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UPGRADE OF A DETERMINISTIC MULTI-ENERGY GROUP DIFFUSION REACTOR PHYSICS CODE

by

Bilguun Byambadorj

A thesis

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To the Graduate Faculty:

The members of the committee appointed to examine the thesis of BILGUUN BYAMBADORJ find it satisfactory and recommend that it be accepted.

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Vita

Bilguun Byambadorj was born in Ulaanbaatar, Mongolia, in 1988. After graduating high school in 2005, he attended National University of Mongolia for two years as nuclear technology major. He then enrolled at Dickinson State University in North Dakota, and received a Bachelor of Science in Mathematics and a minor in Information and Technology. He enrolled at ISU in nuclear engineering in Fall 2011 first as an undergraduate. After completing certain undergraduate engineering courses, he then enrolled as a graduate student in Fall 2012.

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Abstract

The aim of this thesis is to upgrade a Deterministic Multi-Energy Diffusion Reactor Physics Code “DISNEL”. The program DISNEL, Diffusion Iterative Solution using Nineteen Energy Levels, is specifically designed to be able to effectively calculate a wide variety of reactor configurations from the very fast spectrum type to the conventional thermal reactor. The DISNEL code is written in FORTRAN and was originally compiled with a FORTRAN IV compiler. Originally it was used to run on Windows 32-bit machine and limited to 120 mesh points. The new version of the code resulting from this work can be compiled with any GNU FORTRAN 90/95 compiler. The code was upgraded to run on current Windows 64-bit machine. The allowed number of mesh points was increased from 120 to 1000. The output of the calculation was improved to be more readable and printer friendly.

DOSBox is no longer needed to use DISNEL. Same results were obtained from both old and new DISNEL versions with the exact same mesh points and mesh spacing.

1. Introduction

The DISNEL code is specifically designed to be able to effectively calculate a wide variety of reactor configurations from the very fast spectrum type to the conventional thermal reactor. DISNEL is one-dimensional diffusion code, providing built-in cross sections for diffusion calculations. The code has built-in 19 energy-group cross-sections, based on ENDF-II (Evaluated Nuclear Data File) data, which has been modified recently for some of the rare earth metals to correspond to more recent version of ENDF data. Modification to the built-in cross sections can be made, where better data is now available.

The code obviously has geometric limitations, though it does allow for two dimensional solutions in radial cylindrical coordinates, uniform spherical coordinates and one dimensional slab coordinates. Its advantage is that it can provide design and analysis calculations quickly and easily, with deterministic mathematical precision.

The flow chart of the program is shown in Figure 1.

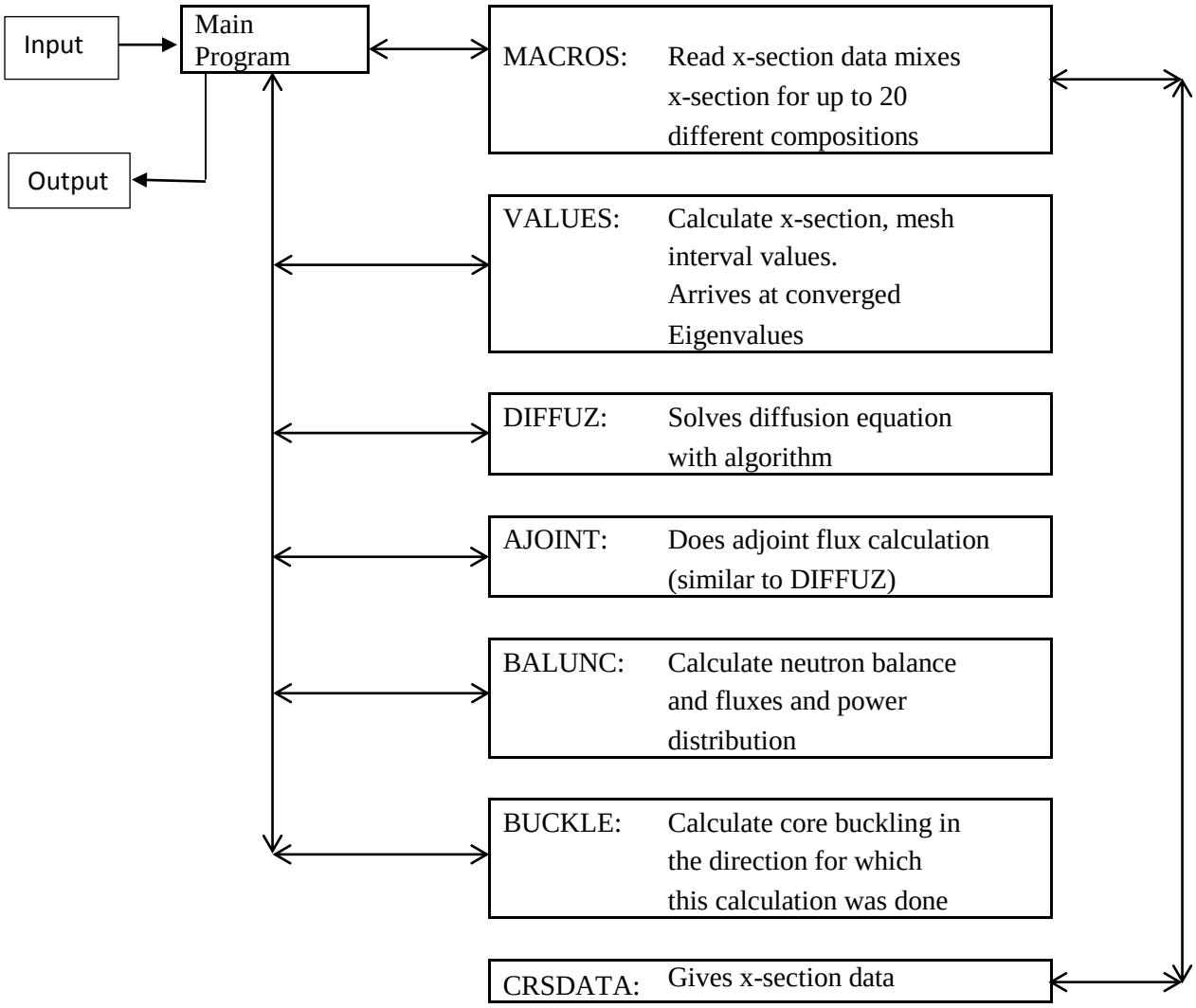


Figure 1. DISNEL Program Flowchart

The DISNEL code uses numerical methods for solving the steady state neutron diffusion equation.

$$\sum_a \Phi \ - D\nabla^2\Phi = \ \nu\sum_f \Phi \tag{1}$$

"The general procedure is to rewrite the differential diffusion equation in finite difference form and then solve the resulting system of differential equations on a digital computer."[1] The core must be divided into N mesh intervals, thus we need N+1 mesh points to do so.

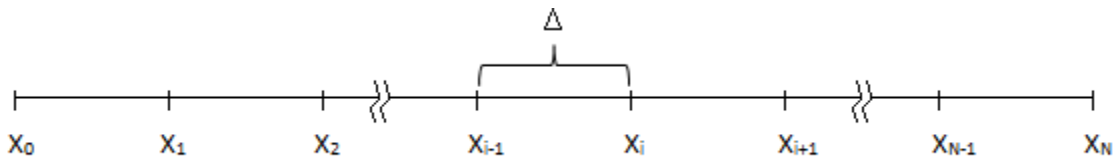


Figure 1. Mesh Interval

As shown in Figure 1, the core is divided into N mesh intervals such that

$$\Delta = \frac{core(region)length\ or\ radius}{N} \tag{2}$$

As mentioned in before, differential equation will be rewritten into finite difference:

$$\left(\frac{d^2\Phi}{dx^2}\right)_i \cong \frac{\Phi_{i-1} - 2\Phi_i + \Phi_{i+1}}{\Delta^2} \tag{3}$$

This approximation comes from Taylor expansion of Φ in one dimensional Cartesian coordinates. Equation 1 can be solved by substituting Equation 3.

