the data

```
MREG 2,1,-3=1,2
```

```
MXS 5,6
```

will result in output for 3 materials. The 1st will be for regions filled with $M(2)$ but with cross sections of $M(6)$ used instead of $M(2)$, the 2nd will be for regions filled with $M(1)$ but using cross sections of $M(5)$ and the 3rd will be for the union of the regions filled for $M(1)$ and $M(2)$ but with cross sections of $M(5)$ and $M(6)$ used respectively. The default value of the vector MXS is $MXS=1,2,3,\dots$

and simple edit calculations will not require this to be changed.

As an example say we are considering an OD reactor filled with $M(1)$. In order to obtain output for materials $M(2)$, $M(3)$... collapsed using the reactor spectrum we could use the data:

```
START
```

```
GROUPS ...
```

```
MREG 1
```

```
MXS 2
```

```
EDIT ...
```

```
MXS 3
```

```
EDIT ...
```

5.24.4 EDIT, initiates the edit calculation

The required edit options are specified with the EDIT data thus ...

```
EDIT 1,m,n,p
```

where $1(>0)$ is an identifying number for output,

m indicates the required output	$\left\{ \begin{array}{l} 0 = \text{no data produced} \\ 1 = \text{reaction rate} \\ 2 = \text{cross section} \\ 3 = \text{both} \end{array} \right.$
n indicates the destination for output	$\left\{ \begin{array}{l} -ve = \text{data prepared in core} \\ 0 = \text{no data prepared} \\ +ve = \text{unit number for output} \end{array} \right.$
p indicates the weighting spectrum and is normally not specified	$\left\{ \begin{array}{l} 0 = \text{FLX (default option)} \\ 1 = \text{FLX and ADJOINT weighting} \\ \quad (\text{FSCE array, Section 5.18}) - \\ \quad \text{if MAXF=0 then } \phi^2 \text{ weighting} \\ \quad \text{is obtained} \end{array} \right.$

With data produced in core ($n < 0$) then provided $m \geq 2$ cross sections for all the materials on the MREG card are replaced. For example using

MREG 1,2,-3=4,5

then data for M(1), M(2) and M(3) are replaced in core except that the replacement is interpreted via the MXS array (previous Section). Continuing the example, with the additional data

MXS 11,12,13,14,15

then data for M(11), M(12) and M(13) are replaced rather than M(1), M(2) and M(3). In addition the fission spectrum, SP, is collapsed and NG is set to the collapsed number of groups when $n=-2$ is used. (Then we could obviously not carry out any further editing and for any subsequent calculation we would need to force regeneration of a trial flux solution using the data FLX=0. before the next START card - Section 5.23.)

The various quantities produced as output are based on the following formulae. We use an imagined continuous spatial representation (rather than the finite difference form used in POW) in order to simplify the presentation. Let us define

$$(\sigma, \phi, \phi^*) (M, G' \rightarrow G) = \sum_{g' \in G'} \sum_{g \in G} \int_M \sigma(\underline{r}, g' \rightarrow g) \phi(\underline{r}, g') \phi^*(\underline{r}, g) d\underline{r}$$

$$\text{and } (\sigma, \phi, \phi^*) (M, G') = \sum_{g' \in G'} \int_M \sigma(\underline{r}, g') \phi(\underline{r}, g') \phi^*(\underline{r}, g') d\underline{r},$$

where on the left G' and G represent collapsed group numbers and on the right they represent sets of numbers of groups to be collapsed, M designates a region of the reactor and the remaining notation is clear. For example

volume flux $(M,G)=(1,\varnothing,1)(M,G)$

When only flux weighting is specified we take $\varnothing^*=1$ in the formulae below.

We then have the following ...

(i) additional reactions

$$RR(M,G')=(\sigma,\varnothing,\varnothing^*)(M,G') \quad (\text{reaction rate})$$

$$XS(M,G')=RR(M,G')/(1,\varnothing,\varnothing^*)(M,G'), \quad (\text{cross section})$$

and the above holds for all reactions,

(ii) transport

$$(TR)RR(M,G') = \{(1,\varnothing,\varnothing^*)(M,G')\}^2 / \sum_{g' \in G'} \left[\frac{\{(1,\varnothing,\varnothing^*)(M,g')\}^2}{(\sigma_{tr},\varnothing,\varnothing^*)(M,g')} \right],$$

(iii) removal and scattering

$$(REM)RR(M,G') = (\sigma_{rem},\varnothing,\varnothing^*)(M,G') - \sum_G (\sigma_s,\varnothing\varnothing^*,1)(M,G' \rightarrow G)$$

(i.e. absorption)

$$+ \sum_G (\sigma_s,\varnothing,\varnothing^*)(M,G' \rightarrow G) - (\sigma_s,\varnothing,\varnothing^*)(M,G' \rightarrow G')$$

(i.e. outscatters)

$$(S)RR(M,G' \rightarrow G) = (\sigma_s,\varnothing,\varnothing^*)(M,G' \rightarrow G), \quad G \neq G' \quad (\text{also } G = G' \text{ for } P_n \text{ data, } n \neq 0)$$

$$(S)RR(M,G' \rightarrow G') = - \left\{ \sum_G (\sigma_s,\varnothing\varnothing^*,1)(M,G' \rightarrow G) - (\sigma_s,\varnothing,\varnothing^*)(M,G' \rightarrow G') \right\} \text{ for}$$

perturbation theory data)

$$= 0 \quad (\text{for in-core } P_0 \text{ data})$$

and,

$$(iv) \text{ fission emission } (\sigma(\tilde{r},g' \rightarrow g) = \nu\sigma_{f,g'}(\tilde{r})\chi_g)$$

$$(\nu F)RR(M,G') = \sum_G (\nu\sigma_f,\varnothing,\chi\varnothing^*)(M,G' \rightarrow G)$$

where χ denotes the normalised fission spectrum ($\sum_g \chi_g = 1$) and undefined summation is taken over all groups. When adjoint weighting is used, we obtain a region dependent fission spectrum

$$\chi(M,G) = \sum_{G'} (\nu\sigma_f,\varnothing,\chi\varnothing^*)(M,G' \rightarrow G) / \sum_{G'} \sum_G (\nu\sigma_f,\varnothing,\chi\varnothing^*)(M,G' \rightarrow G),$$

however the spectrum

$$\chi(G) = \chi(A,G),$$

where A denotes all of the reactor, should be used in subsequent calculation with POW. We force calculation of the above spectrum by defining a region consisting of all the reactor (say, MREG -1=1,2,3) and this region should be

the last defined since the last calculated spectrum will be used if CARD, AUS or core libraries are required.

As an example of a region edit say we require print out of a 4-group region edit of reaction rates for all materials, including a mixture of all materials, in the MOATA calculation of Section 5.3. We would use the edit data:

```
GROUPS 4 1,1(1)4
MREG 1,2,3,-1=1,2,3
EDIT 1,1 3
```

5.24.5 WRITE LIB, AUS XSLIB creation

As part of the AUS scheme requirement POW can both read and write AUS cross section libraries. The libraries read (Section 5.9.4) may contain tabular resonance shielded cross sections, however the libraries written can only contain shielding for one composition. A library is created from data held in core (perhaps prepared with EDIT 1,2, -2 - previous Section).

The data required for the AUS XSLIB creation is the following:

```
MREG i1,i2,...
WRITE name LIB ON unit, extra
```

where

i_1, i_2, \dots are the numbers of the required materials (-ve numbers and 0 are not permitted with this application),
 name is the user's choice of name for the library (however CARD is not permitted - see Note (4)),
 unit is the FORTRAN unit number for the library, usually 10, and
 extra is the FORTRAN unit number of the library from which the original data was derived if we want group energy boundaries, burn up information etc. (Note (3)) to be passed to the newly created library, or 0 (the default value) if the feature is not required.

Notes:

- (1) If data for P_1, P_2, \dots , scattering matrices is held in core (Section 5.10) then we do not specify these pseudo materials on the MREG card as single material data for AUS includes P_0, P_1, \dots scattering. (If we do not want P_1, P_2, \dots data we simply change the names of the pseudo materials from DITTO to something else.)
- (2) If we require the library to contain averaged group velocities, v_g (particularly for kinetic studies) we must
 - (i) have extracted the data from a library, in the form of cross section data for INV455B, Section 5.9.1

- (ii) have averaged INV455B data over the reactor spectrum if a group collapse is involved.

The material number corresponding to IVN455B should not appear on the MREG card unless the data is also required in the body of the cross section part of the library.

- (3) Using the 'extra' feature above we use a correspondence of cross section data for $M(i)$ with burn up information for a material with library name corresponding to $M(I_i)$ set with MXS data (Section 5.24.3). For normal use $I_i=i$ and the names of the materials to be created also identify materials in the 'extra' library.

- (4) For compatability with the data

READ CARD LIB ON 7,1 (Section 5.8)

the data

WRITE CARD LIB ON 7,0

is equivalent to

EDIT 99,2 7,0

5.25 Perturbation EDIT

Perturbation analysis provides a formula for calculating the change in effective multiplication δk , resulting from slight changes (perturbations) to cross sections of materials constituting the reactor. Indeed for not so small changes, we may calculate δk simply by carrying out two normal calculations (CALC=REAL, EIGENV); one with normal data and the second with perturbed data. This approach is adequate when δk is much greater than the accuracy requested (ACCLAM, Section 5.21.1) and only a few cases are to be studied. For small perturbations however (δk of the order of say 10^{-5}) or when many cases are to be studied the perturbation analysis approach discussed here is necessary.

Central to perturbation analysis is having available the REAL and ADJOINT flux for the unperturbed system. We collapse the system under study to one material (over the whole reactor) and one group (from all groups). Except for the leakage term this collapse is straight forward. Before we continue with the perturbation edit proper we elaborate further on this leakage term (and in more general context).

5.25.1 Group dependent leakage from each region

Earlier (Section 5.13) we introduced the way DB^2 leakage could be added to the removal cross section to represent leakage for directions not included in the calculation in hand. For the MOATA calculation for example (Section 5.3) an axial buckling of

$$B^2 = 0.00184$$

was required and this was entered as the data

BSQ(0) 1,2,3 1,2,3 3*0.00184

which modified the removal cross section of all materials (1,2 and 3) constituting the reactor.

A more precise way to approximate leakage not accounted for in the current calculation (when the data is available!) is to use a group dependent buckling for each material $B_g^2(m)$. We may enter this data for use by POW thus ...

GBSQ (($B_g^2(m)$, $g=1,2,\dots,MAXG$), $m=1,2,\dots,MAXM$).

With the data

BSQ (additional reaction number) =

{set L of material numbers to have leakage added},

{set M of material numbers for required transport cross sections},

{set N of required bucklings, B^2 },

POW uses the extended interpretation from our earlier work (Section 5.13)

if $B^2=0$ for the k^{th} element of set N

then $B_g^2(m(k))$ is used instead,

where $m(k)$ is the k^{th} element of set M

For example if $MAXG=4$ and $MAXM=4$ then the data (given in the indicated order and immediately following each other)

GBSQ 4*0.,1.2-3,0.72-3,0.11-3,-0.23-3,8*0.

BSQ(3) 2 2 0.

would result in the generation of a 3rd additional reaction for material 2,

$$\sigma_{\text{reac3},g}(2) = B_g^2(2)/(3\sigma_{\text{tr},g}(2)), \quad g=1,2,\dots,NG \text{ (which may be less than MAXG).}$$

If this were the whole story the feature would hardly be worthwhile. However POW itself can calculate the group dependent bucklings for each material constituting the reactor following a flux (and possibly adjoint) calculation (and this is why we have deferred consideration of the feature until now).

The requirement for POW generation of group dependent bucklings is indicated with a short list of data thus

GBSQ ℓ ,

where $\ell = \begin{cases} 0 & \text{- flux } (\phi) \text{ weighting only (adjoint flux, } \phi^*, \text{ set to 1 in equation below)} \\ 1 & \text{- } \phi \text{ and } \phi^* \text{ weighting as for region EDIT, Section 5.24.4 and this is the required option for perturbation analysis.} \end{cases}$

POW calculates (in a finite difference formulation)

$$B_g^2(m') = 3\sigma_{\text{tr},g}(m') \int_M \phi_g^* \nabla \cdot \mathbf{D}_{n,g}(m') \nabla \phi_g \, dV / \int_M \phi_g \phi_g^* \, dV,$$

where

- M is all of the reactor filled by material m,
 m' = MXS(m), i.e. we may use the cross sections of another material
 (Section 5.24.3) although normally m'=m, and
 D_{n,g}(m') denotes the possibly directional diffusion coefficients of
 material m' (Section 5.8.3).

Considering further the example above we may use instead the data

... START GBSQ 0 BSQ(3) 2 2 0 ...

5.25.2 Perturbation analysis

Using the GBSQ 1 feature of the previous Section we may enter the leakage cross section

$$B_g^2(m)/(3\sigma_{tr,g}(m)) = -\int_M \phi_g^* \nabla \cdot D_{n,g}(m) \nabla \phi_g \, dV / \int_M \phi_g \phi_g^* \, dV$$

as an additional reaction for each material constituting the reactor. The leakage reaction rate

$$(\text{LEAK})RR(M,G') = - \sum_{g' \in G'} \int_M \phi_{g'}^* \nabla \cdot D_{n,g'}(m) \nabla \phi_{g'} \, dV$$

is hence calculated by a region edit in the same way as any other additional reaction (Section 5.24.4). The expression we seek for the change in effective multiplication consequent to a perturbation of cross sections - readily obtained by considering

- (i) the REAL equation with unperturbed cross sections,
 - (ii) the ADJOINT equation with perturbed cross sections (designated by a prime), and
 - (iii) with the ADJOINT flux approximated by the unperturbed values -
- is then

$$\frac{\delta k}{k} = \{ (\text{COMP})RR'(A,1) - (\text{COMP})RR(A,1) \} k / (\text{VF})RR(A,1)$$

where

$$(\text{COMP})RR'(A,1) = \frac{(\text{VF})RR'(A,1)}{k} +$$

$$+ (\text{S})RR'(A,1+1) - (\text{REM})RR'(A,1) - (\text{LEAK})RR'(A,1)$$

with the prime dropped for (COMP)RR(A,1),
 A designates all of the reactor, and
 1 designates the one group obtained from collapsing all groups.

All of the component terms of the above expression may be produced by a region edit (Section 5.24) using a one material (all the reactor considered) one

group (all the groups collapsed) option. Even so in order to avoid unnecessary roundoff errors (as the reaction rates are only printed to single precision accuracy although they are calculated to double precision accuracy) and to save the user unnecessary arithmetic, an automated way of carrying out the computation is available as described in the next Section,

EDIT 0,...

5.25.3 Automated perturbation EDIT (1st word 0)

5.25.3.1 General material replacement

In order to simplify the data requirement for a standard type region edit we may simply follow a calculation (START) with the Keyword

EDIT (\equiv EDIT 0,1,0,0)

which will generate input for region edit data (on FORTRAN unit 7) for an all reactor (A) 1 group edit. In addition the component terms of (COMP)RR(A,1) are printed. The same feature may also be used for a perturbation edit which prints the component terms of $\delta k/k$. For either requirement we use the data ...