The number of mesh points should be carefully chosen such that the mesh interval length is shorter than mean free path. "Since the spatial variation of the flux is essentially characterized by the diffusion length L, one generally chooses a mesh spacing Δ less than L."[2]

$$L = \sqrt{\frac{D}{\sum_a}} \tag{4}$$

where,

D −Diffusion Coefficient (cm)

$\sum_a$ − Absorption Cross Section (cm^{-1})

The diffusion coefficient can be shown as:

$$D = \frac{1}{3\sum_{tr}} \tag{5}$$

where,

$\sum_{tr}$ −Transport Cross Section

Note that the root-mean-square distance that a thermal neutron travels from birth to being absorbed is

$$\bar{r}_{th}^2 = 6\,L^2 \tag{6}$$

So choosing mesh intervals less than L, assures that there are many mesh intervals in the range "r".

Similarly, for slowing down root-mean-square distance:

$$\bar{r}_{SD}^2 = 6\,\tau \tag{7}$$

where,

τ – Fermi Age (cm^2)

2. Code Conversion to Current FORTRAN

FORTRAN is a structured programming language. It is a common choice for numeric computation and scientific computing. In 1957, IBM developed FORTRAN and its compiler. It was used in numerical calculation of large variety of areas such as weather calculation, fluid dynamics, computational physics and chemistry. The DISNEL code was written in FORTRAN 77. FORTRAN started with 32 statements. Since FORTRAN is adaptive, newer versions of FORTRAN can compile previous versions. Some statements are no longer used in newer versions, but it still does the job. There were some changes needed to be done in order to use newer compiler. In this project, a FORTRAN compiler was required to compile the code. The GNU FORTRAN compiler *gfortran* was used. "GNU is a Unix-like operating system that is free software (It respects your freedom). You can install versions of GNU (more precisely, GNU/Linux systems) which are entirely free software".[3] GNU stands for "GNU's Not Unix".

The DISNEL code consists of the following ten subroutines: *ajoint.for, balunc.for, buckle.for, datape.for, diffuz.for, fdisnel.for, macros.for, picktm.for, rdwrte.for,* and *valuesv.for.* Each subroutine had *common* blocks where the variables were declared. These *common* blocks were removed and a new text file (Figure 2) was created which has all the *common* blocks from each subroutine. Instead of big *common* blocks, the *include* statement is used, which can call the *common.txt* file and use necessary variables. (Figure 3) Some '*do statement'* loops were changed to *'do statement end do'*, so that *gfortran* compiler would have no issue with the syntax (Figure 3). FORMAT statements in the code have been changed in various places. The reason to

change the *format* statement was that the output file was not printer friendly. The last number on each line was carried to the next line making it difficult to read the output file. In the *macros.for* subroutine, cell correction factors in each material had four significant digits and there were four blank spaces between each other. The significant digits printed in the output were reduced to three and the blank spaces were reduced to two. The code also prints the scatter-transfer matrix for each composition from group one to group 19. The floating point numbers' significant digits were reduced to three and column spacing also reduced to one. In each composition, 19 group absorption, slowing-down, production, and scattering cross sections were printed out. The column spacing was reduced to five, so that the output can be more readable, when printed in landscape mode.

The code had geometric limitations because of early computer computing power. The mesh points were limited to 120 in order to get answers in a reasonable amount of time on computers in the 1970s and early 1980s era. It calculated effective multiplication factor and neutron flux reasonably close to actual amount. Current computer power has increased significantly, so that the DISNEL code now runs much faster than before. Reduced number of mesh points is no longer required. All the mesh points and mesh intervals were increased to 1001 and 1000, respectively. Sizes of certain arrays were increased to 1000 and *for* loops for effective multiplication factor and neutron flux calculation has also increased to 1000.

```
      COMMON/HOLITH/IDEM(4),IPAGE(2),GEOM(9),KORSE(6),IBOUND(15),
     1 KORE(4),LABEL(2),EN(26),
     2 SKIPA(335),SKP1(63),SKP2(26)

C     in MACROS.FOR COMMON/HOLITH/ISKIPA(42)

      COMMON/MULTIG/DIFF(19,20,2),SPECT(19),LWORD1,ISP,IS,SIGS(19,20),
     1 NUSIGF(19,20),SIGA(19,20),TRANS(10,19,10),LEAP(20),SCAT(19,20),
     2 NCALC,IDENT(20),LEVEL(19)

C     in values.for common/multig/iskipa(6481)
C     variables IS & ISP in COMMON/MULTIG/ may not be used
C     ISKIPA(420) in DIFFUZ.FOR

      COMMON/SCRACH/SKIPC(330),ELEMI(50),RTRAN(19,10,5),RNTRAN,RKTRAN,
     1 RKERGY,RIERGY,BUKLE(20,2),RADR(21,2),WIDTH(20,2),RNVALS(20,2),
     2 BUCKL(19),RLIBRY,DBUCKL(19),RCODE(125),TAU(1000),VALUC(2),
     3 DIFT(2),SOUR(2),SKIPF(1514),FEE(19),PARLEL(19),ABSORB(19),
     4 SCATER(19),PERPEN(19),PRODUC(19),BALNCE(19),XFERS(19),RATE(19),
     5 FEEBAR(19),VA(19,2),VB(19),SUM(8),RSKIPD(4),ETRAN(5),RSKIP(0148),
     6 R(26),ELEM(19),RELEM(19),CELLA(19,10,2),RETRAN(5),RNELEM,
     7 nelemt,ntran,libry,ktran,nvals(20,2),facta(20)

      COMMON/MISCEL/NERGY,LWORD2,KEFF(2),NREG(2),LIML,LIMU,NINT(2),KAY,
     1 ISKIPA(420),NORG(2),NEND(2),ID,JUMP,JUMT,M,N,L,LWORD3,ACC,CONVK,
     2 INTER,LCORE,LUMP,ISORE,ISTART(2),IEND(2),ISKIPB(15),ISKIPC(7),
     3 KORO(2),KOR(2),KOREM(2),ISKIPD(15)

C     in values.for common/miscel/kskipc(15),time

      COMMON/DENS/DENSR(1000,2),DENSL(1000,2),RADI(1001,2),RIREG(20,2),
     1 DBSQK(19,20,2),WE(19,2),WO(19,2),RLODE(20,2),RIVAL(20,2),
     2 FLUX(19,1001,2),SKIPB(10642),SKIPD(836),SKIPE(1560),
     3 DELSQ(19,1000),TEMS(26,5,125),HYDRO(19,19),A(19,4,2),SAVEI(26),
     4 SAVEJ(5),ATOMK(10,2),ELEK(10,2),WIDE(19),V(19),JK(2),
     5 IREG(20,2),LODE(20,2),IVAL(20,2)

       in MACROS.FOR COMMON ABSORB(19),SKIPC(25)

      COMMON/ADENS/ADENSR(1000,2),ADENSL(1000,2),AFLUX(19,1001,2),
     1 FACTB(1001,2),FACTC(1000,2),FACTD(1000,2),FACTZ(20,2),
     2 OMEGA(19,1001),SKP3(7581)
```

Figure 2. common.txt

```
      SUBROUTINE AJOINT
      IMPLICIT REAL*8(A-H,O-Z)
      include 'common.txt'
      DIMENSION SPECTK(19)
      ! DIMENSION SUM(20)!,IREG(20,2),LODE(20,2),IVAL(20,2)
      INTEGER I,SKP3
C**** DOUBLE PRECISION OMEGA,TAU,VALUC,DIFT,SOUR,CON
      REAL*8 KEFF,NUSIGF
C
C TRANSFER REAL TO INTEGER
C
      DO 101 IP=1,2
      DO 101 IPP=1,20
      LODE(IPP,IP)=RLODE(IPP,IP)
  101 IVAL(IPP,IP)=RIVAL(IPP,IP)
      WRITE(6,1040)
 1040 FORMAT(31H1ADJOINT EIGENVALUE CALCULATION)
      ID=LIML
      DO I=1,1000
        ADENSR(I,ID)=1.0
        ADENSL(I,ID)=1.0
      end do
      DO 3 J=1,20
    3 SUM(J)=0.0
```

Figure 3. *include* common.txt

3. Adaption to Current Windows Computers

The earlier DISNEL code was used to run on 32-bit machine using Windows Command Prompt. In order to run on 64-bit machine, external software, DOSBox, was required to be installed (Figure 4).