EDIT 0,m,n,p

where

- | | | |
|---|---|---|
| m | indicates the data type | $\left\{ \begin{array}{l} 1 = \text{unperturbed (default)} \\ 2 = \text{perturbed} \end{array} \right.$ |
| n | indicates an additional reaction number for the storage of $D_g B_g^2$ leakage (Section 5.25.1) or 0 (default) if leakage is to be ignored, and | |
| p | indicates the weighting spectrum and must be 1 for a perturbation edit | $\left\{ \begin{array}{l} 0 = \text{FLX (default)} \\ 1 = \text{FLX and ADJOINT weighting as for a region edit.} \end{array} \right.$ |

Should data exist for a material INV455B (Section 5.9.1) then $10^{-8} \sigma_{\text{remg}}$ (i.e. $1/v_g$ with v_g expressed in units of cm sec^{-1}) is always stored as additional reaction n+1 for calculation of prompt neutron lifetime in seconds, \bar{l} , of the unperturbed system (and then MAXS (Section 5.6) \geq n+1 for storage of the data). The calculation uses

$$\bar{l} = (\text{ADD.REAC.n+1})\text{RR}(A,1) k / (\sqrt{F})\text{RR}(A,1) .$$

As an additional feature when studying (X,Y) geometry systems with axial (Z) leakage added, it is possible to attribute axial leakage correctly to a gross leakage term rather than to have it unidentified as part of absorption. For this situation we take n-ve in the above, then

- | | |
|---------|--|
| $ n $ | indicates an additional reaction number for POW storage of $(X,Y) D_g B_g^2$, and |
| $ n -1$ | is the reaction number where the user has stored axial (Z) $D_g B_g^2$ in addition to the same quantity being added to the removals. |

Here, for example, say we have 3 materials filling the reactor then we might use the data

```
BSQ(1) 1,2,3 1,2,3 3*0.00184
```

followed by

```
BSQ(-1) (and no more data)
```

which causes the removals to also be updated similarly (Section 5.13). Later we would use $n=-2$ as part of our automated perturbation edit.

As an example of the use of the present feature we extend the MOATA calculation of Section 5.3 to include calculation of δk for perturbations of the basic cross sections.

```
//JPPMOATA JOB...
PRELUDE...MAXM=4,MAXF=1 END
BSQ(1) 1,2,3 1,2,3 3*0.00184 BSQ(-1)
START
CALC=ADJOINT START EDIT 0,1,-2,1
XSD FUEL350 M(4)
... perturbed cross section data supplied and then leakage added
BSQ(1) 4 4 0.00184 BSQ(-1)
MXS 4,2,3 (M(4) data is used for regions filled by M(1), Section 5.24.3)
EDIT 0,2,-2,1
XSD C350 M(4)
... perturbed cross section data supplied and then leakage added
BSQ(1) 4 4 0.00184 BSQ(-1)
MXS 1,2,4 EDIT 0,2,-2,1
etc.
```

A user intent simply on obtaining an idea of the sensitivity of the reactor calculation to particular cross sections may modify cross sections using the feature described in Section 5.11 and may otherwise proceed with a perturbation study as in the example above.

5.25.3.2 Detector response

When a specific type of edit is required associated with small reactivity effects ($\delta k/k < 10^{-6}$) of a detector material to be taken over different parts of the reactor the preceding feature proves to be inadequate as $\delta k/k$ is calculated from the differences of the unperturbed and perturbed system. Here a feature is made available to work directly with the cross section changes associated with effectively adding a detector to the material filling a single region mesh cell. The same type of EDIT 0 data must be supplied as in the previous Section along with additional data that also supplies information for

the generation of the data perturbation. We have

AEDIT i,j,m'=m,a,(ℓ) (AEDIT 0 is default for EDIT 0 as in Section 5.25.3.1) where

the material m" filling the single REGION mesh cell at i,j (Section 5.15.4) has effectively added to it the perturbed material m' (a spare cross section location) made up of (10^{24} a) atoms of the required detector m in the reactor segment being considered, and the optimal data ℓ=1 forces the printing of a REGION layout picture not normally printed (default ℓ=0).

Here previous data held in m' is lost and m' must not appear anywhere in a REGION filling the reactor. The perturbed data is made up thus...

concentration, $c=a/(\text{volume of cell at } i,j)$

cross sections, $\sigma(m')=c\sigma(m)$ is stored, $\delta\sigma=\sigma(m')$ is used

diffusion coefficients, $D_n(m')=D_n(m)/c$ is stored, $\delta D_n=D_n^2(m'')/D_n(m')$ is used, and

$\delta k/k$ per (10^{24} a) atoms per reactor segment is printed as a result of the calculation along with component terms. Note that, for example, if the reactor segment being considered is $\frac{1}{2}$ of the entire reactor as a reflective boundary condition is used we then have $\frac{1}{2}\delta k/k$ as the reactivity effect per (10^{24} a) atoms for the entire reactor.

Considering our earlier MOATA example (Sections 5.3 and 5.25.3.1) say the detector required for comparison of reactivities at the centre and edge of the fuel is M(4) (with data to be stored in M(5)) then we could use the data

```

CALC=ADJOINT START EDIT 0,1,-2,1

```

```

AEDIT 9,3,5=4,1.-6 EDIT 0,2,-2,1

```

```

AEDIT 7,5,5=4,1.-6 EDIT 0,2,-2,1

```

5.26 Point EDIT (1st Word -ve)

For the point edit mode a map of reaction rates of materials is produced on the printer in the same style as a detailed flux map. The option uses similar data keywords to the region edit (Section 5.24) except that the data may be slightly differently interpreted. The data keywords are

- (1) GROUPS... interpreted the same as before
- (2) MREG... regions to be included in map
- (3) MXS... interpreted the same as before
- (4) PLOT... this data must be supplied for each use
- (5) EDIT...

5.26.1 GROUPS, collapsed group structure

With the point edit option we always obtain an entire map of a selected reaction rate (chosen with the EDIT card) for boxes about the points of

intersection of mesh lines for the collapsed groups indicated with the GROUPS card (interpreted the same as before, Section 5.24.1).

5.26.2 MREG, material regions

In the calculation of reaction rates a cross section is only included if the corresponding material is indicated on the MREG card. We may thus map out the reaction rates of material 1 for all regions containing the material using the data

MREG 1

Outside of the region filled by M(1) we would have zero reaction rates. We may however have reaction rates printed for a region which is the union of regions filled by M(1) and M(2) using the data

MREG -3=1,2

Also several items may be given on the one card as for the region edit.

5.26.3 MXS, cross section correspondence

As for the region option we may select a region on the basis of whether the material number for the material filling the region is given on the MREG card, but then we may substitute the cross section for a different material as implied with MXS data. For example if we use the data

MREG 2,1

MXS 5,6

then the cross sections of M(5) are used instead of M(1) and the cross sections of M(6) are used instead of M(2).

5.26.4 PLOT, plotting specification

Along with a print out of flux or reaction rate we may obtain plots of corresponding quantities on the CALCOMP plotter connected to the site IBM360/50 through a PDP9/L (Richardson 1971). The types of plot available are

- (i) $f_G(x,y)$ against x or y (XYPLOT, B.E. Clancy and G.D. Trimble, AAEC unpublished report), or
- (ii) $f_G(x,y)$ against x and y (contour XYCONT, B.E. Clancy and G.D. Trimble, AAEC unpublished report and 2D PUREJOY, Kubert et al. 1968)

where G denotes collapsed groups. The plotting requirement is set with the data

PLOT $p_1, p_2, \dots, 0$ (terminating data indication)

where p_1 makes the basic plot selection thus...

$$|P_1| = \begin{cases} 0 & , \text{ no plot (default)} \\ 1 & , \text{ x plot} \\ 2 & , \text{ y plot} \\ 3 & , \text{ contour and 2D plot} \end{cases}$$

and if $p_1 < 0$, printed output is not produced, only a plot.

Note:

- (1) When any plotting is required we must remember to provide additional JCL (Section 5.5) thus


```
//JPPMOATA JOB...
//          CLASS=J,...
// EXEC    BUFFPROG,PRG=AEPLLOT - insert this card -
// EXEC    AUS
```
- (2) On exit from the point edit in hand POW sets $p_1=0$ in order that subsequent accidental production of unwanted graphs may be thereby avoided. We must thus supply new PLOT data with every plot requirement, or we must at least restore the erased p_1 data thus PLOT p_1 (and the remainder of the previous list is used).

We now look more closely at the available options.

- (i) The XYPLOT option uses the remainder of PLOT data in the following way. The p 's designate selected lines for plotting parallel to the chosen axis and must be ordered

$$P_{i-1} < P_i < P_{i+1}, \quad i = 3, 4, \dots$$

Each plot produced consists of data for 1 line and all collapsed groups (plotted with different types of lines). For example to plot the thermal flux for the MOATA example (Section 5.3) parallel to the x axis for 2 lines, (a) along the axis, and (b) on the edge of the FUEL we would use the data

```
GROUPS 1 4,4
```

```
MREG -1=1,2,3
```

```
PLOT 1 1,6,0
```

```
EDIT -1,0,0,0 (as described in the next Section).
```

(Plot (a) obtained from the above is reproduced as Figure 1.)

The user may change the physical size and mode of plotting using the additional data

```
XYPLT x,y
```

where

$|x|$ = x size of required grid in inches ($|x| < 100$)

$|y|$ = y size of required grid in inches

and the sign of x and y determines the mode of plotting,

+ = log scale, and

- = linear scale.

The default data is

XYPLT -12,8

- (ii) The PUREJOY option for the simplest mode of use would consist of the data

PLOT $\pm 3, p_2, 0$

where p_2 is the viewing angle (in degrees) measured in an anticlockwise direction from the x axis. If however we require plots of part of the reactor, or a number of plots at different viewing angles, we need to supply 5 values of p for each plot. For the k^{th} plot we would have

p_{5k-3} = viewing angle

p_{5k-2} = from this x mesh line (1 for the axis)

p_{5k-1} = to this x mesh line (NYM for the boundary)

p_{5k} = from this y mesh line (1 for the axis)

p_{5k+1} = to this y mesh line (NXM for the boundary)

except that the last 4 numbers may be $4*-1$ for the whole reactor.

Again we use an extension of the MOATA example (Section 5.3).

Say we want an x,y plot of the thermal flux. We would simply use the data

GROUPS 1 4,4

MREG -1=1,2,3

PLOT 3,120,0

EDIT -1,0,0,0 (as described in the next Section).

(The PUREJOY plot obtained from the above is reproduced as Figure 3 and a corresponding contour plot is given as Figure 2.)

The user may change details of the PUREJOY plot, particularly the box containing the plot, using the additional data.

PUREJY x_1, x_2, \dots, x_3

where

x_1 = size of y direction of contour plot in inches (default -9)
 - if $x_1=0$ then a contour plot is not produced,

x_2 = factor forcing interpolation in x direction (default 2 and

$$x_2 \leq \sqrt{8} \frac{\text{MAXX}}{\text{NXM}}$$

- if $x_2=0$ then a PUREJOY plot is not produced,

x_3 = factor forcing interpolation in y direction (default 2 and

$$x_3 \leq \sqrt{8} \frac{\text{MAXY}}{\text{NYM}}$$

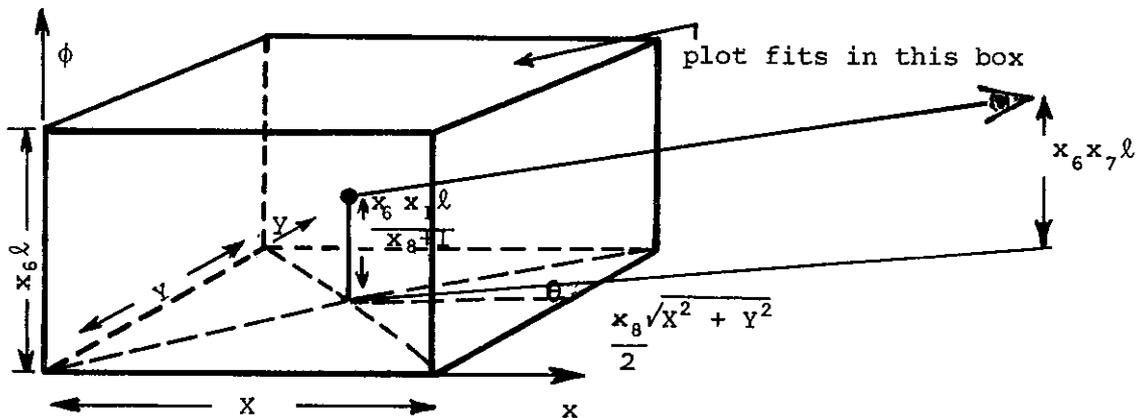
x_4 = horizontal size of frame for PUREJOY plot in inches
(default 10),

x_5 = vertical size of frame for PUREJOY plot in inches (default
10),

x_6 = box factor (default 0.7) such that the height of the box
= $\max(X, Y) * x_6$ where X and Y are the lengths of the
sides of the box,

x_7 = height factor such that the viewer's eyes are at the height
= $x_7 * x_6 * \max(X, Y)$ (default 0.8), and

x_8 = radius of viewing position (r) in terms of $\frac{1}{2}$ the length of
the diagonal (default 3), i.e. $r = x_8 (\frac{1}{2} \sqrt{X^2 + Y^2})$.



Here $\ell = \max(X, Y)$

and $\theta =$ viewing angle.

5.26.5 EDIT, initiates the edit calculation

The required edit options are specified with the EDIT data thus...

EDIT ℓ, m, n, p

where

$\ell (<0)$	is an identifying number for output,
m	+ve indicates the required additional reaction number
	0 specifies absorption (removals - outscatters)
	-ve indicates that reaction -m is required (e.g. -3 for fission emission),

the weighting flux option is set with

n	{	0 = flux only (\emptyset if $p=0$, $\emptyset\emptyset^*$ if $p=1$)			
		1 = reaction rate			
		2 = reaction rate with weighting factor FER_k (the fission energy release) - for a power map			
		3 = reaction rate with weighting factor of $WSEA_k$ (the user's array)			
		4 = reaction rate with weighting factor of $WSEA_{g+(k-1)MAXG}$ and			
p		indicates the weighting spectrum and is normally not specified			
		<table style="border-collapse: collapse;"> <tr> <td rowspan="2" style="font-size: 3em; vertical-align: middle; padding-right: 10px;">{</td> <td>0 = FLX (default option)</td> </tr> <tr> <td>1 = FLX and ADJOINT weighting as for region edit, Section 5.24.4</td> </tr> </table>	{	0 = FLX (default option)	1 = FLX and ADJOINT weighting as for region edit, Section 5.24.4
{	0 = FLX (default option)				
	1 = FLX and ADJOINT weighting as for region edit, Section 5.24.4				

with k being the material number of the actual cross section used (after interpretation via the MXS, and

g an index for energy group (of the original set).

As an additional, but important, option reaction rates may be calculated per unit volume (the usual choice) by setting $n=-n'$, where n' is an entry in the above list.

As a simple example say we want print out of the (collapsed) flux. We would simply use the data

```
GROUPS ...
MREG -l=1,2,...
EDIT -l,0,0,0
```

5.27 Possible User Written Subroutines

Using the temporary update feature (Section 5.5) a user may supply additional FORTRAN coding for the user subroutines

```
SUB4,SUB5,...,SUB9,UEDIT
```

The subroutines SUB_n may be used for specialised criticality SEARCHes (Section 5.17), however the manner of inclusion for this use will not be considered here. We may, however, call in the SUB_n subroutines with the data (supplied as part of normal POW card input)

```
CALL SUB9 , for example.
```

The subroutines may be written then for pre-editing or post-editing a flux calculation. On the other hand the subroutine UEDIT may be called during, or at the termination of a calculation - set with the data

```
OUTPUT PRINT,...,UEDIT (Section 5.22)
```

Here we will be content to provide some skeleton ideas for writing these subroutines using the following simple example. Considering the MOATA calculation again (Section 5.3) say we want to print the thermal flux at point (9,3) after each outer iteration. We would supply the data indicated below.

Note: Every subroutine must have a side entry for variable 'COMMON' of POW and we obtain all COMMON data using a special update programme which inserts the required FORTRAN statements with the data, for example,

```

CINSERT COMMON ENTRY SSUB9

//JPPMOATA JOB ...
//          CLASS=J,TIME=10
// EXEC    POW,POW='&&POW',GO=0
//FORT.SYSIN DD *
    SUBROUTINE UEDIT
C PRINTS THERMAL FLUX AT POINT (9,3)
CINSERT COMMON ENTRY SUEDIT - this inserts COMMON and variable
    WRITE(3,1)FLX(9,3,4,1)      dimension setting side entry SUEDIT
    1 FORMAT('OFLX(9,3,4,1)=' ,1PE15.6/)
    RETURN
    END

/*
// EXEC AUS,POW='&&POW'
:
PRELUDE ... PRINT END      - PRINT forces listing of address table
:
OUTPUT DATA PRINT UEDIT
IOUT      0      0      1
START
:
STOP
/*
//

```

5.28 Termination Data

In the Section on PRELUDE data (5.6) we were introduced to the termination data

- (i) END, and
- (ii) STOP

Here we simply reiterate what was said earlier.