Figure 4. DOSBox

The DOSBox command prompt (Figure 5) can be confusing for those who are not completely familiar with a windows command prompt. Extra steps were required to run *disnel.exe*. DISNEL 2014 was compiled on a 64-bit machine, so a 64-bit machine users no longer struggle with DOSBox. It only works on 64-bit machine. “If the program is specifically designed for the 64-bit version of Windows or other operating systems, it won’t work on the 32 bit version of Windows or other operating systems. However, most programs designed for the 32-bit version of Windows do work on the 64-bit version of Windows”. [4]

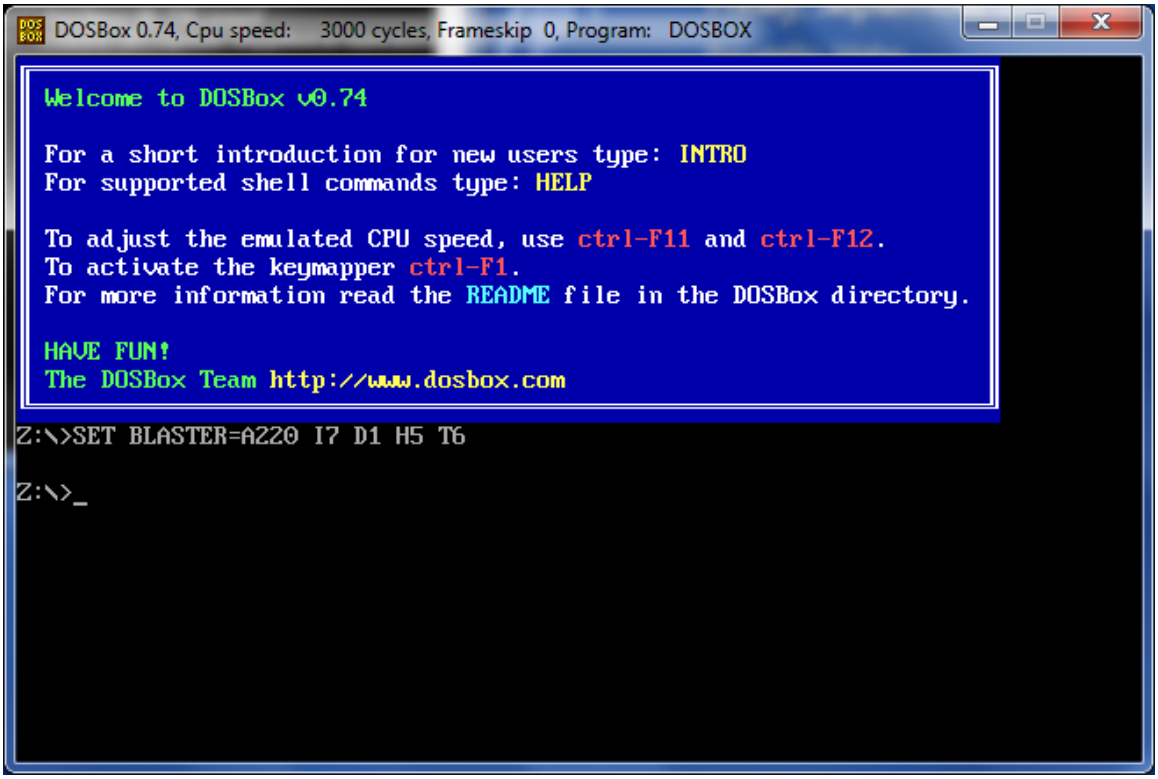


Figure 5. DOSBox Command Prompt

Currently, most desktop computers use 64-bit operating systems and 32-bit operating system is no longer on the market.

4. Test Cases, Benchmarks and Advantages of Upgrade

After making changes to the DISNEL code, obtaining a properly running the code was challenging. The initial DISNEL 2014 compiled cross section calculation for 19th energy group was much different than previous DISNEL calculation (Figure 6). The difference was about 25%, which implied serious differences in the new compiled version. The multiplication factor and the neutron fluxes were significantly affected by these changes.

COMPOSITION 1 CONSTANTS

ENERGY GROUP	ABSORPTION CROSS SECTION	SLOWING-DOWN CROSS SECTION	PRODUCTION CROSS SECTION	SCATTERING CROSS SECTION	AXIAL DIFFUSION	RADIAL DIFFUSION
1	8.0723E-04	1.4204E-01	2.8482E-03	1.3777E-01	4.9778E+00	4.9778E+00
2	5.8229E-04	1.2134E-01	1.8546E-03	1.6121E-01	4.4275E+00	4.4275E+00
3	4.8911E-04	1.5429E-01	1.3739E-03	2.4060E-01	2.5579E+00	2.5579E+00
4	5.1209E-04	1.9380E-01	1.3100E-03	2.9094E-01	2.4079E+00	2.4079E+00
5	3.3326E-04	2.5070E-01	6.8863E-04	3.7307E-01	1.8675E+00	1.8675E+00
6	2.7034E-04	3.3275E-01	4.1888E-04	4.9231E-01	1.4213E+00	1.4213E+00
7	2.6968E-04	4.2835E-01	4.1509E-04	6.2910E-01	1.1323E+00	1.1323E+00
8	3.0618E-04	5.4277E-01	4.5563E-04	7.8779E-01	9.2530E-01	9.2530E-01
9	4.4015E-04	5.4448E-01	5.7321E-04	1.0957E+00	7.0188E-01	7.0188E-01
10	8.1221E-04	6.0252E-01	9.3675E-04	1.5525E+00	5.2430E-01	5.2430E-01
11	1.7210E-03	6.9165E-01	1.7685E-03	1.7615E+00	4.7070E-01	4.7070E-01
12	5.4100E-03	6.9889E-01	4.7061E-03	1.7801E+00	4.6313E-01	4.6313E-01
13	1.6963E-02	6.9863E-01	1.1715E-02	1.7865E+00	4.5156E-01	4.5156E-01
14	4.1582E-02	7.6783E-01	1.2413E-02	1.7868E+00	4.4030E-01	4.4030E-01
15	8.2711E-03	9.5691E-01	9.1298E-03	1.8294E+00	4.5242E-01	4.5242E-01
16	1.6660E-02	1.0912E+00	2.3247E-02	1.8744E+00	3.9635E-01	3.9635E-01
17	3.7225E-02	1.3273E+00	5.6524E-02	2.2487E+00	2.8515E-01	2.8515E-01
18	5.7512E-02	1.6867E+00	8.8276E-02	2.8524E+00	1.8570E-01	1.8570E-01
19	1.0454E-01	0.0000E+00	1.6553E-01	3.7699E+00	1.1928E-01	1.1928E-01

Figure 6. Cross Section Calculation for Composition 1

In the *gfortran* compiler, the second part of the subroutine was not read by the compiler, which is anything after "*end"* keyword. (Figure 7) In the second part of *fdisnel.for*, *DATA* blocks were defined. Only the last *DATA* block was required for cross section calculation

```
 9000 STOP
      END
C     THIS DECK FOR NDATA=1 READS TAPE ONLY,   =2 TAPE AND CARDS,   = 3
C     CARDS ONLY
      BLOCK DATA
      IMPLICIT REAL*8(A-H,O-Z)
      include 'common.txt'
      REAL*8 NUSIGF
      CHARACTER*6 IDEM,KORE,JOIN,IPAGE,LABEL,GEOM,KORSE,IBOUND,
     1 SPCNME,TITLE,EN,SKIPA,SKP1,SKP2
!      DIMENSION R(26),NVALS(20,2)
!      EQUIVALENCE (RNVALS(14,2),R)
      DATA IDEM/'   A  ','  RA  ','XIAL  ','DIAL  '/
      DATA IPAGE/'0     ','0     '/
      DATA GEOM/'SEMI-I','RADIAL','      ','NFINIT',' CYLIN','  SPHE',
     1' SLAB ','DRICAL','ERICAL'/
      DATA KORSE/'   CON','FROM P','STANT ','REVIOU',
     1'SOURCE','S CASE'/
      DATA IBOUND/'      ','ZERO S','EXTRAP','EXTRAP','INPUT',
     1'   ZER','LOPE,C','OLATED','OLATED','FLUX V',
     2'O FLUX','URRENT',',INPUT',',CALC.','ALUES '/
      DATA KORE/'**CO  ','KOR2  ','RE**  ','KOR4  '/
      DATA LABEL/'     G','ROUP  '/

      DATA LEVEL/1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19/
      DATA EN/'     1','     2','     3','     4','     5','     6',
     1'     7','     8','     9','    10','    11','    12','    13',
     2'    14','    15','    16','    17','    18','.025EV','3000 F',
     3'2500 F','2000 F','1500 F','1000 F',' 500 F','  68 F'/
      DATA R/0.0,0.5,1.0,1.5,2.0,2.5,3.0,3.5,4.0,6.0,8.0,10.0,12.0,14.0,
     115.5,16.5,17.5,18.5,19.795,17.675,17.831,18.016,18.243,18.537,18.9
     259,19.555/
      END
```

Figure 7. Second Part of FDISNEL.FOR Subroutine

in *macros.for*. The *R* is an array of length of 26 cross sections for absorption, 19 energy levels plus 7 higher temperature cross sections. The correction was to redefine R array in *macros.for*, so that the cross section calculation does not need to go back to *fdisnel.for* and look for this *DATA* block. By doing this, the not-so-obvious error was corrected.

An AGN 201 spherical model was used for test and benchmark work (Figure 8). Five compositions were used. The input file was run on original DISNEL with 69 mesh points and on new DISNEL with 690 mesh points. The effective multiplication factor was calculated to be 1.008911 on new DISNEL with 690 mesh points. The previous

calculation shows that effective multiplication factor is 1.008428. More mesh points allow better neutron flux distribution. Figure 9 shows neutron flux as a function of distance. In Figure 9.a, the distance is divided into 690 equally spaced locations. On the other hand, Figure 9.b shows gap between neutron fluxes, so that there are some gap spaces between points.

```
0
19 1    AGN 201, spherical model, 14.54 cm radius
    5    1    1
    1    2    2    3     68.00
    1   95  0.000135
    1   98  0.000546   12
      0.70      0.46      0.50       1.0       1.0       1.0       1.0       1.0
    0    6    0.0396
    0    1    0.0791
    2    2    2    3      68.0
    1   95  0.000270
    1   98  0.001092   12
      0.89      0.46      0.50       1.0       1.0       1.0       1.0       1.0
    0    6    0.0396
    0    1    0.0791
    3    2    3    3     68.00
    1   95  0.000135
    1   98  0.000791   12
      0.89      0.46      0.50       1.0       1.0       1.0       1.0       1.0
    0    6    0.0396
    0    1    0.0791
    0   13   0.00052
    4    0    1    3     68.00
    0    6    0.0878
    5    0    1    3     68.00
    0   79   0.00591
    4    0    3    4    4    2    4    1    1   20    1    1    0   100
      0.0       0.0    0.0000  .0000100    0.0001         0
    2   50       0.5   0.00000    1  250     14.04  0.000000
    4  390      20.0   0.00000
```

Figure 8. Input Deck

See Appendix E for detailed explanation for input deck.

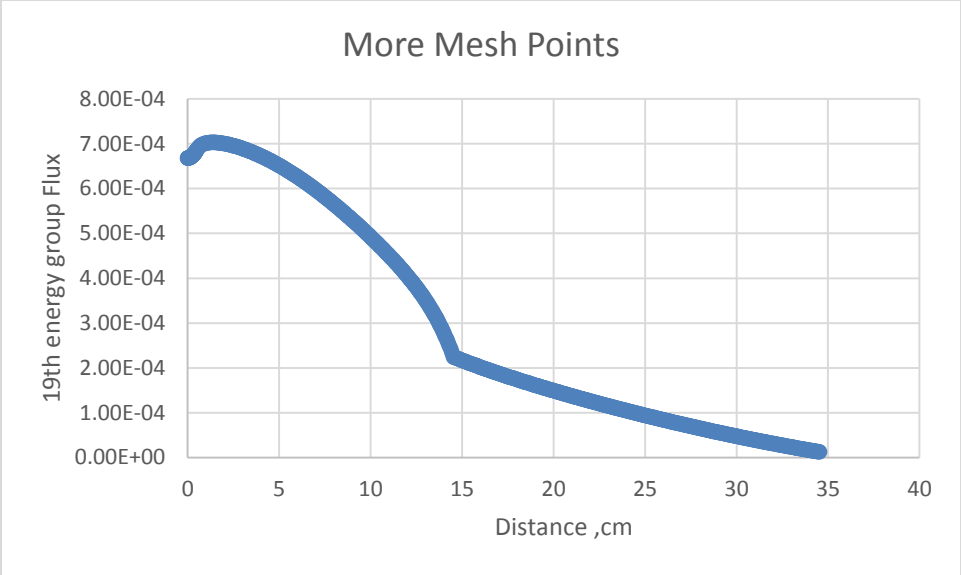


Figure 9.a. More Mesh Point Plot

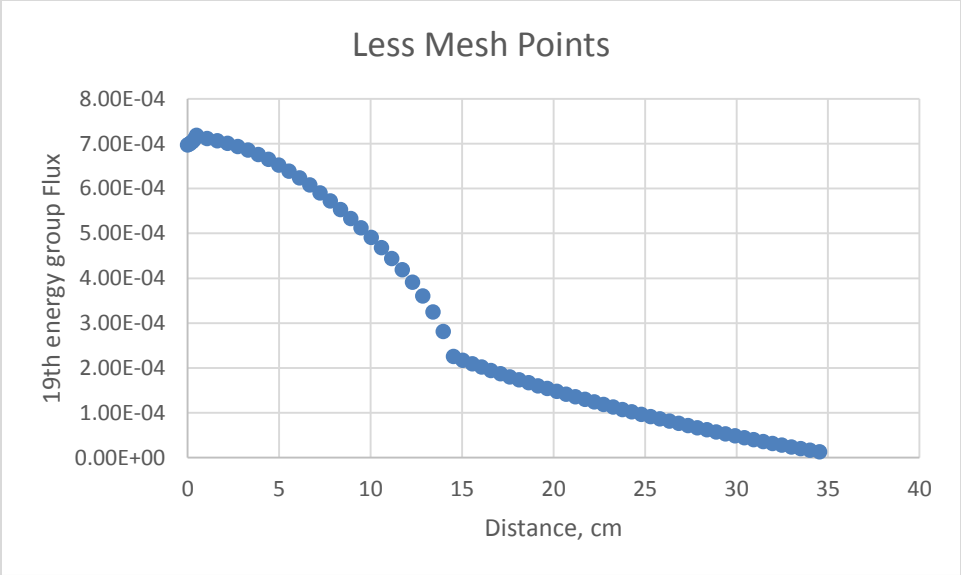


Figure 9.b. Less Mesh Point Plot

According to Figure 9.b data, the difference in flux was less than 4.7% in region 1, at position 0.5 cm, and was less than 0.6% in regions 2 and 3. The 4.7% difference was at

the boundary between “fuse” and the main core, where the smaller mesh spacing was of considerable importance.