(i) END occurring somewhere in the data (other than at the termination of PRELUDE data itself) causes cessation of the present calculation. A new PRELUDE is assumed to follow and a completely independent calculation may be undertaken.

(ii) STOP occurring somewhere in the data causes POW to exit (that is to return to the AUSYS control programme if run under AUS or to the operating system if run stand alone). STOP is thus effectively equivalent to an end of file on

the input unit (1). The main advantage of having a special code detectable termination keyword is that we may simply move the STOP card around in a deck when only a partial run is required. The cards after STOP are ignored, however they are left undisturbed for future restoration of the original run.

6. POW KINETICS DATA

6.1 Introduction

In Section 2 we were introduced to the kinetics equations solved by POW. The usual kinetics study starts with a steady state calculation first. Data needed for this calculation was detailed in Section 5 and we also met some neutron reaction data required for a kinetics calculation proper (Section 5.8.5 to Section 5.8.10) as well as data required to specify the intention of pursuing a KINETICS CALCULATION, Section 5.16.

A steady state consists of the initial conditions

$$\frac{\partial \phi}{\partial t} = 0, \quad \frac{\partial C_i}{\partial t} = 0, \quad S_g = 0, \quad t \leq 0 \text{ for all groups,}$$

however the POW flux normalisation is somewhat arbitrary (to a total fission source of unity) and, prior to starting the time dependent part of the calculation, the code (usually) applies the normalisation

$$\sum_g \int_{\text{reactor}} f \sigma_{fg} \phi_g \, dV = P, \text{ given power for } t=0,$$

where

f is the fission energy release for each reactor material (FER, Section 5.8.6), and

σ_{fg} is the (macroscopic) fission cross section.

An exception arises however, if we are studying a purely time dependent external source problem (perhaps including fissile material) where the initial conditions are the shutdown ones,

$$\phi_g = 0 \text{ (POW substitutes instead } 10^{-40}), \quad C_i = 0, \quad S_g = 0, \quad t \leq 0 \text{ for all groups.}$$

To the code user this exception is achieved simply by not carrying out a steady state calculation first. (We may however need

FLX=0, Section 5.19,

if other calculations precede the current one.)

The present version of POW calculates the time variation of the flux following a prescribed pulsed (feedback-free) variation of some, usually physical, parameter from the steady state value. Two types of reactivity variation, $\lambda(t)$, are permitted:

(1) $\lambda(t)$ may be interpreted the same as λ used in a criticality SEARCH (Section 5.17)

or (2) $\lambda(t)$ may simply weight the effective number of neutrons produced from fission, $\lambda(t) \frac{\nu}{k}$ instead of the 'actual' $\frac{\nu}{k}$.

With a variation of type (1) we may thus carry out physical changes to

(i) vary concentrations (SUB1),

(ii) vary mesh spacing (SUB2),

or (iii) vary control absorber positions (SUB3).

On the other hand the variation of type (2) (normal for OD calculations) represents the response of the reactor following an unspecified physical change and may perhaps be attributable by an astute code user to a real cause.

In addition to a reactivity pulse we may specify a source pulse, that is we may follow the time variation of the flux following time variation of an external source (i.e. one not dependent of the neutron flux). Further, both reactivity and source type pulses are permitted concurrently in the one calculation, although this feature is probably of little use.

As before we start the main presentation with data required of a sample run (Section 6.2) for user familiarisation.

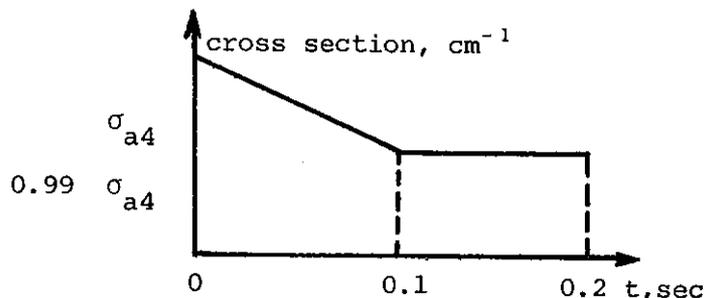
Notes:

(1) POW is not recommended for OD calculations. The reason is simply this - POW concentrates on not slowing down the normal lengthy part of the kinetics calculation, the point flux solution, and when this is trivial the overhead on data setting up is excessive.

(2) Future developments of POW should concentrate on speeding up of the kinetics calculation and the inclusion of feedback terms depending on the needs of reactor studies at the Research Establishment.

6.2 A Sample Run (MOATA)

Here we consider the sample run of Section 5.3 extended to follow the flux variation resulting from a time pulse of the FUEL thermal absorption cross section as sketched below



The steady state data is the same as before except as indicated.

Notes:

- (1) The neutron reaction data is given after the steady state calculation as we do not provide delayed fission spectrum data different to prompt.
- (2) Only 1 delayed group is considered here although normally we would use 6 (with data available from Keepin 1967).
- (3) We set up the required data pulse using both the XSD MODIFY feature (Section 5.11) and the post mixing feature available with the concentration SEARCH option (Section 5.17).

```
//JPPMOATA ...
//          CLASS=J,TIME=60
PRELUDE ... ,MAXM=5,MAXGD=1,MAXF=1  END
DEFN FUELV M(4)=M(1)  1          - FUEL  $\sigma$  without added leakage
BSQ(0) ...
START                          - steady state calculation
* KINETICS DATA FOLLOWS
VEL  1.84+9,7.04+6,5.91+5,2.39+5
IGD=1                          - only 1 delayed neutron group
BETAD=6.4-3
DLAMDA=0.08
SD                              - delayed spectrum the same as
                              prompt
DEFN FUEL M(5)=M(1)  1          - original FUEL with added leakage
XSD  MODIFY M(4)                - to set up  $0.01\sigma_{a4}$ 
4*1.-20                        remaining  $\sigma$  to be small
3*1.-20,0.01
20*1.-20
SEARCH(-0.01)                  - concentration SEARCH
WSEA  3*0,1,0
DEFN FUEL WSEA M(1)=M(5)  1 M(4)  -1  - we have  $\sigma_{a4}(M(1))=\sigma_{a4}(M(5))-$ 
                               $0.01\lambda\sigma_{a4}(M(4))$  otherwise
                               $\sigma(M(1))=\sigma(M(5))$ 
PULSE(21)=(0,0),(0.1,1),(0.2,1) - straight line segments describing
                              reactivity pulse
REACP  -21,1,0,0
DTS  8,0.015
CALC=REAL,KINETICS
ACCLAM=1.-3,ACCFO=1.-3
```

```

OUTPUT DATA PRINT
IOUT 0 1 - print every time step
START
* FOR ASYMPTOTIC REACTIVITY CALCULATION
CALC=REAL,EIGENV
ACCLAM=1.-4,ACCFO=1.-4 - restore usual accuracies
IOUT 0 0 - turn off PRINT (here every outer
           otherwise)
SEARCH(0) - turn off SEARCH
START - steady state calculation with
       thermal group
STOP FUEL absorption cross section of
: 0.99  $\sigma_{a4}$ 

```

6.3 The Functional Data Blocks in Brief

The sample run of the previous Section introduced us to the kinetic data of POW. Here we briefly look at the functional blocks required to be put together to carry out a kinetics calculation. All or some of the previously introduced blocks (Section 5.4) will be needed for the steady state calculation. Even so we will only emphasise functional blocks introduced earlier that contain new data that is specifically needed for the kinetics calculation proper. In subsequent Sections we detail the newly introduced functional blocks one by one.

As a further guide the user is reminded that an index is provided (Section 10).

The functional blocks consist of the following - essentially entered in indicated order:

- PRELUDE data - MAXF,MAXGD and MAXP (Section 5.6),
- Card group data - VEL,FER,IGD,BETAD,DLAMDA and SD(i) (Sections 5.8.5-5.8.10),
- Calculation type- CALC = REAL,KINETICS (Section 5.16),
- (6.4) Initial power specification - not necessarily required,
- (6.5) Time dependent pulses - data for setting up reactivity and source pulse descriptions,
- (6.6) Time integration step length - may be variable and must be user specified,
- (6.7) Calculation termination data - accuracy (see also Section 5.21),
- (6.8) Output requirement specification - to set content of output (see also Section 5.22),
- (6.9) Calculation START - may use a flux dump (RESTART) (see also Section 5.23), and

(6.10) EDIT data - essentially as before (Sections 5.24.5-5.27).

6.4 Initial Power Specification

The initial power is specified with the data

POWER = P,i (default values 0.,0)

where

- P is the required power in watts (per cm for slab geometry), except that if P=0 no change is made to the existing flux level, and
- i is an index nominating the additional reaction containing σ_f (3 for AUS libraries), which is multiplied by the corresponding material fission energy release FER (Section 5.8.6), except that if i=0 then P(\neq 0) is taken instead to be the required flux level.

6.5 Time Dependent Pulses

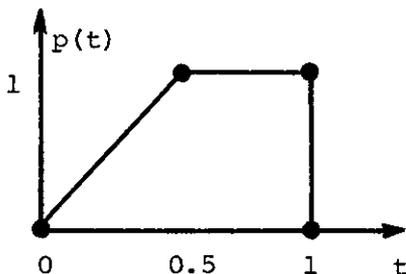
Neutrons may be injected into a reactor system in the form of pulses of either, or both, reactivity (say in the form of movement of control absorbers) or an external source (the emission from which is not dependent on the neutron flux in the reactor). We build up a pulse description as follows:

- (1) We describe the type of pulses we required with data following the keyword PULSE.
- (2) We relate reactivity variation with a particular train of pulses (REACP).
- (3) We relate the external source variation with a train of pulses (SCEP).

Each data item will be described in turn

6.5.1 PULSE description

- (i) We generate basic shapes (amplitude p as a function of time t), which are not necessarily scaled to the eventually required scale, using straight line segments or special functions as detailed later. Each basic shape, or combination of shapes, is entered in the form $\text{PULSE}(n) = (t_1, p_1), (t_2, p_2), \dots, (t_m, p_m)$ which describes PULSE type n ($21 \leq n \leq 40$) as consisting of straight line segments between the points indicated and obviously here all $t_\ell, \ell=1,2,\dots,m$ must be non-negative and given in non-descending order. For example



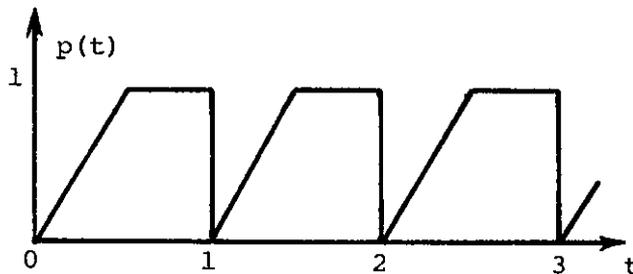
PULSE (21) = (0,0), (0.5,1), (1,1), (1,0)

Here and elsewhere all pulse types are treated as being cyclic so that the time used, t' , is given as

$$t < t_1, t' = t_m + (t - t_m) \bmod (t_m - t_1); \quad t_1 \leq t \leq t_m, t' = t;$$

$$t > t_m, t' = t_1 + (t - t_1) \bmod (t_m - t_1)$$

which makes the pulse periodic with period (perhaps as large as) $(t_m - t_1)$. The above example is thus interpreted as...



and we could well have taken the equivalent more compact definition
 $\text{PULSE}(21) = (0,0), (0.5,1), (1,1)$

(ii) We combine basic shapes n' to form a new pulse train $n (\neq n')$ thus

$$\text{PULSE}(n) = -n', r, (t_f, p_f),$$

where for most purposes

$(r > 0)$ is the number of required repeats of the basic shape n' ,

t_f = scale factor for the time, and

p_f = scale factor for the amplitude.

Thus if we have

$$\text{PULSE}(n') = (t_1, p_1), (t_2, p_2), \dots, (t_m, p_m)$$

then the interpretation for the new pulse train $n (r > 0)$ is

$$\text{PULSE}(n) = (t_f t_1, p_f p_1), (t_f t_2, p_f p_2), \dots, (t_f t_m, p_f p_m); (t_f (t_m + t_1), p_f p_1),$$

$$(t_f (t_m + t_2), p_f p_2), \dots, (t_f r t_m, p_f p_m)$$

For the situation $r=0$ we take the meaning

t_f = amount to be added to the time

p_f = amount to be added to the amplitude

then we have the interpretation

$$\text{PULSE}(n) = (t_f + t_1, p_f + p_1), (t_f + t_2, p_f + p_2), \dots, (t_f + t_m, p_f + p_m).$$

We multiply amplitudes of pulse trains using the indicator $r < 0$, where

$n'(\neq n)$ is the 1st pulse shape and $-r(\neq n)$ is the 2nd pulse shape. For this option (t_f, p_f) must be supplied as data, but the values are ignored. Thus if we have

$$\text{PULSE}(n') = (t_1, p_1'), (t_2, p_2'), \dots, (t_m, p_m')$$

$$\text{PULSE}(n'') = (t_1, p_1''), (t_2, p_2''), \dots, (t_m, p_m'')$$

then we have the interpretation, with $r=-n''$,

$$\text{PULSE}(n) = (t_1, p_1' p_1''), (t_2, p_2' p_2''), \dots, (t_m, p_m' p_m'') .$$

When the times t_ℓ for the two pulse trains do not coincide we use the elements of both as basis that is

$$\{t_\ell\} = \{t'_\ell\} \cup \{t''_\ell\}$$

and the values of p' and p'' are obtained on the new basis using linear interpolation (extrapolation is unnecessary since the PULSES are cyclic).

The definitions for basic shapes may be given in any order, however, for combinations the referenced pulse shapes must have been previously defined as the interpreted meaning is generated by the code when the definition is encountered. Any definition may include both basic shapes and combinations except combinations which would modify the definition being built up. For example, say we require 3 pulses of the type illustrated in (i) with $p(t)=0, t>3$ then we could achieve the required pulse train ($n=22$) using the data

$$\text{PULSE}(21) = (0,0), (0.5,1), (1,1)$$

$$\text{PULSE}(22) = -21 \quad 3, (1,1) \quad (3,0), (1.E20,0)$$

however the definition

$$\text{PULSE}(22) = (0,0), (0.5,1), (1,1) \quad -22 \quad 3, (1,1) \quad (3,0), (1.E20,0)$$

would be illegal.

- (iii) Some standard basic shapes are also available. These are identified with pulse type $n' < 20$. The general structure is a basic FORTRAN coded form

$$\text{PULSE}(n') = p_n(t)$$

which must be computed on a designated ordered point set t_1, t_2, \dots, t_m before the shape can be used further (as a table of values rather than as a function). The required point set is indicated in a special way with $\text{PULSE}(0)$ thus ...

$$\text{PULSE}(0) = t_1, t_2, \dots, t_m$$

We then take

$$\text{PULSE}(n) = \underbrace{-n' \ 0 \ (t_a, p_a)}_{\text{optional}} \ -n' \ 1 \ (t_f, p_f)$$

(the underlined is optional and if not given $t_a=0$ and $t_b=0$)
which gives us the interpretation

$$\text{PULSE}(n) = (t_1, p_1), (t_2, p_2), \dots, (t_m, p_m)$$

$$\text{where } p_\ell = p_f p_n (t_f t_\ell + t_a) + p_a$$

For example

$$\text{PULSE}(2) = \sin 2\pi t$$

hence if we use the data

$$\text{PULSE}(0) = 0. (0.01) 1.$$

$$\text{PULSE}(21) = -2.0, (0.02, 0) \ -2, 1, (0.5, 0.1)$$

we have the interpretation

$$\text{PULSE}(21) = 0.1 \sin(\pi t + 0.02)$$

evaluated at $t=0., 0.01, \dots, 1.$

The presently available standard shapes are listed below.