In AGN-201 reactor model, fuel and reflector regions are included in the input file. There are two fuel regions, one, the “fuse”, had five mesh intervals and the other had 25 mesh intervals. The reflector region had 39 mesh intervals. Since the maximum number of mesh points was 120, we were not able to design entire reactor effectively. Now that we have 1000 mesh points, the entire reactor model can be designed with adequate mesh intervals on the range of slowing down or thermal diffusion distances. The mesh interval length should be much smaller than the diffusion length or slowing down length. The diffusion length for region 1 is calculated to be 1.85975 cm (Appendix D). The radius of this region is 14.04 cm and we had 25 mesh points, which will give us 0.5616 cm per mesh interval. Compared to the mean free path in this region, which is 0.3125 cm, the mesh interval is larger, and hence not an ideal situation. But now 250 mesh points can easily be selected, and the mesh interval is much better than “just adequate”.

5. Conclusion

There were two primary reasons for undertaking this thesis:

1. To convert the FORTRAN program to a current version of FORTRAN, so that any free compiler can be used to compile the code.

2. To enhance the usefulness of the program by increasing the finite element detail so as to not compromise the adequacy of the finite element deterministic solution to the diffusion equation. Reduced mesh spacing will also make the "transport theory" approximations in the code more reliable, especially for high absorption materials where the flux is changing very rapidly.

Both of these improvements have been implemented successfully. The increase in the number of mesh points has not had any dramatic effect of the primary outcome of the calculation, the k-effective and the flux shape. As reported on page 15, a 10 fold decrease in mesh point spacing had minimal effect on k-effective, the result differing by only 5 parts in 10,000 (5 in the fourth decimal place).

6. Possible Future Upgrades

1. Number of compositions could be increased depending on the reactor configuration complexity, and to provide the user with more flexibility in easily making changes to compositions.
2. Input format could be changed to free-format or comma delimited, thus making the input more user friendly
3. Cross section data can be updated, as needed, especially for the rare earth elements and transuranic isotopes, to ENDF-7. This will require using cross section averaging code.
4. A flux plotter should be added.
5. Convert the entire code to FORTRAN 90, C++, or Python.

Appendix A

Installing and Running DISNEL

Two kinds of DISNEL disk were created, one for those who need to use DISNEL for effective multiplication factor calculation and neutron flux calculation, and the other for those who need to make changes in the code and recompile it.

The folder, which is named *DISNEL*, should be copied from the disc to C drive. It includes executable file *disnel.exe*, cross section data *CRSDATA.DAT*, and input file *DISNEL.INP*. There are two ways to run DISNEL. Double clicking on *disnel.exe* would run the code, but if there are any errors in the input file, it would not give any warning or error. The output file will have no calculated values. In order to diagnose such errors, Windows Command Prompt or Linux Terminal are required to run DISNEL.

- Open Windows Command Prompt, or Linux Terminal
- Change directory to C:\DISNEL\
- Type disnel.exe and hit enter

If the code runs without any error, there will not be any message in the screen. (Figure 10)

The *Notepad++* is suggested to use for better input and output purpose. *npp.6.4.5.Installer.exe* is included in the disk to install *Notepad++* . Printer configuration must be changed to landscape; otherwise, the output will be hard to read.

The *Wordpad* can be used to open the output file, but font size should be decreased so that all the information can fit in one line.

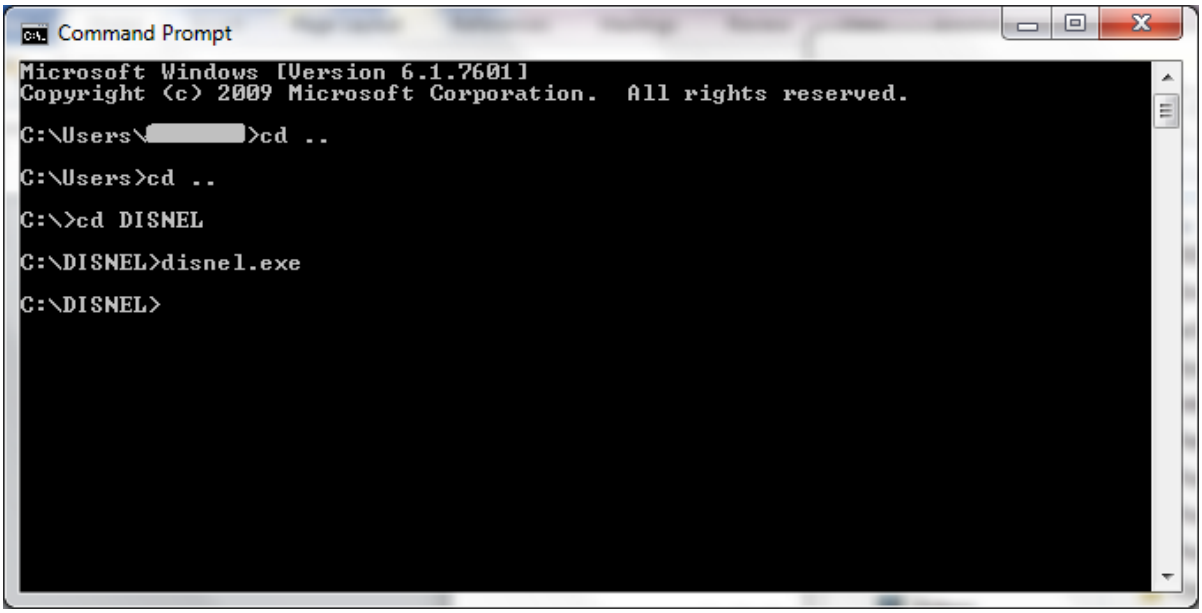


Figure 10. Running DISNEL on Windows Machine

A different disk is provided for those who need to recompile the code. The disk includes a folder *DISNEL.FOR*, which has all the FORTRAN subroutines and *common.txt*. Same installing processes should be followed. The gFortran compiler, *gfortran-windows-20130301.exe*, needs to be installed on the machine. It is included in the disk. In order to compile the code, the following line should be typed in the Command Prompt: *gfortran -O2 -fno-align-commons AJOINT.FOR BALUNC.FOR BUCKLE.FOR DATAPE.FOR DIFFUZ.FOR EXIT.FOR MACROS.FOR PICKTM.FOR RDWRTE.FOR valuesV.FOR FDISNEL.FOR -o disnel.exe*. It will give new *disnel*.exe inside the *DISNEL.FOR* folder. An extra command is required for portable executable, which is *objdump -p disnel.exe | grep "cygwin1.dll"*. This will help us to copy *disnel*.exe to any other machine and run. The cross section library file, CRSDATA.DAT, must be copied with *disnel*.exe.