$\text{PULSE}(1)$ = amplitude returned from a user supplied (REAL*4)FUNCTION

$\text{PULSE},$

$P = \text{PULSE}(T)$ (which must be written in the style of the user subroutines,
Section 5.27, with a side entry SPULSE provided for variable
'COMMON')

$$\text{PULSE}(2) = \sin 2\pi t$$

$$\text{PULSE}(3) = \cos 2\pi t$$

$$\text{PULSE}(4) = e^t$$

As a further example say we require the pulse shape,

$$p(t) = 0.1 e^{-0.01t} \cos 2\pi t, 0 \leq t \leq 5, \text{ zero otherwise.}$$

We could generate the required data thus

$$\text{PULSE}(0) = 0. (0.05) 5. \quad t_1=0, t_1=0.05, \dots, t_{101}=5$$

$$\text{PULSE}(21) = -3 \ 1, (1, 0.1) \quad p_{21}(t) = 0.1 \cos 2\pi t$$

$$\text{PULSE}(22) = -4 \ 1, (-0.01, 1) \quad p_{22}(t) = e^{-0.01t}$$

$$\text{PULSE}(23) = -21 \ -22, (1, 1) \quad p_{23}(t) = 0.1 e^{-0.01t} \cos 2\pi t' \text{ but with}$$

$t' = t \bmod 5$ (that is the pulse repeats
again for $t < 5$)

$\text{PULSE}(21) = -23 \ 1, (1, 1), (5, 0), (1.E20, 0)$ as above but with $p_{21}(t) = 0$
for $t < 5.$

Here we emphasise the fact that the PULSE data must all be
contained in the PULS array dimensioned

REAL*4 PULS(2,MAXP) (equivalent to the array IPULS(2,MAXP))

with MAXP (default value 50) assigned in the user's PRELUDE (Section 8.1.2). The array is used thus...

IPULS(1&2,1) = index for next PULSE entry, length of index table
(default 22)

IPULS(1&2,2) = index for PULSE(0) entry, length of compacted PULSE(0)
definition

IPULS(1&2,3) = index for PULSE(21), length of PULSE(21) definition

IPULS(1&2,22) = index for PULSE(40), length of PULSE(40) definition

PULS(1&2,23) = 1st PULSE used t_1 , 1st PULSE used p_1

PULS(1&2,IPULS(1,n-18)) = PULSE(n, $21 \leq n \leq 40$) t_1 , PULSE(n, $21 \leq n \leq 40$) p_1

PULS(1&2,IPULS(1,2)) = PULSE(0) t_1 , PULSE(0) t_2 (or t_1 if t_2 is not
given)

For the preceding example we must thus have at least

MAXP=378 (i.e. 22+51 (PULSE(0) times) +101+101+101+2)

We may save core storage by redefining a PULSE no longer required even to the extent of providing no data with the definition, for example, PULSE(21), or if we require the whole table to be cleared for subsequent use we simply use the data PULSE by itself. An adjustment of length of a definition is automatically made if redefinition occurs and the size of the table is adjusted accordingly. (We should perhaps note that whenever PULSE(n) data is encountered the data for n goes at the end of the table, even if PULSE(n) is being redefined.)

6.5.2 REACP, REACTivity Pulse

Reactivity is inserted (or removed) from the reactor under study following a specified variation of $\lambda(t)$, where λ variation is interpreted in the same way as for a criticality SEARCH (Section 5.17) and indeed the same SEARCH data must be provided (except that if we have SEARCH(0), the default option, the effective multiplication is adjusted. We may thus

- (i) vary concentration of a material constituting part of material filling the reactor (SEARCH(-0.01))
- (ii) vary the size of indicated regions (SEARCH(-0.02)), or
- (iii) vary the positions of banks of control absorbers (SEARCH(-0.03)) as a function of time following a selected PULSE train (Section 6.5.1).
As additional features we may also
- (iv) vary the effective multiplication ($\lambda(t)/k$ multiplies the fission emission), or
- (v) vary quantities coded by the user in SUB4,...,SUB9.

Selection of the required reactivity option is made with the data

REACP n, r₂, r₃, r₄ (default values 0,1.,1.,0.)

where

-|n| designates a PULSE train, except that zero implies that forced reactivity variation is not required, and

$$\lambda(t) = \beta^* r_2 p_{|n|}(t) + r_3 + r_4 \lambda_s$$

with $\beta^* = \begin{cases} 1 & \text{if } n < 0 \\ \beta, & \text{the total delayed neutron fraction, if } n > 0 \end{cases}$
and,

λ_s = eigenvalue from previous steady state calculation (for control absorber SEARCH).

We should note that when a criticality SEARCH is carried out the eigenvalue multiplying say the concentration (SEARCH(-0.01)) or the mesh widths (SEARCH(-0.02)) is absorbed into data held in core. (That is before a criticality SEARCH we have $\lambda=1$ and if after a SEARCH $\lambda=2$ then the concentration or mesh widths would be twice the values supplied by the user and λ would start again at 1 for any subsequent calculation). With the adjustment of control absorbers, however (SEARCH(-0.03) - Section 5.17), λ specifies an absolute value rather than a relative value and we should note that POW does not correctly cope with moving fuel regions as the precursors do not move with the fuel.

The specification of $\lambda(t)$, the reactivity pulse, then becomes clear. For a pulse about the critical position we require

$$\lambda(t) = \beta^* r_2 p_{|n|}(t) + 1 \text{ (SEARCH(-0.01) or SEARCH(-0.02))}$$

or $\lambda(t) = \beta^* r_2 p_{|n|}(t) + \lambda_s$ (SEARCH(-0.03)) (say control absorber moved out 10 cm from critical position)

and for a pulse of a desired physical magnitude (say control absorber completely out of the reactor) we require

$$\lambda(t) = \beta^* r_2 p_{|n|}(t).$$

6.5.3 SCEP, fixed external Source Pulse

We enter the spatial fixed external source shape and group dependence into the array FSCE using either direct entry (FSCE) or element entry (FSCEL) as for a SOURCE calculation - Section 5.18. Selection of the required PULSE train to be associated with the spatial and group data held in the FSCE array at the time of encountering the present Keyword is made with the data

SCEP -n (default value is 0)

where n designates a PULSE train, except that zero implies that an external source is not required.

In addition to selecting the required PULSE train (or 0 if not required) the data held in the FSCE array is written onto disk (FORTRAN unit 12) for ease of recall when required. During a kinetics calculation the array FSCE contains all sources in addition to any external source. The time dependent external source is then given by

$$S(I,J,G,t) = \underset{\text{disk}}{\text{FSCE}(I,J,G)} p_n(t).$$

As a simple example say we require PULSE train 23 and a centre source with strength 0.8 in group 1 and 0.2 in group 2 then we could use the data FSCE 100000*0 (if this is not the 1st calculation since kinetics calculations use FSCE)

FSCEL (1,1,1-2) = 0.8,0.2

SCEP -23

6.6 Time Integration Step Length

For the present version of the code the user must supply the time integration step lengths, δt seconds, to be used during the course of the calculation. The specification is carried out thus...

DTS n,d,T (default values all zero)

where $n = \begin{cases} \text{-ve selects PULSE } (|n|), \text{ a train of all +ve amplitudes,} \\ \text{then } \delta t = p_{|n|}(t) d, \\ 0 \text{ selects PULSE}(0) \text{ as the set of required } t\text{'s for the calculation,} \\ \text{+ve sets } \delta t=d, T=n\delta t \text{ (if } T \text{ not given), and} \end{cases}$

T = time at or beyond which the calculation is to terminate. The calculation also terminates (as an error) if

$\delta t \leq 0$ for any time encountered in the calculation (say at the end of PULSE(0) data).

For example say we require the following time steps

$0 \leq t < 0.01$, $\delta t = 5.-3$

$0.01 \leq t < 0.1$, $\delta t = 0.05$

$0.1 \leq t < \infty$, $\delta t = 0.1$

then we could use the data

PULSE(21) = (0,5.-3),(0.01,5.-3),(0.01,0.05),(0.1,0.05),(0.1,0.1),(1.E20,0.1)

DTS -21,1,0.3

As a guide in the selection of step length we should attempt to choose δt so that the power (or flux) does not increase by more than say 20% in the step. Larger time steps may however be tolerable as the method used is stable.

6.7 Calculation Termination Data

The calculation termination data is the same as introduced earlier (Section 5.21), however, on account of errors introduced by the (generally large) time step length the normal accuracy used for neutron balance (ACCLAM=1.-4) and fission source (ACCFO=1.-4) are usually warranted. After the steady state calculation we should perhaps change the accuracies thus

ACCLAM=1.-3 ACCFO=1.-3

which have been found to be usually adequate. We may also limit the number of outer (fission source) iterations per time step compared to the code default value of NOL=100. If the limit is exceeded the code continues with the next time step. Normally changing NOL is only necessary with OD calculations where 2 iterations are always carried out on account of the way POW assesses convergence. With OD calculations we may thus use

NOL=1

to save some computer time.

6.8 Output Requirement Specification

The same type of OUTPUT is possible with a kinetics calculation as for a steady state calculation (Section 5.22). With the kinetics calculation however, unless otherwise set, OUTPUT is not produced after each convergence of the flux (that is every time step) but only if the specific kinetics time limit or computer run time limit is exceeded. We may however produce intermediate OUTPUT after every so many time steps. For example with

```
OUTPUT DATA PRINT FLUX
IOUT      0      5      10
```

we would obtain PRINTed flux OUTPUT for time steps 5,10,15,... and the final step and RESTARTable FLUX OUTPUT on disk for time steps 10,20,30,... and the final step.

In order to understand a flux dump the user should note that volume integrated precursor concentrations are stored (at least during part of the calculation) as if they were flux for additional groups ϕ_{NG+i} , $i=1,2,\dots,IGD$ (and the additional groups may be forced to PRINT if we use the data underlined NSD=0,1).

6.9 Calculation START

We start a kinetics calculation with exactly the same data as before, START or RESTART (Section 5.23).

Note: A flux dump is only produced at the completion of a time step and hence a RESTART begins for the step following the last completed time step. We may however begin earlier using the AFTER option

(Section 5.23), for example

AFTER 2 RESTART

6.10 EDIT Data

We may EDIT data as for a steady state calculation (Sections 5.24-5.27), that is after the calculation is finished (the specified time limit has been exceeded) or we may interrupt the calculation by specifying a time limit short of that ultimately required. After EDITing we may continue the calculation by simply specifying a time limit further along towards the ultimate time required and by using the data

RESTART CONTINUE

which is equivalent to a RESTART from a disk FLUX dump except that information in core is used. Alternatively we may save up a series of FLUX dumps for different time steps and we may EDIT these after the calculation has finished (provided any required time dependent data is available) thus

NIL=0 (no inner iteration, thereby preventing further computation)

AFTER 1 RESTART EDIT...

AFTER 2 RESTART EDIT...

⋮

NIL=100 (restoring the limit to the number of inner iterations).

7. CONCLUSIONS

The writing of POW was necessary as a module of the AUS scheme and as such the undertaking has proven to be worthwhile. To what extent the code will be extended will very much depend on needs of our reactor studies on site.

Future developments of the AUS scheme should include interactive (terminal oriented) input/output. To what extent POW will directly share in the interactive input output is not clear at present.

8. ACKNOWLEDGEMENTS

The general encouragement and detailed help of fellow AUS module writers, particularly Mrs. Baiba Harrington and Mr. Graham Robinson, is gratefully acknowledged. As well Baiba wrote some of the output and edit routines of POW and Graham undertook extensive calculations on fast critical experiments. Thanks are also due to Applied Mathematics and Computer Section staff, particularly Dr. Gordon Cox for the Assembler version of the SLOR routine and second shift computer operators for hastening debugging runs through the queue.

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MOATA (X,Y) CALCULATION, GYMER DATA

M(-1)

EDIT -1 0 0 0

LEGEND

— X PLOT 1, GROUP 1
- - - X PLOT 6, GROUP 1

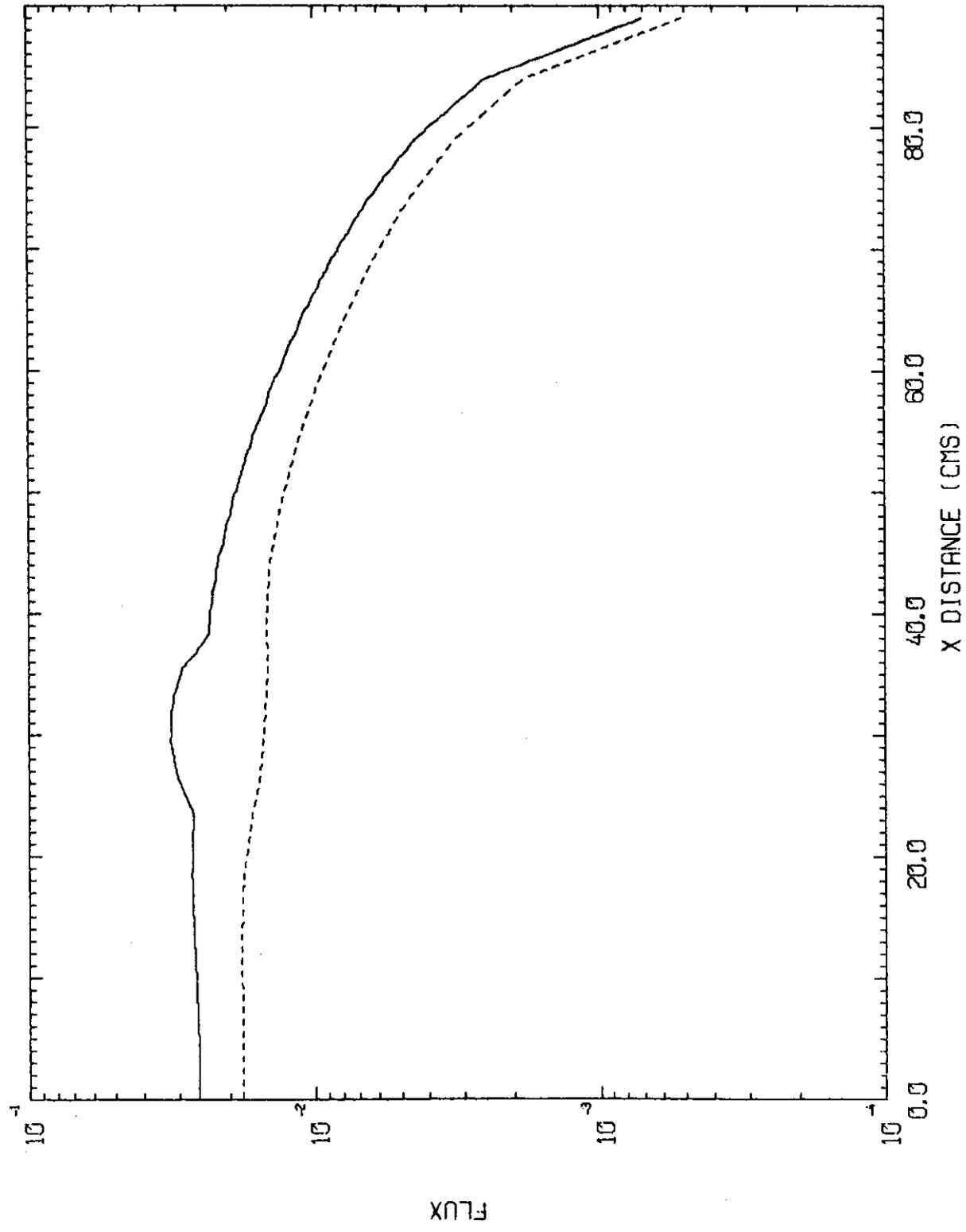


FIGURE 1. X-DIRECTION PLOTS OF MOATA THERMAL FLUX

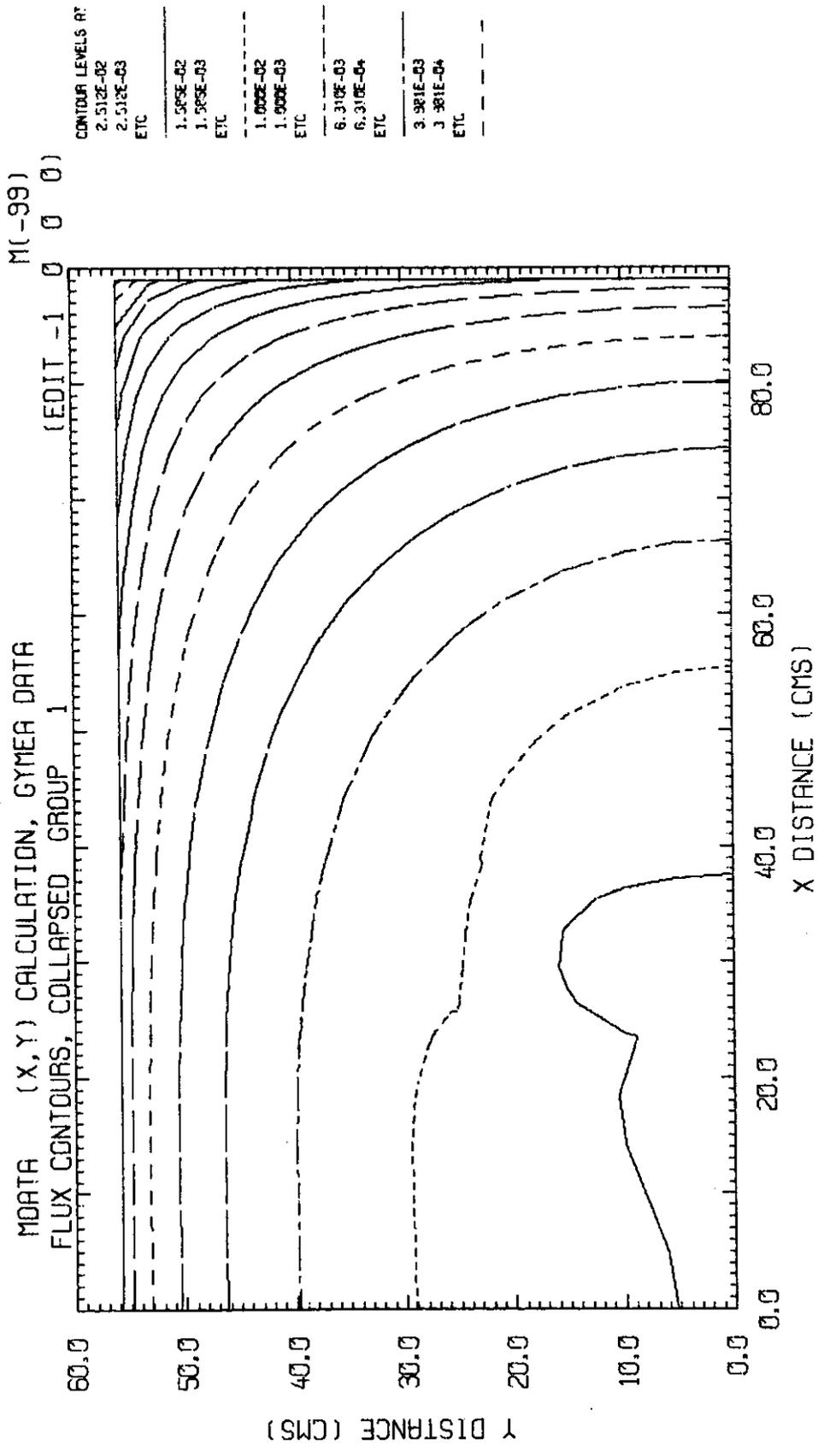


FIGURE 2. CONTOUR PLOT OF MOATA THERMAL FLUX

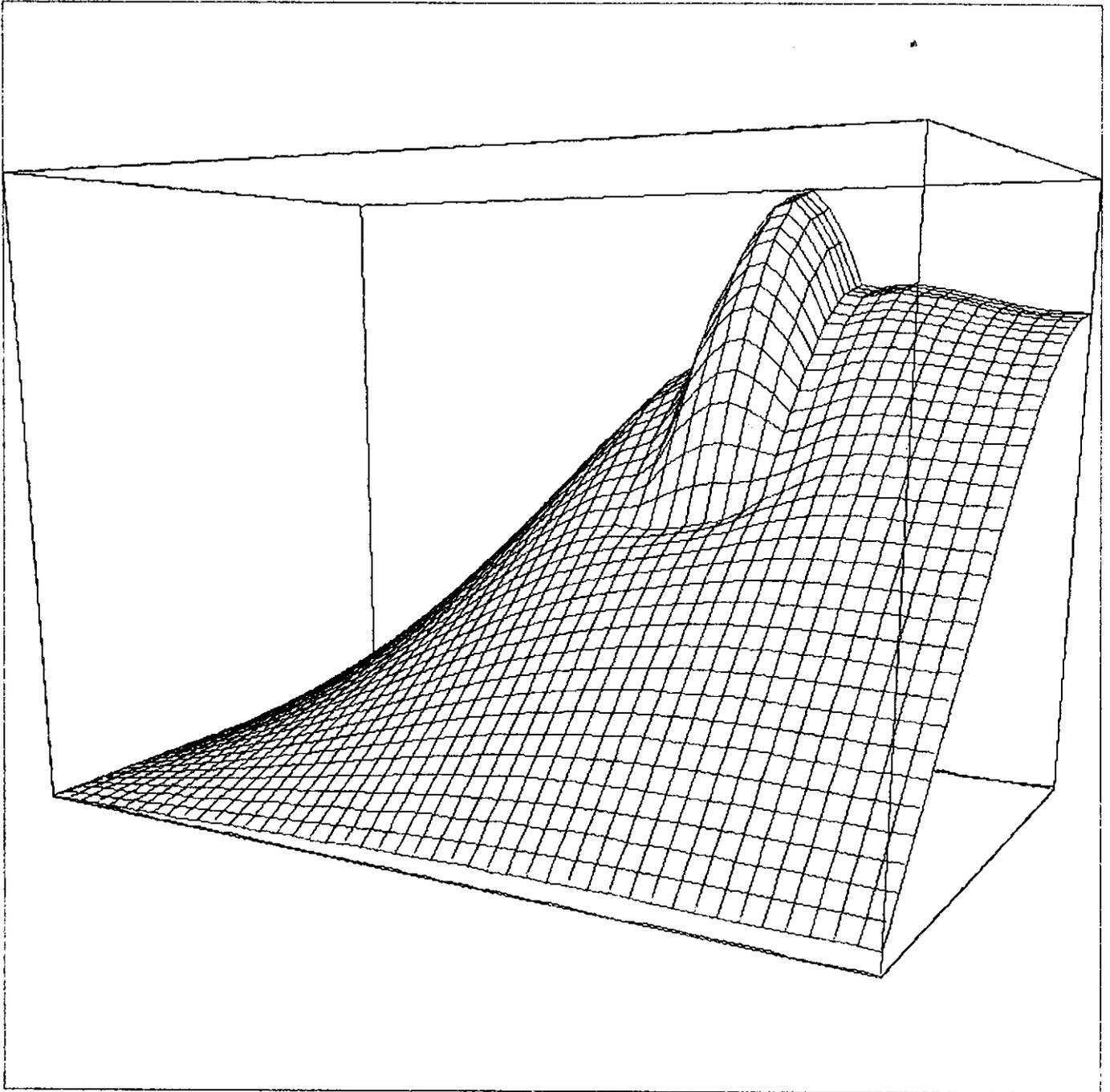


FIGURE 3. (X,Y) PLOT OF MOATA THERMAL FLUX

APPENDIX A

AUS MODULE ASPECTS OF POW

A1 System Aspects

AUS, A modular Scheme for reactor neutronics computations, was designed, and is being evolved, to undertake general reactor calculations required as support to the site experimental programme. On account of the developing nature of the work on AUS, documentation will exist only for local use until modules, such as POW, are sufficiently stabilised in their growth. The scheme, unlike some overseas, uses loosely linked reasonably self-contained modules. The modules may run as stand alone or as part of the AUS scheme. The choice of this type of structure arose out of the following considerations...

- (1) modules of the GYMEA system (Pollard and Robinson 1969) could be used with non-extensive modification,
- (2) the scheme could be quickly implemented to a minimal working stage (3 people were originally involved for about 6 months each), and
- (3) the scheme can include borrowed codes without extensive modification being involved.

Unlike the GYMEA system which relied on programme creation of exact copy card input data for each module AUS uses some well defined data pools (libraries). A figure (see p.A4) sketches the way 4 of the modules (GYMEA, Pollard and Robinson 1969; POW, this report; WDSN, Francescon 1963; ICPP, Doherty 1969) are coupled together along with required data pools.

The POW default coupling of FORTRAN units (e.g. 1) to disk data sets (e.g. DD2) is the following...

LINK POW

(1,DD2),	card input follows *DD2 card
(2,DD12),	card punch output
(3,DD13),	printer output
(4,DD57),	%COMMON and standard POW data
(5,DD21),	SCRATCH for coefficient matrix (if insufficient core and kinetics)
(6,DD35),	GEOM data (READ REG)
(7,DD14),	SCRATCH for alternate card input or output (READ CARD LIB) - also used by EDIT 0
(8,DD31),	Hansen-Roach (or ABBN) library
(9,DD36),	FLUX dump (FL1)
(10,DD33),	temporary XSLIB (XS1)
(11,DD34),	temporary XSLIB (XS2)

(12,DD22), SCRATCH for external source (kinetics)
 (13,DD23), SCRATCH for precursor concentrations (kinetics)
 (14,DD24), SCRATCH for all XS (kinetics)
 (15,DD25), SCRATCH for fission source (kinetics)
 (16,DD98), dummy data set used with EDIT 0
 (AEPLOT,DD11) plotter output

A POW user may for example require the card punch output to be switched to temporary data set DD20. He would enter the required path statement (written in the FOREX language, Robinson 1968) thus

```
*DD1
STEP *
      LINK POW (2,DD20)
      END
```

STOP

*DD2

PRELUDE...

which as an example in no way indicates the dynamic path selection possible with AUSYS (an AELINK, Mason and Richardson 1969, control programme).

A2. Datapool Aspects

Datapools of the AUS system are simple structured sequential disk data sets which can normally be read using FORTRAN. The XSLIB, however, is specially compacted for easy skipping of materials and special AUS routines are necessary to unbuffer the data. The special routines can also filter out data not interpreted by some modules. As far as a POW user is concerned the main interest here would be in the cross section library (XSLIB) and then probably only in the reaction cross sections available.

In addition to scattering matrices (P_0, P_1, \dots), for each group and potential scattering cross section a material can have up to 20 reaction entries (mostly cross sections) of which the first 10 are dedicated to the following reactions...

- 1 ~ σ_{tr} , transport cross section,
- 2 ~ σ_a , absorption cross section,
- 3 ~ $\nu\sigma$, fission emission cross section,
- 4 ~ σ_p , potential scattering cross section,
- 5 ~ σ_{tot} , total cross section,
- 6 ~ σ_f , fission cross section,
- 7 ~ σ_{b1} , 1st burnup reaction, usually σ_γ , radioactive capture
- 8 ~ σ_{b2} , 2nd burnup reaction,

9 ~ D_r , r direction anisotropic diffusion coefficient, and
 10 ~ D_z , z direction anisotropic diffusion coefficient.

Reactions 1 to 3 are required as standard data for POW. Up to MAXS (PRELUDE data, Section 5.6) additional reactions are stored in core thus...

$$\sigma_{r1} = \sigma_p ,$$

$$\sigma_{r2} = \sigma_{tot} ,$$

$$\sigma_{r3} = \sigma_f ,$$

$$\sigma_{r4} = \sigma_{b1} ,$$

$$\sigma_{r5} = \sigma_{b2} ,$$

$$\sigma_{r6} = \text{11th entry} ,$$

$$\sigma_{r7} = \text{12th entry, etc.} ,$$

and if D_r and D_z are available they are entered into the appropriate POW data array (DCX(i) and DCY(i), Section 5.8.3).

Note: With a resonance tabular library we must have $\text{MAXS} \geq 2$.

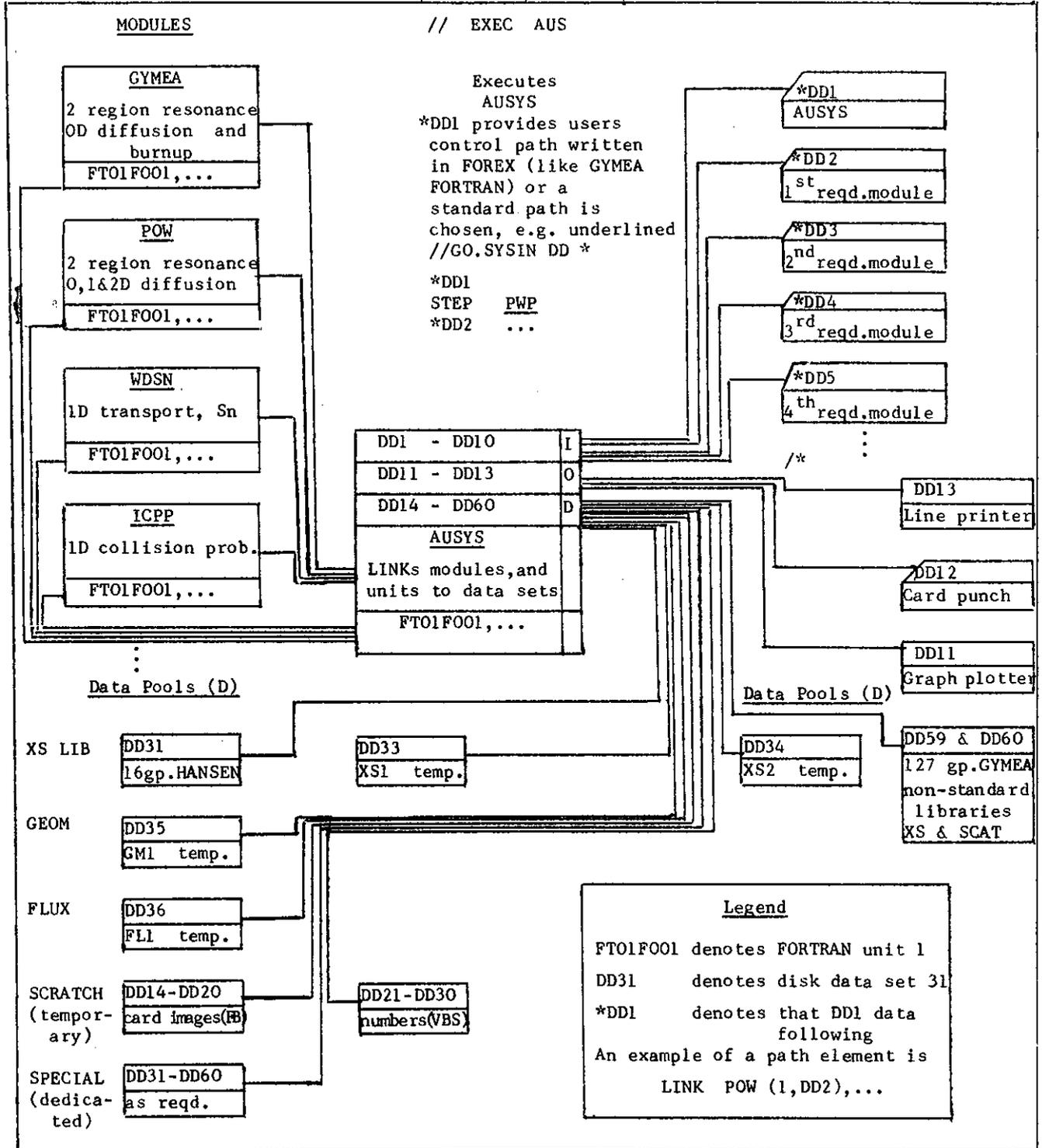
IBM 360/50
Operating System (OS)
HASP or MVT

Card
Inputs (I)

Readable
Outputs (O)

AUS cat. procedure

//GO.SYSIN DD *



A SKETCH OF THE COUPLING OF SOME AUS MODULES AND DATA POOLS

APPENDIX B
26 GROUP ABBN XSLIB

The well known Russian cross section set (Bondarenko et al. 1964) is available as an AUS library and may be obtained on POW's FORTRAN unit 8 by using:

```
// EXEC AUS,LIB=ABBN
```

Data in the library is for three temperatures (300, 900, 2100 K) and cross sections for various materials are shown in Table B1.