Appendix B

Absorption Cross Section Calculation for Core Region 2

$$N_{U-235} = \frac{0.6023 * 10^{24} atoms}{235\ gm} * \frac{672\ gm}{12.7 * 10^{3} cm^{3}} = 0.000135 * 10^{24}\ \frac{atoms}{cm\text{^}3}$$

Similarly, $N_{U-238} = 0.000546\ \frac{atoms}{b*cm}$

$\sigma_{a_{U-235}} = 585\ b$

$\sigma_{a_{U-238}} = 2.78\ b$

$\sigma_{a_H} = 0.33\ b$

$\sigma_{a_C} = 0.004\ b$

$$\sum_{a_{U-235}} = N_{U-235} * \sigma_{a_{U-235}} = 0.000135\ \frac{atoms}{b * cm} * 585\ b = 7.8975 * 10^{-2}\ cm^{-1}$$

$$\sum_{a_{U-238}} = N_{U-238} * \sigma_{a\ U-238} = 0.000546\ \frac{atoms}{b * cm} * 2.78\ b = 1.51788 * 10^{-3}\ cm^{-1}$$

Absorption cross section is dominated by U-235 and U-238, thus:

$$\sum_a \cong \sum_{a_{U-235}} + \sum_{a_{U-238}} = 8.0493 * 10^{-2}\ cm^{-1}$$

Appendix C

Diffusion Coefficient Calculation for Core Region 2

$\bar{\mu}_{0_C} = 0.0556$

$\sigma_{t_C} = 4.80\ b$ total microscopic cross section of carbon

$\sigma_{s_C} = 4.80\ b$ scattering cross section of carbon

$N_C = 0.0396 \frac{atoms}{b * cm}$

$\sum_{t_C} = N_C * \sigma_{t_C} = 0.0396 \frac{atoms}{b * cm} * 4.80\ b = 1.9008 * 10^{-1}\ cm^{-1}$

$\sum_{s_C} = N_C * \sigma_{s_C} = 0.0396 \frac{atoms}{b * cm} * 4.80\ b = 1.9008 * 10^{-1}\ cm^{-1}$

$\sum_{tr_C} = \sum_{t_C} - \bar{\mu}_{0_C} * \sum_{s_C} = 1.9008 * 10^{-1}\ cm^{-1} - 0.0556 * 1.9008 * 10^{-1}\ cm^{-1} =$

$= 1.79511552\ cm^{-1}$

$\bar{\mu}_{0_H} = 0.6614$

$\sigma_{t_H} = 38\ b$

$\sigma_{s_H} = 38\ b$

$N_H = 0.0791 \frac{atoms}{b * cm}$

$\sum_{t_H} = N_H * \sigma_{t_H} = 0.0791 \frac{atoms}{b * cm} * 38\ b = 3.0058\ cm^{-1}$

$\sum_{s_H} = N_H * \sigma_{s_H} = 0.0791 \frac{atoms}{b * cm} * 38\ b = 3.0058\ cm^{-1}$

$\sum_{tr_H} = \sum_{t_H} - \bar{\mu}_{0_H} * \sum_{s_H} = 3.0058\ cm^{-1} - 0.6614 * 3.0058\ cm^{-1} =$

$= 1.01776388\ cm^{-1}$

U-235 and U-238 scattering cross section is negligible compared to C and H

Appendix D

Mesh Interval Length Calculation for AGN-201 Core Region 2

$$D = \frac{1}{3 * \sum_{tr}}$$

Since transport cross section is dominated by carbon and hydrogen, we have:

$$D = \frac{1}{3 * (\sum_{tr_C} + \sum_{tr_H})} = \frac{1}{3 * (1.79511552\ cm^{-1} + 1.01776388\ cm^{-1})} = 0.2784\ cm$$

$$L = \sqrt{\frac{D}{\sum_a}} = \sqrt{\frac{0.2784\ cm}{8.0493 * 10^{-2}\ cm^{-1}}} = 1.85975\ cm$$

Hence, mesh intervals should be approximately 1 cm or less.

For slowing down distance:

$\tau_{CH_2} \sim 18\ cm^2$

$\sqrt{\tau} \sim 4.24\ cm$

Hence, 1 cm mesh interval should be adequate, as was the case for the original calculations with the 120 mesh interval limitation, except for flux distribution at boundaries.

Appendix E

Input File Explanation

```
      0
printer alingment indicator
    19          1    AGN 201, spherical model, 14.54 cm radius
1=page control, 9=type of neutron spectrum,
Spaces 9 through 80 are for case
description
      5         1         1
5=5 compositions, 1=give listing of mixed compositions, 1=flashes the library
      1         2         2              3              68.00
1=composition #1, 2=number of fuel elements, 2=number of non-fuel elements, 3=no Behren's correction, temperature 68 F
      1        95              0.000135
1=fuel element, 95=U-235, atom density of 0.000135*10^24 atoms per cm^3
      1        98              0.000546         12
1=fuel element, 98=U-238, atom density of 0.000546*10^24 atoms per cm^3, cell correction factors start at
level 12
            0.70     0.46         0.50        1.0       1.0         1.0       1.0       1.0
The 8 cell correction factors, energy level 12 through 19*
      0         6              0.0396
0=non-fuel element, 6=carbon, atom density of 0.0396*10^24 atoms per cm^3
      0         1              0.0791
0=non-fuel element, 1=hydrogen, atom density of 0.0791*10^24 atoms per cm^3
      2         2         2              3              68.00
2=composition #2, 2=number of fuel elements, 2=number of non-fuel elements, 3=no Behren's correction, temperature 68 F
      1        95              0.000270
1=fuel element, 95=U-235, atom density of 0.000270*10^24 atoms per cm^3
```

```
      1        98              0.001092         12
1=fuel element, 98=U-238, atom density of 0.001092*10^24 atoms per cm^3, cell correction factors start at
level 12
            0.89     0.46          0.50       1.00     1.00         1.00      1.00       1.00
The 8 cell correction factors, energy level 12 through 19
      0        6               0.0396
0=non-fuel element, 6=carbon, atom density of 0.0396*10^24 atoms per cm^3
      0        1               0.0791
0=non-fuel element, 1=hydrogen, atom density of 0.0791*10^24 atoms per cm^3
      3        2        3              3               68.00
3=composition #3, 2=number of fuel elements, 3=number of non-fuel elements, 3=no Behren's correction, temperature 68 F
      1        95              0.000135
1=fuel element, 95=U-235, atom density of 0.000135*10^24 atoms per cm^3
      1        98              0.000791
1=fuel element, 98=U-238, atom density of 0.000791*10^24 atoms per cm^3, cell correction factors start at
level 12
            0.89     0.46          0.50       1.00     1.00         1.00      1.00       1.00
The 8 cell correction factors, energy level 12 through 19
      0        6               0.0396
0=non-fuel element, 6=carbon, atom density of 0.0396*10^24 atoms per cm^3
      0        1               0.0791
0=non-fuel element, 1=hydrogen, atom density of 0.0791*10^24 atoms per cm^3
      0       13              0.00052
0=non-fuel element, 13=aluminum, atom density of 0.00052*10^24 atoms per cm^3
      4        0        1              3               68.00
4=composition #4, 0=number of fuel elements, 1=number of non-fuel elements, 3=no Behren's correction, temperature 68 F
      0        6               0.0878
0=non-fuel element, 6=carbon, atom density of 0.0878*10^24 atoms per cm^3
      5        0        1              3                68
```

5=composition #5, 0=number of fuel elements, 1=number of non-fuel elements, 3=no Behren's correction, temperature 68 F

```
      0        79              0.00591
```

0=non-fuel element, 79=gold, atom density of 0.00591*10^24 atoms/cm^3

```
      4        0        3            4          4        2          4        1          1       20         1         1         0      100
```