TABLE B1
ABBN DATA SET

No.	Mat.	Co Range	Temps.	Scat.*
1	H	-	1	2
2	D	-	1	2
3	LI6	-	1	2
4	LI7	-	1	2
5	BE	$\infty, 10, 1, 0$	1	2
6	B10	-	1	2
7	B11	-	1	2
8	C	$\infty, 10, 1, 0$	1	2
9	N	$\infty, 10, 1, 0$	1	2
10	O	$\infty, 10, 1, 0$	1	2
11	NA	$\infty, 10^3, 10^2, 10$	1	1
12	MG	$\infty, 10^3, 10^2, 10$	1	1
13	AL	$\infty, 10^3, 10^2, 10, 1, 0$	1	1
14	SI	-	1	1
15	K	$\infty, 10^3, 10^2, 10$	1	1
16	CA	-	1	1
17	TI	$\infty, 10^3, 10^2, 10$	1	1
18	V	$\infty, 10^3, 10^2, 10$	1	1

TABLE B1 (Cont'd.)

No.	Mat.	σ Range	Temps.	Scat.*
19	CR	$\infty, 10^2, 10, 1, 0$	1	1
20	FE	$\infty, 10^2, 10, 1, 0$	1	1
21	NI	$\infty, 10^2, 10, 1, 0$	1	1
22	CU	$\infty, 10^3, 10^2, 10, 0$	1	1
23	ZR	$\infty, 10^3, 10^2, 10, 0$	3	1
24	NB	$\infty, 10^3, 10^2, 10, 0$	3	1
25	MO	$\infty, 10^3, 10^2, 10, 0$	3	1
26	TA	$\infty, 10^5, 10^4, 10^3, 10^2, 10, 0$	3	1
27	W	$\infty, 10^4, 10^3, 10^2, 10, 0$	3	1
28	RE	$\infty, 10^4, 10^3, 10^2$	3	1
29	PB	$\infty, 10^2, 10, 0$	1	1
30	BI	$\infty, 10^3, 10^2, 10, 0$	1	1
31	TH232	$\infty, 10^4, 10^3, 10^2, 10, 0$	3	1
32	U233	$\infty, 10^3, 10^2, 10, 0$	3	1
33	U234	$\infty, 10^5, 10^4, 10^3, 10^2$	3	1
34	U235	$\infty, 10^3, 10^2, 10, 0$	3	1
35	U236	$\infty, 10^5, 10^4, 10^3, 10^2$	3	1
36	U238	$\infty, 10^4, 10^3, 10^2, 10, 0$	3	1
37	PU239	$\infty, 10^3, 10^2, 10, 0$	3	1
38	PU240	$\infty, 10^6, 10^5, 10^4, 10^3, 10^2$	3	1
39	PU241	-	1	1
40	PU242	$\infty, 10^5, 10^4, 10^3$	3	1

*Scat. 1 = P₀, 2 = P₀ & P₁

The group boundaries are given in Table B2.

TABLE B2
GROUP BOUNDARIES FOR THE ABBN DATA SET

No.	Energy, E	Lethargy, u	δu
1	10.0 - 6.5 MeV	0.0 - 0.43	0.43
2	6.5 - 4.0 MeV	0.43 - 0.92	0.48
3	4.0 - 2.5 MeV	0.92 - 1.39	0.48
4	2.5 - 1.4 MeV	1.39 - 1.97	0.57
5	1.4 - 0.8 MeV	1.97 - 2.52	0.57
6	0.8 - 0.4 MeV	2.52 - 3.22	0.69
7	0.4 - 0.2 MeV	3.22 - 3.91	0.69
8	0.2 - 0.1 MeV	3.91 - 4.60	0.69
9	100. - 46.5 KeV	4.60 - 5.37	0.77
10	46.5 - 21.5 KeV	5.37 - 6.14	0.77
11	21.5 - 10.0 KeV	6.14 - 6.91	0.77
12	10.0 - 4.65 KeV	6.91 - 7.67	0.77
13	4.65 - 2.15 KeV	7.67 - 8.44	0.77
14	2.15 - 1.0 KeV	8.44 - 9.21	0.77
15	1000. - 465. eV	9.21 - 9.98	0.77
16	465. - 215. eV	9.98 - 10.75	0.77
17	215. - 100. eV	10.75 - 11.51	0.77
18	100. - 46.5 eV	11.51 - 12.28	0.77
19	46.5 - 21.5 eV	12.28 - 13.05	0.77
20	21.5 - 10.0 eV	13.05 - 13.82	0.77
21	10.0 - 4.65 eV	13.82 - 14.58	0.77
22	4.65 - 2.15 eV	14.58 - 15.35	0.77
23	2.15 - 1.0 eV	15.35 - 16.12	0.77
24	1.0 - 0.465 eV	16.12 - 16.88	0.77
25	0.465 - 0.215 eV	16.88 - 17.66	0.77
26	0.0253 eV	-	

Note: Calculations on fast reactor experiments (Robinson, unpublished) indicate that the fissionable materials are somewhat too reactive. No adjustments have been made to the library however.

APPENDIX C

16 GROUP HANSEN-ROACH XSLIB

The Hansen-Roach data set (1961), found to be very reasonably accurate for fast reactor critical mass assessments, is available to POW on FORTRAN unit 8.

Data in the library is given in Table C1 at one temperature (300 K) and only two additional reactions (σ_p and σ_{tot}) are available here.

TABLE C1
HANSEN-ROACH DATA SET

No.	Mat.	Data Source	Mod.	σ_p Range	Scat.*	Recom. No.
1	H	HANSEN	ORIG	-	1	2
2	HP01	"	"	-	2	1
3	D	"	"	-	1	2
4	DP01	"	"	-	2	1
5	LI6	"	"	-	1	1
6	LI7	"	"	-	1	1
7	BE	"	"	-	1	1
8	B	"	"	-	1	1
9	C	"	"	-	1	1
10	N	"	"	-	1	1
11	O	"	"	-	1	1
12	F	"	"	-	1	1
13	NA	"	"	-	1	1
14	AL	"	"	-	1	1
15	CL	"	"	-	1	1
16	K	"	"	-	1	1
17	CR	AEROJET	"	-	1	1
18	FE	HANSEN	"	-	1	1
19	CO	"	"	-	1	1
20	NI	"	"	-	1	1
21	ZR	"	"	-	1	1
22	NB	"	"	-	1	1
23	MO	"	"	-	1	1
24	CD	"	"	-	0	1
25	CE	"	"	-	1	1

TABLE C1 (Cont'd.)

No.	Mat.	Data Source	Mod.	σ_p Range	Scat.*	Recom. No.
26	TA	HANSEN	ORIG	-	1	1
27	PBP01	EDISON	"	-	2	1
28	TH	HANSEN	"	-	1	1
29	U233	"	"	$10^{20}-20$	1	1
30	U235	"	"	"	1	1
31	U235	REVHAN	"	"	1	2
32	U238	HANSEN	"	"	1	1
33	U238	REVHAN	"	"	1	2
34	PU239	HANSEN	"	"	1	1
35	PU240	"	"	$10^{20}-50$	1	1

* Scat. 1 = P_0 , 2 = P_0 & P_1

The group boundaries are given in Table C2.

TABLE C2
GROUP BOUNDARIES FOR HANSEN-ROACH DATA SET

No.	Energy, E	Lethargy, u	δu
1	10.0 - 3.0 MeV	0. - 1.20397	1.20
2	3.0 - 1.4 MeV	1.20397 - 1.96611	0.76
3	1.4 - 0.9 MeV	1.96611 - 2.40795	0.44
4	0.9 - 0.4 MeV	2.40795 - 3.21888	0.81
5	0.4 - 0.1 MeV	3.21888 - 4.60517	1.39
6	100 - 17 keV	4.60517 - 6.37713	1.77
7	17 - 3 keV	6.37713 - 8.11173	1.73
8	3000 - 550 eV	8.11173 - 9.80818	1.70
9	550 - 100 eV	9.80818 - 11.5129	1.70
10	100 - 30 eV	11.5129 - 12.7169	1.20
11	30 - 10 eV	12.7169 - 13.8155	1.10
12	10 - 3 eV	13.8155 - 15.0195	1.20
13	3 - 1 eV	15.0195 - 16.1181	1.10
14	1 - 0.4 eV	16.1181 - 17.0344	0.92
15	0.4 - 0.1 eV	17.0344 - 18.4207	1.39
16	0.1 - 0.001 eV	18.4207 - 23.	4.58

Note: The default option for a material with more than one data entry corresponds to the material with the highest recommendation number.

Thus

XSD U238 M(1) \equiv XSD U238,REVHAN,ORIG M(1)

(Section 5.9.1)

APPENDIX D

DTAV FREE INPUT AND DUMP ROUTINES

D1 Introduction

The use of free format input for neutronics codes is now no longer disputed even by the hardened FORMAT (6E12.5) 'fans'. For codes like POW requiring extensive amounts of data, some of which may be optional, several approaches have been available for some time. Most of the features of existing routines developed overseas were incorporated into the site SCAN (Bennett and Pollard 1967) so that SCAN could do almost any free input task. The main bugbear with SCAN is that it requires an extensive driving routine to do even the simplest job. For example with the data used by XSEEDIT (GYMEA report of Pollard and Robinson 1969)

DATA U235,...

1.23-2,...

...

...

DATA U238,...

the underlined keyword not only had to be read and identified but also had to not be passed over should a short extent of data be given for one nuclide (the data overrun problem). With GYMEA (Pollard and Robinson 1969) certain keywords such as

GSCE

also required data following to be stored in an array of the same name. The POW routines DTAV (Pollard unpublished) were written as a driver control routine for SCAN to greatly simplify the identification and storage of data, thereby easing the task of the programme author (as well as the programme user).

D2 Overview of DTAV

Data for the DTAV input routines consists of essentially two parts, (1) DTACOM data to set up a table of keywords (which actually includes the programme COMMON or labelled COMMON cards) and (2) DTAIN data consisting of KEYWORD data where KEYWORD is (usually) the FORTRAN variable name of an array to contain data to follow and data is (usually) numeric data punched in any mode (i.e. 1E1.31.DO) but which is converted to the mode of KEYWORD.

In addition to the free input feature briefly described, the DTAV routines also include a printer dump routine (DTADMP) which labels the variables and prints data contained by the variables (COMMON is zeroised first to prevent rubbish data from being printed here) and a PRELUDE generating routine (or the name indicated) for setting up 'variable dimensioned COMMON'.

In the next few Sections we introduce certain user oriented features (as distinct from programmer oriented features) of DTAV as a possible help to system minded POW users - others have read far enough.

D3 DTAIN Input

The DTAIN input routine has itself 3 special keywords,

- (i) %COMMON,
- (ii) %OPT, and
- (iii) %MOD

described below.

(i) If %COMMON appears as first data (starting column 7), rather than PRELUDE, the remaining data to the keyword %END (starting column 7) replaces the POW special data held on FORTRAN unit 4. The layout of (part of) the data POW requires between the special keywords %COMMON and %END is given on the printer if we use the control word

PRINT

in the user's PRELUDE (Section 5.6).

(ii) The listing of all input data is vital to a code such as POW. A user tends to keep output listings but not input decks (since these are usually being continually evolved). A user may however change the listing option (perhaps to prevent cross section data from being printed for many group problems) with the data (given anywhere in non-PRELUDE input)

%OPT *l,m,n* %

where

- l* = 1st column of card to be scanned, usually 1,
- m* = last column of card to be scanned usually 72, and
- n* = listing option, 0 for no listing, ≠ 0 for listing.

(iii) A quick perusal of %MOD output made to PRINT as in (i) shows the structure of separate data items of the general form

(Keyword, address, (*4) length, mode, option)

where

- mode 1 = fixed point,
- 2 = *4 floating point,
- 3 = *8 floating point, and
- 4 = alphanumeric, and option is tested in POW's DTAIN control routine.

As a simple example of a possible application say we want to supply data to a user written subroutine, SUB9 (Section 5.27). We could set up data to be stored in the 4 (*8) neighbouring temporary data variables of COMMON WA, WB, WC and WD thus

```
§MOD (SUB9D,WA,8,3,0) §
```

The data would then be entered (as *8 type) in the successive variables WA,WB,WC,WD using

```
SUB9D 5,1.723D2,0.003,0 CALL SUB9
```

For alphanumeric data we would similarly use

```
§MOD (SUB9A,WA,4,4,0) §
```

```
SUB9A MOATA,MOATA1 CALL SUB9
```

As a further less desirable possibility a user could change standard keywords to names of his own choosing. If many new keywords are added using the feature described here we may need to increase the table size set in the subroutine SZECOM. Presently we have

```
SUBROUTINE SZECOM
```

```
COMMON/CSIZE/LBCOM,LSCOM
```

```
COMMON/SCANT/S(1806)          - 6 words for each keyword
```

```
LSCOM=1806
```

```
CALL CMSIZE(LBCOM)
```

```
RETURN
```

```
END
```

D4 DTADMP Printer Dump

Vital to development of a large code is ready print out of labelled variables of the programme during initial stages. Much of the usefulness of POW's printer dump feature is now lost, however we give brief details here.

The POW data required to set up the dump consists of

- (i) LIST, which sets a list of the variables required
- (ii) IDMP, which selects the portion of LIST required for a dump at different stages during the calculation (called, for example, with the FORTRAN coding

```
CALL DTADMP (LIST, IDMP(2),2)
```

where the last argument is simply an indicative number to head the dump).

(i) The way LIST is specified is best followed using the example of the default LIST of POW keywords (more easily understood when compared with the table obtained using the PRINT option set in user's PRELUDE, Section 5.6)

```
LIST 1 ANAME TO DNAME,SCE TO MY,XM TO AM,WSEA TO MXINOT,INPULS TO STOP
```

```
LIST 2 ANAME TO MY,XM TO AM,WSEA TO MXINOT,IPULS TO STOP
```

```
LIST 3 ANAME TO AM,CF TO MXINOT,IPULS TO STOP
```

```
END
```

which is of length MIST = 28 set in the standard PRELUDE (Section 5.6).

A dump then produces a labelled listing on the printer of all variables in a segment of the full LIST array.

Segment 1, following LIST 1, produces all variables except the flux array, the layout array and the coefficient array.

Segment 2, following LIST 2, produces all variables except the layout array and the coefficient array.

Segment 3, following LIST 3, produces all variables, although only including the coefficient matrix if MAXC=MAXG is used in the PRELUDE (Section 5.6).

(ii) The choice of whether a dump is required at different stages of the calculation and which segment of LIST is to be used is specified using the array

IDMP. We have the interpretation

IDMP(K) \leq 0 then stage K dump is not produced,

IDMP(K) > 0 then stage K dump is produced following segment IDMP of LIST

The various stages K (and default values IDMP(K)) are...

- 1 ~ after all data read and before the calculation commences (0),
- 2 ~ prior to 1st inner or outer iteration (0),
- 3 ~ dumps every inner iteration (0),
- 4 ~ dumps after each group has converged inner iterations (0),
- 5 ~ dumps after all groups have converged upscatter calculation (0),
- 6 ~ dumps every IOUT outer iterations if OUTPUT PDUMP is used (1),
- 7 ~ dumps if outer iteration count limit, NOL, is exceeded (OUTPUT PDUMP) (1),
- 8 ~ dumps if outer iteration converged (OUTPUT PDUMP) (1),
- 9 ~ dumps if TLIM exceeded for latest outer iteration (OUTPUT PDUMP) (1),
- 10-18 ~ not used (0)
- 19 ~ dumps for some types of input data errors (0), and
- 20 ~ dumps after STOP encountered in data (0).

Data is specified in the usual way, for example,

IDMP 5*0,4*1,11*0

Note: As a possible help in recovering from input data errors POW can give printer dumps following segment 1 of LIST after some types of errors are detected (IDMP (19)). Scanning of data continues although no calculation is carried out.

2*0.0 9.C7922-3 0.0
 SP 7.53564-1 2.46436-1 2*0.0
 HSC(0) 1,2,3 1,2,3 3*.00184
 XM=C,5*4.572,C,6.25,5*2.968,0.625,10*5,0.71
 YM=0.5*5.0*4,.636,10*2.984,.71
 REG MX=1(1)22 MY=1(1)16 M(3)
 REG MX=6(1)12 MY=1(1)6 M(2)
 REG MX=7(1)11 MY=1(1)5 M(1)
 START

LAST VAR M
 LAST VAR M
 LAST VAR SP
 LAST VAR BSC
 LAST VAR XM
 LAST VAR YM
 LAST VAR M
 LAST VAR M
 LAST VAR M

PCW MOATA (X,Y) CALCULATION, GYMEA DATA

LAYOUT OF XY REACTOR SEGMENT

0.71
 Y****
 EXTRAPOLATION DISTANCES 0.0 Y * 0.71 IN TR.M.F.PATHS (0.0 IMPLIES ZERO CURRENT CONDITION)
 *XXXX
 0.0
 NOTE THAT I=M(1),A=M(10),10=M(16) AND THAT THE FISSILE MATS ARE IN HEAVY TYPE

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

SOLN METHOD TO BE USED FOR 2D DIFFUSION EQN

SLOR WITH LINE= ?, I.E. * * * * * , GROUP AND REGION REBALANCE WITH * * * * *
 LLLLLL * * * * *
 * LX= 4 SEG BET LINES 1 7 12 17 23
 * LY= 4 SEG BET LINES 1 6 11 14 17

PCW MOATA (X,Y) CALCULATION, GYMEA DATA

MESH POINT COORDINATES

*** DESIGNATES BOUNDARY CONDITION -TR.M.F.PATHS (0.0 IMPLIES ZERO CURRENT CONDITION)

X MESH POINT	MESH WIDTH (CMS)	POSITION (CMS)	Y MESH POINT	MESH WIDTH (CMS)	POSITION (CMS)
***	0.0	0.0	***	0.0	0.0
1	4.57200E+00	0.0	1	5.06400E+00	0.0
2	4.57200E+00	4.57200E+00	2	5.06400E+00	5.06400E+00
3	4.57200E+00	9.14400E+00	3	5.06400E+00	1.01280E+01
4	4.57200E+00	1.37160E+01	4	5.06400E+00	1.51920E+01
5	4.57200E+00	1.82880E+01	5	5.06400E+00	2.02560E+01
6	5.35000E-01	2.28600E+01	6	5.36000E-01	2.53200E+01
7	2.96800E+00	2.74320E+01	7	2.98400E+00	2.55860E+01
8	2.96800E+00	2.64630E+01	8	2.98400E+00	2.85400E+01
9	2.96800E+00	2.54910E+01	9	2.98400E+00	3.14940E+01
10	2.96800E+00	2.45190E+01	10	2.98400E+00	3.44480E+01
11	2.96800E+00	2.35470E+01	11	2.98400E+00	3.74020E+01
12	6.35000E-01	2.25750E+01	12	2.98400E+00	4.03560E+01
13	5.00000E+00	2.16030E+01	13	2.98400E+00	4.33100E+01
14	5.00000E+00	2.06310E+01	14	2.98400E+00	4.62640E+01
15	5.00000E+00	1.96590E+01	15	2.98400E+00	4.92180E+01
16	5.00000E+00	1.86870E+01	16	2.98400E+00	5.21720E+01
17	5.00000E+00	1.77150E+01	17	7.10000E-01	5.51260E+01
18	5.00000E+00	1.67430E+01	***		
19	5.00000E+00	1.57710E+01			
20	5.00000E+00	1.47990E+01			
21	5.00000E+00	1.38270E+01			
22	5.00000E+00	1.28550E+01			
23	7.10000E-01	1.18830E+01			

OUTPUT DATA FOR POW MCATA (X,Y) CALCULATION, GYMEA DATA

```

XSD FUEL      M( 1)
1.64481E-01  3.68630E-01  9.02355E-01  2.00955E+00
C.81315E-02  6.18992E-02  6.81700E-01  1.13082E-01
3.72274E-04  3.30167E-03  3.96448E-02  9.77554E-02
0.0          9.37282E-02  0.0          0.0
0.0          0.0          4.88109E-02  8.75701E-03
0.0          5.09412E-03  0.0          6.48822E-01
0.0          1.66342E-07  4.77318E-02  0.0
SIGTR
SIGREM
NLSIGF
CUTS 1
CUTS 2
CUTS 3
CUTS 4

CCX( 1)
2.15776E+00  9.04249E-01  3.65404E-01  1.65975E-01
CCY( 1)
2.15776E+00  9.04249E-01  3.69404E-01  1.65375E-01

XSD AL        M( 2)
1.16556E-01  3.05169E-01  9.05011E-02  9.34384E-02
2.16776E-02  7.04039E-03  2.52295E-02  1.99981E-02
0.0          0.0          0.0          0.0
0.0          1.61320E-02  0.0          0.0
0.0          0.0          5.06778E-04  0.0
0.0          5.36885E-04  0.0          1.29782E-02
0.0          0.0          1.27736E-03  0.0
SIGTR
SIGREM
NLSIGF
CUTS 1
CUTS 2
CUTS 3
CUTS 4

CCX( 2)
2.85985E+00  3.16950E+00  3.68319E+00  3.56740E+00
CCY( 2)
2.85985E+00  3.16550E+00  3.68319E+00  3.56740E+00

XSD C         M( 3)
1.45824E-01  3.44623E-01  3.74146E-01  3.63541E-01
2.65968E-02  6.01283E-03  9.59091E-02  1.00150E-02
0.0          0.0          0.0          0.0
0.0          2.24898E-02  0.0          0.0
0.0          0.0          4.22309E-03  4.23284E-08
0.0          1.58544E-03  0.0          9.65788E-02
0.0          0.0          8.07923E-03  0.0
SIGTR
SIGREM
NLSIGF
CUTS 1
CUTS 2
CUTS 3
CUTS 4

CCX( 3)
2.22483E+00  9.67802E-01  8.90918E-01  9.16907E-01
CCY( 3)
2.22483E+00  9.67802E-01  8.90918E-01  9.16907E-01

F-R
3.17200E-11  0.0          0.0
SP
7.52564E-01  2.46436E-01  0.0          0.0

```

POW MCATA (X,Y) CALCULATION, GYMEA DATA CALC= REAL EIGENV FRCLEN

```

INNER IT EIGENV-GP E(SCMEGA) E(1.) F(CMEGA) MIN
SEARCH( 0.0 ) GP IT EPP .....FOR INNER ITERATION, 0 NO OF GP PASSES 6 MAX ERR 3 GPS WITH UPSCAT
CUTER KEFF SCE-FRR N-BALANCE DOMINANCE CRIT-EIGENV TN STAGE GO-MINS GBAL-ERR REAL-ERR
0 1.000000
1 0.846591 0.846594 0.437120 3
2 0.903672 0.903673 0.526292 4
3 0.624999 0.625006 0.240412 3
4 0.886249 0.886251 0.495588 4
1 26 0.0573691 2 21 0.0421200 3 12 0.0330933 4 14 0.0602879 0 2 0.0602879
1 0.069157 0.2857066 0.569157 0.0 1.000000E+00 0 3 1.17 0.851422 0.283232
1 5 0.0173664 2 7 0.0100674 3 6 0.0127509 4 8 0.0126030 0 2 0.0127909
2 0.990754 0.1254352 1.022285 0.0 1.000000E+00 0 3 1.57 0.022960 0.181130
1 7 0.0074466 2 8 0.0044067 3 6 0.0044252 4 8 0.0054894 0 2 0.0054894
3 0.994211 0.0816546 1.003489 0.0 1.000000E+00 0 3 1.58 0.015994 0.068983
1 6 0.0050247 2 8 0.0024938 3 6 0.0021072 4 7 0.0048851 0 2 0.0048851
4 0.997083 0.0481036 1.002888 0.0 1.000000E+00 0 3 2.39 0.007218 0.028725
1 6 0.0032153 2 8 0.0015773 3 6 0.0013380 4 7 0.0030473 0 2 0.0030473
5 0.997946 0.0304101 1.000667 0.6234885 1.000000E+00 1 2 2.80 0.004626 0.013229
1 9 0.0015157 2 9 0.0010964 3 6 0.0010832 4 8 0.0020833 0 2 0.0020833
6 0.999731 0.0096904 1.000764 0.6234885 1.000000E+00 2 2 3.23 0.002762 0.007034
1 11 0.0003995 2 12 0.0002357 3 7 0.0000653 4 11 0.0005467 0 2 0.0006053
7 0.998766 0.0040133 1.000035 0.6234885 1.000000E+00 3 2 3.70 0.001666 0.004076
1 9 0.0001883 2 9 0.0001450 3 7 0.0002177 4 10 0.0002179 0 2 0.0002179
9 0.998906 0.0019669 1.000139 0.6234885 1.000000E+00 4 2 4.15 0.000584 0.002087
1 9 0.0001124 2 10 0.0000777 3 7 0.0001009 4 10 0.0001008 0 2 0.0001009
9 0.998982 0.0010406 1.000075 0.7294192 1.000000E+00 1 2 4.60 0.000273 0.000981
1 9 0.0000526 2 9 0.0000394 3 7 0.0000466 4 10 0.0000472 0 2 0.0000472
10 0.999040 0.0005564 1.000057 0.7294192 1.000000E+00 2 1 4.98 0.000273 0.000451
1 11 0.0000231 2 12 0.0000161 3 7 0.0000277 4 10 0.0000276 0 2 0.0000277
11 0.999053 0.0000992 1.000023 0.7294192 1.000000E+00 0 0 5.39 0.000273 0.000250
CONVERGED

```

CONVERGED

(X, Y) CALCULATION, GYMEA DATA

OUTPUT PRINT FOR POW MDATA

EDGE REAL FLX (MULTIPLIED BY 1.E+08) FROM SOURCE OF IN/SEC FOLLOWS

ERCUP 1

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
17	6443	6753	7640	8574	10516	11921	12076	12655	12923	12838	12398	11662	11449	9558	7458
14	10712	11241	12762	15059	17726	20172	20441	21435	21527	21784	21024	19718	19383	16122	12526
15	15669	16503	18912	22588	26915	30945	31393	33084	33886	33672	32440	30318	29776	24521	18830
14	21584	22549	26535	32243	39099	45618	46348	49131	50480	50170	48209	44824	43965	35684	26548
13	28717	30595	36120	44839	55584	66091	67275	71858	74120	73676	70548	65145	63789	50807	37565
12	37307	40642	48189	61344	78086	95053	86998	104572	108382	107735	102687	94004	91837	71428	51481
11	47537	51445	62251	82648	108801	136350	139558	152218	158661	157708	145427	135263	131775	99484	69575
10	59494	64558	81724	110460	150412	195491	200846	222326	233382	231848	218012	194480	188782	147279	92710
9	73126	80569	103794	145048	205845	280313	289417	326626	345444	347004	319600	279559	270067	182510	121513
8	88199	98330	129229	186745	277356	401638	417677	484068	516480	512004	471922	401588	385216	250951	155990
7	104281	116819	157205	234213	364038	572284	604655	727394	779257	771378	705059	576658	544732	37395	195011
6	12762	140898	193313	284644	438202	611593	646959	792746	837751	828577	787617	615322	581212	344280	203581
5	135521	153598	213240	330371	539850	908315	945914	119768	132670	1312525	1180235	914482	855252	482540	274024
4	161381	183787	257496	404045	666886	1125246	1195055	1519332	1662100	1645067	1471682	1132762	1065607	596140	335108
3	181518	208556	291703	458668	758423	1277055	1359435	1726883	1893397	1874426	1674125	1286415	1210959	676119	380872
2	193517	221519	312287	492382	813611	1368020	1451618	1851078	2031281	2011362	1795412	1378774	1298105	728525	408954
1	198215	226475	316384	503643	832064	1398411	1483767	1892567	2077220	2057070	1895951	1409472	1327281	745234	418404

	16	17	18	19	20	21	22	22
17	5502	3878	2633	1723	1106	680	389	180
16	9201	6459	4370	2847	1826	1120	640	296
15	13670	9494	6364	4142	2621	1600	910	420
14	15244	10166	6712	4508	3017	2131	1207	586
13	26287	17661	11505	7310	4535	2725	1534	705
12	35192	23155	14825	9284	5692	3385	1895	869
11	46298	25798	18728	11552	6996	4126	2291	1048
10	59528	37676	23236	14116	8645	4932	2720	1242
9	74183	46781	28323	16554	10023	5799	3177	1447
8	94773	56565	33998	20015	11703	6712	3655	1661
7	115390	70925	39809	21221	13445	7652	4144	1879
6	119870	70304	41085	23911	13818	7853	4248	1925
5	156498	85625	51380	25432	16787	9439	5066	2290
4	185123	107647	60701	34430	19468	10866	5800	2616
3	214150	120620	68032	38390	21590	11995	6380	2873
2	225723	129163	72682	40658	22946	12718	6751	3038
1	234595	132071	74272	41762	23413	12967	6875	3095

GRCUP 2

17	50803	51732	54344	58120	62237	65673	66017	67166	67364	66501	64557	61607	60865	53715	14	15
16	126606	126911	133394	142778	153024	161596	162557	163939	165660	163742	158941	151644	145908	132119	111410	45333
15	200722	204602	215539	231477	248902	263642	255134	270198	271249	267841	259899	247755	244697	215231	180899	
14	280748	286540	302824	326851	353464	376176	378402	386499	388479	383719	372135	354264	349761	306358	256168	
13	366010	374192	397435	431721	470193	503598	507062	519164	522638	516431	500452	475535	465257	408700	335404	
12	457461	468646	500585	543162	602380	650310	655342	673185	678556	671167	649743	615955	607432	525262	432512	
11	553568	570485	613353	678002	752912	820975	827752	853509	862428	853068	824810	779750	788366	658651	536937	
10	660199	679672	735984	821672	923889	1018179	1028237	1064567	1076295	1056679	1029874	970626	955620	810764	652404	
9	770528	795382	867755	980033	1115977	1245907	1259706	1309255	1324602	1314738	1267484	1191171	1171692	981899	781569	
8	884990	915974	1006812	1145789	1327371	1544977	1523411	1586652	1612443	1595488	1536141	1442138	1417480	1170453	919446	
7	1004315	1038085	1150079	1327147	1552073	1794932	1820302	1882449	1923206	1898025	1824244	1723578	1692843	1370924	1064144	
6	1025681	1065113	1180639	1365162	1559944	1840184	1843752	1906011	1941439	1919928	1843013	1743554	1737010	1412673	1095139	
5	1215712	1270827	1422752	1666645	1987168	2321484	2332421	2542147	2652552	2623452	2457516	2201222	2187127	1758331	1342798	
4	1392220	1454325	1639634	1941551	2339155	2769586	2786324	3086678	3248747	3214478	2986705	2631094	2611918	2073037	1566571	
3	1527824	1598567	1809995	2154122	2613349	3113585	3132327	3490313	3684559	3647082	3375940	2962225	2930840	2319277	1742497	
2	1614258	1690447	1918286	2291675	2785436	3327144	3348515	3737183	3950102	3910135	3620122	3168087	3143892	2474410	1854084	
1	1643917	1721560	1955370	2337972	2844242	3393368	3421278	3820215	4039065	3998397	3701755	3237752	3212967	2727242	1992233	

BU

17	36775	28809	21853	16029	11264	7368	4097	1185								
16	90302	70686	53591	35281	27592	18947	10030	2899								
15	146128	114023	86193	62044	44201	28862	16030	4631								
14	205839	159829	120302	87678	61238	39942	22152	6397								
13	270834	208557	156410	113465	79038	51341	28435	8208								
12	342239	262043	194861	140567	97512	63163	34897	10068								
11	420790	319473	235806	165116	116733	75345	41534	11977								
10	505676	381105	279157	198535	136625	87856	48315	13925								
9	595383	446598	324560	225802	157019	100588	55182	15895								
8	657557	514366	371379	261202	17653	11332	62054	17865								
7	758082	584799	418122	252175	168181	126099	68824	19904								
6	820645	555641	428738	295126	202489	128687	70238	20209								
5	922600	716614	507116	351234	235792	149062	81081	23310								
4	1147094	821112	576593	396435	264977	156822	90497	26001								
3	1266747	903254	531339	432542	287752	180637	97802	28089								
2	1346189	955785	666176	455282	302234	189407	102436	29412								
1	1372727	973775	678134	463086	307201	192413	104023	29865								