4=spherical-radial, 0=no axial, 3=number of radial region, 4=extrapolated zero flux, 4=axial final boundary conditions, 2=radial initial boundary conditions, 4=radial final boundary condition, 1=identification of core region, 1=fission densities are assumed equal to 1.0, 20=maximum number of buckling iterations, 1=neutron balance will be made and printed for each region, 1=flux and adjoint printout, 0=no adjoint flux calculation, 100=maximum number of diffusion calculation

```
              0.0      0.0              0.0000          0.00001          0.0001                0
```

Starting axial dimension is 0.0, starting radial dimension is 0.0, starting value for core transverse buckling is 0, effective multiplication factor convergence criteria is 0.00001, buckling convergence criterion is 0.0001, source convergence factor is 0. **

```
      2        50       0.5              0.0000        1        250             14.04           0.0000
```

2=region composition identification, 50=number of intervals in region, width of region is 0.5 cm, transverse buckling for this region is 0
1=region composition identification, 250=number of intervals in region, width of region is 14.04 cm,
transverse buckling for this region is 0

```
      4       390    20.0              0.0000
```

4=region composition identification, 390=number of intervals in region, width of region is 20.0 cm, transverse buckling for this region is 0

* The important cell correction factors are primarily for resonance self-shielding, groups 12, 13 and 14. For all the other groups, 1.0 indicates no self-shielding.

** The spherical size of the reactor was determined by the spherical radius that has the same volume as the cylindrical reactor volume, plus the several extra pieces of core material laid on top of the reactor [8].

References

1. James J. Duderstadt and Louis J. Hamilton, “Nuclear Research Analysis” 1942.

2. Samuel Glasstone and Milton C. Edlund, “The Elements of Nuclear Reactor Theory” 1952.

3. http://www.Gnu.org

4. http://windows.microsoft.com/en-us/windows/32-bit-and-64-bit-windows#1TC=windows-7

5. Mackenzie Leigh Gorham, “Experimental Parameterization of the Idaho State University AGN-201 Research and Training Reactor”, Idaho State University, 2012

User's Manual

THE DISNEL* MULTIGROUP NEUTRON DIFFUSION CODE

* DISNEL – Diffusion Iterative Solution for Nineteen Energy Levels

The DISNEL Multi Group Diffusion Reactor Physics Code

1. Introduction

The widespread use of microcomputers with substantial memory capacity has made it more convenient and advantageous to use these microcomputers instead of mainframe computer for many computationally intensive programs.

The program DISNEL had its origin with the Space Nuclear Propulsion Programs of the General Electric Company in the 1960/1970 period.

The program is specifically designed to be able to effectively calculate a wide variety of reactor configurations from the very fast spectrum type to the conventional thermal reactor. The program was subsequently sized to be accommodated by the early generation of the IBM-360 computers at the Idaho National Engineering Laboratory, where the program was used for generalized calculations of conceptual or preliminary design, or for general safety analysis calculations. The code has since routinely been used at the University of Utah (TRIGA reactor) as well as at the University of Missouri (10 MW plate-fuel reactor similar to one lobe of the ATR).

This program was for use on IBM-PC to perform various reactor-physics calculations, based upon the solution of the one-dimensional neutron diffusion equation.

Now, the program has been revised and adapted in Fortran F-77 Microsoft, Version 4.0, for IBM-PC and compatible with 640K bytes of main memory and hard disk, running PC-DOS or MS-DOS version 2.11 or later.

The program itself requires approximately 217 K memory when it has been loaded into IBM-PC. A version of “DISNEL” on floppy disk has been made that can be run on an IBM/PC-XT with two floppy disks (360 K each) and 640 K memory, without a

hard disk. The input data can be typed through the keyboard from the input data file, which has the name of DISNEL.INP. The input could previously have been generated and saved on the floppy or hard diskette.

2. Theoretical Consideration

2.1. General Description

DISNEL is a "one-pass", one-dimensional diffusion code, providing its own cross sections for diffusion calculation. Reactor compositions (not cross sections) are the required input, and consequently the code is very useful for quick, survey calculations of a type usually desired for scoping studies or for calculating effects of changes in reactor structure or composition. The code uses a fixed 19 group energy structure shown in Table 1. The group structure in the resonance region is essentially identical to that given ANL 5800, P 526-529, for computing resonance self-shielding corrections.

The element cross sections are from a Nuclear Data Tape (1) compiled at General Electric, NMPO. Cincinnati.

These cross section libraries are listed in Table 2. The code will handle slab (one dimensional), radial-cylindrical, or spherical coordinates. It also has the provision for cross matching axial slab and radial calculations by iterating on buckling-leakage terms so as to, in-effect, obtain the reactivity and flux distribution of a cylindrical reactor in two dimensional geometry for the core. (Note, this cross matching technique, in effect, results in the equivalence of a true two dimensional calculation for the core.

The later specifically solves both coordinates simultaneously, whereas DISNEL explicitly averages the buckling through the calculation.)

An adjoint calculation option is included. The general input format for the program is shown in user's instruction in Chapter 3.1. The method of solution is as below.

a. Cross sections and number densities (volume fractions) are combined to form composition macroscopic cross sections.
b. The reactor description is used to develop the mesh interval values of size and cross sections.
c. The diffusion equation is solved using an algorithm that is considered standard (2).

Table 1. Energy Group Structure of Disnel

Group NO.	Lethargy Width	Energy (eV)	
		Upper	Lower
1	0.25	10.0×10^6	7.788×10^6
2	0.50	7.788×10^6	4.724×10^6
3	0.50	4.724×10^6	2.865×10^6
4	0.50	2.865×10^6	1.738×10^6
5	0.50	1.738×10^6	1.054×10^6
6	0.50	1.054×10^6	6.393×10^5
7	0.50	6.393×10^5	3.877×10^5
8	0.50	3.877×10^5	2.352×10^5
9	1.25	2.352×10^5	6.738×10^4
10	2.00	6.738×10^4	9.119×10^3
11	2.00	9.119×10^3	1.234×10^3
12	2.00	1.234×10^3	1.670×10^2
13	2.00	1.670×10^2	2.260×10^1
14	1.75	2.260×10^1	3.928
15	1.25	3.928	1.125
16	1.00	1.125	0.414
17	1.00	0.414	0.1523
18	1.03	0.1523	0.05437
19	Maxwell-Boltzman Thermal Average (Temperatures from 68 to 3000 ^{0}F) 0.0254 at room temp		

d. Following the desired convergence* of the solution (convergence on eigenvalue K_{eff} is the only option), region averages for absorption, fission, etc. and grand total are calculated, fluxes and power are normalized, and fluxes are printed, if desired.

Most of the calculations are done in 64 bit arithmetic (REAL*8 in FORTRAN), what would normally be referred to as double precision arithmetic. This was found to be necessary for problems involving very small thickness of low absorption materials.