GROUP 3

17	10733	10775	10902	11062	11201	11251	11245	11181	11027	10807	10488	9987	9106	8072
16	27514	27633	27952	28369	28730	28861	28845	28685	28217	27727	27277	26910	23359	20704
15	44337	44537	45077	45787	46412	46661	46644	46394	45313	44865	44454	41454	37767	33446
14	61334	61630	62434	63500	64459	64886	64873	64585	63770	62471	60625	57705	52523	46450
13	78578	78573	80122	81634	83025	83717	83716	82608	82608	80740	78355	74553	67773	59824
12	56100	96661	98194	100267	102222	103290	103313	102993	101653	99823	96882	92136	83622	73641
11	113986	114625	116658	119436	123121	123723	123786	123524	122252	119861	116335	111700	100146	87937
10	131864	132826	135469	139129	142777	145191	145220	145220	143035	141088	134541	131407	117398	102710
9	149532	151149	154530	159291	164268	168170	168436	168656	167258	164203	159350	152702	134442	117919
8	167500	169421	173681	175851	180763	184185	184876	196129	194582	191557	185726	177259	154442	133477
7	185537	187406	192690	200531	210402	227584	230776	234539	234386	230657	223102	210536	206415	149219
6	189216	191164	196683	204520	215438	23108	234203	237691	237552	233812	226155	213527	178704	152557
5	217402	220032	227608	235435	256159	288701	291380	323720	336282	332183	310605	264377	261300	178819
4	241891	245204	254861	270740	293105	317576	341053	391140	411239	404479	375941	309907	243989	202488
3	260512	264797	276198	294675	322217	375496	379561	441253	464058	460816	424562	345551	268818	221247
2	272977	277235	289754	310173	340701	399299	403715	471038	499436	493910	454428	363145	284666	233247
1	277111	281498	294407	315487	347024	407392	411925	482354	510644	505024	464493	3765703	290099	237370

17	6581	5838	4753	3732	2787	1912	1092	301						
16	17850	14568	12182	8585	7142	4899	2797	772						
15	28807	24131	19621	15394	11486	7875	4494	1240						
14	35542	33404	27170	21250	15939	10951	6185	1708						
13	51332	42835	34708	27148	20207	13830	7882	2175						
12	53018	52446	42391	33088	24588	16807	9572	2641						
11	75012	62233	50158	35057	28967	19772	11252	3104						
10	67289	72163	57578	45026	33324	22711	12911	3561						
9	55785	82172	65796	50552	37626	25601	14535	4039						
8	112300	92166	73535	56778	41831	28415	16120	4444						
7	124943	102012	81095	62430	45889	31119	17636	4861						
6	127584	104071	82668	63601	46727	31676	17948	4947						
5	148087	119592	94661	72476	53049	35864	20287	5589						
4	166246	132710	105020	80074	58423	39406	22258	6131						
3	180522	144084	113037	85318	62435	42106	23757	6542						
2	195633	151732	118115	86603	65120	43799	24696	6800						
1	152762	153681	119850	90662	66002	44376	25016	6887						

GROUP 4

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
17	108054	108187	108435	108730	108545	107576	107395	106035	106184	101761	98748	95145	94306	86785	77980
16	273214	273254	274483	275646	274582	272128	271569	268229	263545	257419	245808	240710	238579	219562	197286
15	435061	435628	440945	441362	441226	437253	436351	430955	423435	413613	401415	388252	383438	352946	317144
14	605445	606267	608144	605645	608632	630300	601765	594259	583858	570351	553634	533675	528994	487127	437759
13	772483	773604	776202	776179	776723	769702	767563	757760	744380	727214	706100	680951	675044	622057	555208
12	945008	941463	944829	947275	945072	934976	932831	920381	902835	883068	857856	827930	820888	757548	681372
11	1107952	1109418	1113641	1116440	1112823	1098805	1095990	1080035	1059334	1035671	1006936	973125	965142	892818	802317
10	1274421	1276761	1291956	1284501	1278699	1258732	1254772	1233144	1208648	1181105	1146583	1114074	1105520	1026898	926308
9	1601589	1605264	1613200	1616656	159839	1545730	1536958	1489197	1451324	1419165	1390340	1365527	1359290	1286799	1168010
8	1759783	1763457	1773701	1777547	1752142	1657937	1648945	155947	1512082	1480616	1456661	1463532	1460817	1411826	1284270
7	2038115	2046368	2064217	2072243	2061667	1965807	1961261	2046605	2111865	2093727	1950332	1715534	1715736	1459642	1506272
6	2252013	2242515	2289707	2317740	2321015	2251731	2248143	2461325	2575585	2546805	2351132	1967184	1965376	1870670	1682979
5	2418772	2430074	2465732	2507167	2528478	2478456	2475357	2771081	2920924	2885580	2650504	2171466	2168410	2041777	1823971
4	2521064	2536294	2577103	2628524	2661336	2623007	2621441	2961610	3128365	3022162	2834882	2302305	2288527	2152247	1914653
3	2556771	2572685	2615505	2666860	2706966	2672434	2671022	3022863	3193444	3161590	2897159	2347151	2190322	1945907	
2	68210	58231	49144	38236	28958	20038	11505	3220							
17	172810	147297	121767	56547	73223	50663	29096	8141							
16	271245	236656	195554	155426	117496	81270	46648	13054							
15	383277	326405	269539	214362	161745	111824	64166	17957							
14	488475	416568	343702	273106	205710	142771	81604	22835							
13	596267	507056	417931	331719	249881	172525	98905	27674							
12	703406	597439	492005	390058	297492	202462	116008	32454							
11	810477	687531	565572	447164	336504	231016	132802	37147							
10	916892	773739	638144	504461	378617	260674	149172	41720							
9	1021527	865262	709092	556336	419447	288478	164970	46130							
8	1124714	940682	777654	612689	458553	315032	180030	50333							
7	1146190	948428	791828	623632	466601	320485	183121	51156							
6	1311211	1102464	899032	705523	526884	361238	206165	57623							
5	1454507	1200331	990748	775140	577716	355449	225660	53001							
4	1576671	1311083	1061363	825122	616396	421392	240060	67068							
3	1643617	1348695	1105917	862689	640633	437639	249172	68505							
2	1668702	1366452	1121163	874145	648803	443128	252271	70468							

GO TIME LEFT= 6.44 MINS

15 FEB 73*

20 MULTIGROUP A DIFF EOM *

LAST VAR GROUPS
LAST VAR MREG
LAST VAR PLCT
LAST VAR XYPLT

GROUPS 1 4,4
MREG -1,1,2,2
PLCT 1 1,6,C
XYPLT -5,7
EDIT -1,0,0,C

EDIT -1 0 0 OUTPUT FOR PCM
DATA (X,Y) CALCULATION, GYMFA DATA
CONVERGED

FLUX FOR AT (-)	(MULTIPLIED BY 1.0*0R)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
17	108054	108187	108205	108730	108544	107576	107355	106035	104183	101761	98744	95145	94306	86785	77980	
14	273314	273654	274442	275646	276582	272128	271569	268229	263544	257619	245806	240710	238579	219562	187286	
15	435661	439627	440545	441562	441226	437253	436351	430965	422425	413612	401619	386852	382438	352946	317144	
14	655443	662267	608183	605665	608631	603029	601748	596769	582858	570551	559633	533671	528993	487127	437758	
17	772483	771604	776201	778179	776723	769202	767543	757760	744380	727215	7065107	680551	675083	622057	555207	
12	945598	941463	944828	947275	945072	934975	932831	920180	903825	883067	857854	827930	820887	757547	681372	
11	1105419	1105419	1113647	1116440	112823	1098863	1095995	1080055	1059934	1035671	1006935	973125	965141	892817	803917	
10	1276420	1276761	1281956	1286501	1278698	1258151	1254271	1233147	1208647	1181164	1145562	1114074	1105519	1026698	926308	
9	1445558	1442482	1448848	1451773	1441142	1409046	1403388	1373364	1343064	1312713	1281192	1246525	1233559	1158565	1047884	
8	1601539	1605254	1613200	1616095	1588838	1565729	1566994	1491194	1451223	1410946	1390339	1365926	1352899	1286799	1168010	
7	176782	1763456	1773456	1773566	1752141	1657936	1648944	1555846	1512080	1483170	1457732	1465025	1474480	1411875	1286270	
5	179389	1792316	1807194	1811632	1785174	1671584	1659506	1556717	1516345	1483170	1457732	1465025	1474480	1438600	1311215	
5	2036514	2046357	2064216	2078242	2061665	1965807	1961261	2046605	2111664	2203727	1950332	1755332	1751536	1659640	1504270	
4	2252018	2262514	2289206	2317759	2321014	2251123	2248143	2461124	2578599	2546805	2351132	1967182	1985376	1870418	1682578	
3	2416172	2430073	2465191	2507166	2478426	2478426	2476394	2771081	2920522	2885575	2650506	2171485	2168409	2041775	1822969	
2	2521064	2536293	2577102	2628253	2661335	2673006	2621439	2961610	3129355	3092162	2834881	2302304	2298527	2152245	1914651	
1	2546770	2572684	2615505	2669660	2706955	2672433	2671021	3025862	3199444	3161589	2807095	2347152	2343151	2190322	1945907	
17	68310	58231	48144	38336	28958	20038	11505	3220								
16	172810	147207	121767	96567	73223	50663	29086	8141								
15	277745	236656	195554	155626	117496	81270	46649	13056								
14	382277	226405	269519	214362	161745	111824	64166	17957								
13	484475	416568	343702	271106	205910	142271	81604	22835								
12	596266	507056	417931	331735	249881	172525	98904	27674								
11	703406	597638	492004	390058	293492	202462	116008	32454								
10	810476	687530	565571	447766	336506	231916	132902	41720								
9	916892	777379	638143	504460	379617	260674	149172	41720								
8	1021527	865267	709051	556324	409446	288478	144970	46130								
7	1124714	950682	777643	612688	458553	315033	140070	50317								
6	1146190	968427	791428	623632	466600	320485	183121	51196								
5	1311209	1103463	893031	705522	526883	361237	206165	57523								
4	1456535	1270229	990747	775739	577715	395449	275440	63001								
3	1576670	1311081	1061342	829125	616395	421391	240059	67068								
2	1647616	1368484	1105916	862689	640633	417608	249171	68605								
1	1668702	1388451	1121163	874145	648892	443128	252271	70468								

FLOT 3 120.C
 PUREJY -5.2,2.7,7
 EDIT -1.C,0.C

LAST VAR
 LAST VAR PLCT
 LAST VAR PUREJY

EDIT -1 0 0 C OUPUT FOR PCM		CONVERGED																			
MOATA (X,Y) CALCULATION, GYMEA DATA																					
FLUX FOR M(-9) (MULTIPLIED BY 1.C*08)																					
GROUP 1																					
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15						
17	108054	108187	108495	108730	108544	107576	107355	106035	104183	101761	98748	95145	94306	86785	77980						
18	273314	273654	274442	275046	274582	272128	271569	268229	263444	257419	249606	240710	238579	219562	197286						
19	439061	439627	440945	441562	441226	437253	436351	430955	423435	413612	401419	394852	382438	352546	317144						
20	605443	606267	608183	608665	608631	603039	601768	594269	583458	570351	553633	533675	528993	487127	437758						
21	772483	773604	776201	776175	776723	769202	767543	757760	744380	727275	706107	680551	675083	622057	559207						
22	945098	944465	944828	947275	945072	934975	932831	920980	903835	883067	857835	827930	820887	757547	681372						
23	1107552	1109418	1113643	1116440	1112823	1098801	1095989	1080055	1059634	1035671	1006935	973125	965141	892817	803917						
24	1274420	1276761	1281956	1284901	1278698	1258121	1254271	1233143	1208647	1181104	1148562	1114072	1105519	1026898	926308						
25	1438553	1442482	1448948	1451133	1441142	1409046	1403386	1373364	1343054	1312718	1281152	1246529	1238559	1158565	1047884						
26	1601589	1605284	1613900	1616655	1588838	1545729	1539994	1489186	14431323	1419165	1390336	1365926	1259299	1286799	1168010						
27	1758782	1753456	1773700	1775866	1752141	1657936	1649944	1555946	1512080	1480616	1456060	1425232	1400816	1411825	1286270						
28	1913814	1906316	1907199	1811632	1785124	1671534	1659508	1556717	1514345	1483170	1457732	1426025	1404480	1438600	1311215						
29	2039914	2046367	2064216	2078242	2061665	1955807	1943261	2046605	2111664	2083727	1950333	1715532	1715736	1655440	1506270						
30	2252018	2262154	2289306	2311759	2321014	2251133	2248142	2461324	2578569	2546805	2351132	1967182	1565376	1370618	1682978						
31	2416772	2430073	2465181	2507166	2528476	2478436	2476396	2771081	2920993	2885576	2650506	2174485	2168409	2641775	1823969						
32	2521064	2536293	2577102	2628753	2661335	2623006	2631435	2961610	3125355	3092142	2834881	2302304	2298527	2152245	1914651						
33	2554770	2572684	2615505	2665860	2706955	2672433	2671021	3025862	3199444	3161589	2897695	2347152	2243151	2190322	1944907						
34	58310	58231	49144	36336	28958	20038	11505	3220													
35	172510	147297	121767	56547	73223	50663	29086	8141													
36	277745	236656	195554	156626	117496	81270	46848	13056													
37	382277	326405	269539	214362	161745	111824	64166	17957													
38	495475	416568	343732	274106	205910	142271	81604	22935													
39	566266	507056	417931	331739	249881	172525	98909	27674													
40	703406	597618	492004	390058	293492	202462	116008	32454													
41	810476	687930	565571	447166	336506	231916	132802	37147													
42	916892	777375	638143	504460	378617	250674	149172	41720													
43	1021527	865262	709041	559436	419446	289478	164970	46130													
44	1124714	950482	777643	612688	458553	315033	180030	50333													
45	1146190	968427	791828	623632	466600	320489	183121	51146													
46	1311209	1103453	899031	705922	526883	361237	206165	57623													
47	1436505	1202025	990747	775739	577715	395469	225460	63001													
48	1570670	1311081	1061342	825125	616395	421391	240055	67068													
49	1643616	1368454	1105916	862685	640633	437608	249171	69605													
50	1666702	1388451	1121163	874145	648892	443128	252271	70468													

E10

PURE JPY OUTPUT

X LIMITS 0.0 88.97C
Y LIMITS 0.0 55.796
Z LIMITS 0.0 62.276
Z OFFSET 0.223222E-04 0.220478E-01
PICT SIZE 7.000 7.000
PLOT ORIGIN 0.0 0.0

CAMERA DATA

LENS LOCATION -34.27455 144.22088 49.82319
AIMING POINT 44.48400 27.80700 12.45580

ROTATION MATRIX

-0.566026E+00 -0.499959E+00 0.0
0.315403E+00 -0.159885E+00 0.973100E+00
0.406459E+00 -0.542643E+00 -0.230807E+00

Z SCALING METHOD -4

CFI INTENSITY 16

Z MULTIPLIER 0.194227E+04, Z ORIGIN SHIFT -0.624373E-01

FOCAL LENGTHS TO FILL X,Y PLOTTER SPACE 0.100300E+02 0.127349E+02, LESSER VALUE CHOSEN

PICTURE SIZE IN X, Y = 7.000 5.513, REQUESTED SIZES 7.000 7.000

NUMBER OF POINTS WITH Z OUTSIDE BOX 0

FRAME WILL BE DRAWN AROUND PICTURE

TIME TAKEN TO DO PLOT= 1.17 MINS

STOP

LAST VAR

STIP. END OF DATA FOR POW MCATA (X,Y) CALCULATION, GYMEA DATA

ALCYS CODE SUPERVISOR * 15 JAN 73*

END OF AUCSYS AFTER 8.18 MINS
*** *****

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