The code limitations are as below:

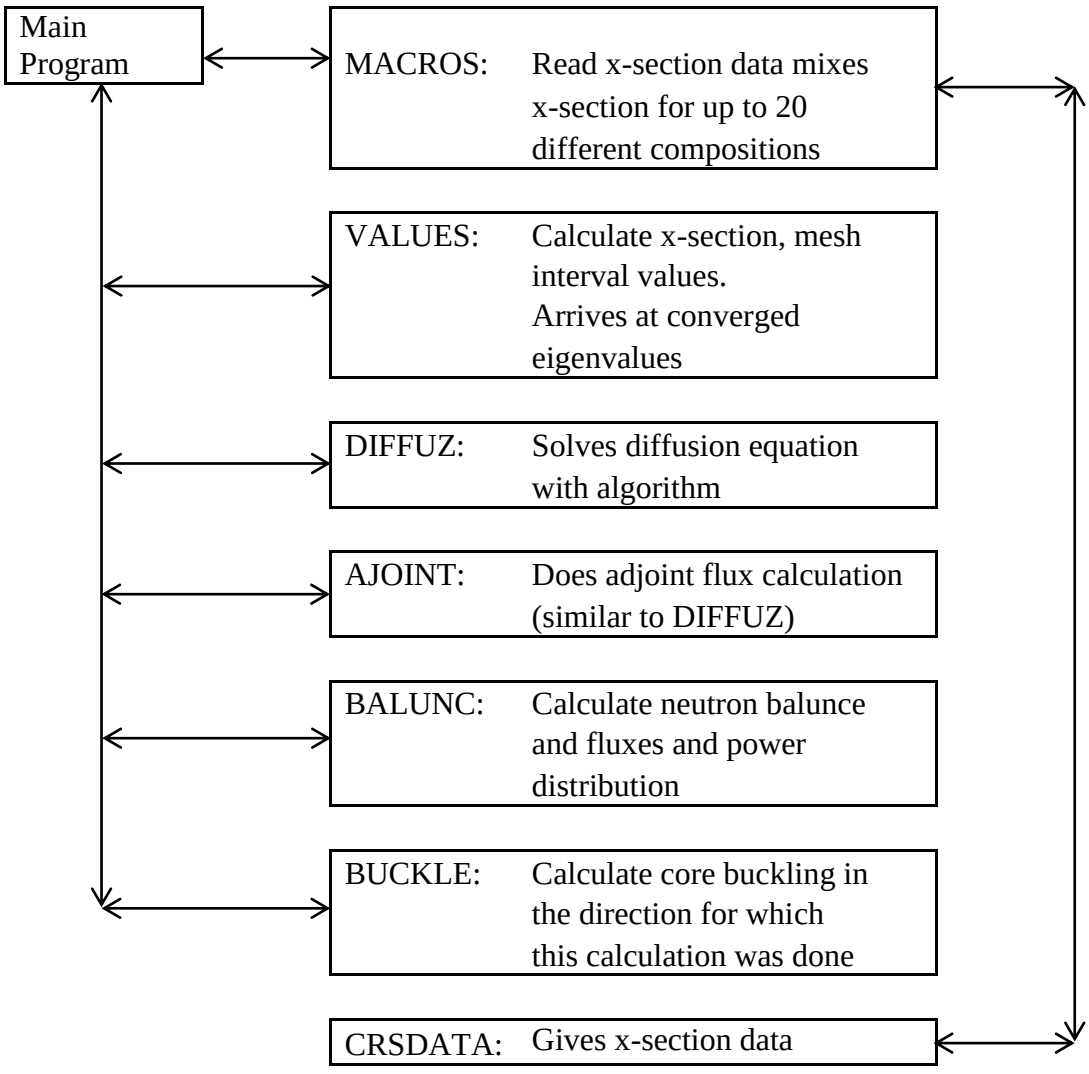
a. The mesh points for any one dimensional calculation must not be more than 1000.
b. The kind of special element for which new cross sections are read must not be more than 20.
c. The kind of different compositions, of which no more than 10 can have scatter transfer matrices, must be not more than 20.
d. The regions for the reactor description for any one dimensional calculation must not be more than 20.

---

*Convergence to 1*E-5 and 1*E-6 on fission source eigenvalue is typical and recommended. Under such conditions, typical problems have all fluxes converged to less than 1%. About 20 to 40 iterations are required to achieve this convergence depending on the type of problem.

2.1.1 Flow Chart

Figure 1 shows a flow chart for the code:



2.2 Cross Section Data

The basic cross-section data is supplied in a set of "lines", for 125 different elements or materials (See table 2). For elements without any production cross-section, there is a title line plus 12 "lines" of data. (See source program of CRSDATA.DAT). Elements with production cross-sections require "17 lines". Elements designated with an asterisk have their cross sections in macroscopic form (cm^{-1} =$\sum$), usually with reference to normal density of that material. All other cross section are in barns, (E-24 cm^2). Hence, concentrations of these should be entered in units of E-24 atoms/cc. The cross-section listing for a given element or material consists of five columns of 26 values. The columns are cross sections for:

a. Scattering – used only when scatter-transfer matrix is required.

b. Slowing down, $\xi \sum_S$. The cross section for down scattering is then computed in the code as these cross sections divided by the lethargy width of the group from which the scattering is occurring. When using this format, all transfers are assumed to occur to the next lower group. However for hydrogen and deuterium, this is a poor approximation, and for these a scatter matrix is calculated, see next page.

c. "Transport" cross section equal to $\sum_S(1-\mu_0)$.

   Note: the usual definition of transport cross section is $\sum_S(1-\mu_0)+ \sum_a$. However, the code adds together column 3 and column 4 to get the usual transport cross section from which the diffusion coefficient is then calculated. There is also an option to adjust this calculation to more accurately approximate a true transport calculation. (See Section 3.1)

d. Absorption cross section (includes fission as well as capture).

e. $\nu\sum_{F,}$ fission cross section times neutron yield per fission (commonly called production cross section). This column is included only with those element codes preceded by a minus sign. Note, Be and BeO have an equivalent production cross section to account for the (n, 2n) reaction.

For hydrogen and deuterium, down scattering will span many groups. To obtain a scatter transfer cross section, the hydrogen material must be separated into its elemental parts. Then transfer cross section matrix, spanning 10 down scatter groups*, is calculated. (The remainder of the down scattering is placed in the tenth group). This treatment produced for elements #100 (water), #1 (hydrogen) and #102 (deuterium, bound as in heavy water). In the case of water, for instance, the scatter-transfer matrix is calculated for its hydrogen and then oxygen is added to the first down-scatter group. All other elements (materials) will be treated in the elastic-scattering single down-scatter group approximation. Note, this approximation is correct for beryllium and all heavier elements. For Be, the maximum energy loss is 0.503 lethargy units. The narrowest group, with the exception of the top group is 0.50 lethargy units.

Lithium is the only element that for which scattering to only the next lower group is not exactly correct for its down scatter treatment. (Hydrogen and deuterium are exceptions, as per above.)

The 26 values in each column are the cross sections for the first 18 groups, the 19^{th} row is an unused reference cross section for 0.03930 eV, and the final 7 rows are thermal cross sections, Maxwell Boltzman averaged, for 3000, 2500, 2000, 1500, 1000, 500, and 68^0F respectively. Cross sections for any temperature selected between these

extremes will be interpolated by the program. However, if an element contains production cross sections that are to be used, then when it is read in, its title line must have a -1 in columns 79 and 80 and be followed by 16 data lines of cross sections.

---

* Ten down scatter groups covers the region of interest and correctly allocates 99% of the hydrogen scatterings (100% of the deuterium scatterings).

Table 2

Cross Section Library Index

Element with * are Macroscopic Sigma (1/cm)

1	BND HYD ATOM	Bound as in the water molecule	0
2	HELIUM		0
3	LITHIUM (NAT)		0
4	BE (with N, 2N)	Metal has 0.1236 BE/CC. See 104 and 114 for BEO	-2
5	BORON (NAT)	See 105 for Boron-10 Isotope	0
6	CARBON	Reactor grade blocks have 0.0855 atoms/cc	0
7	NITROGEN	Nitrogen atom	0
8	OXYGEN ATOM		0
9	FLUORINE	Fluorine atom	0
10	NEON		0
11	SODIUM	Liquid, 200 ^{0}F, has 0.0248 NA/CC, density 0.947	0
12	MAGNESIUM	Metal has 0.0431 Mg/CC, density 1.74	0
13	ALUMINUM	Metal has 0.0602 Al/CC, density 2.7, See 113 for Al203	0
14	SILICON		0
15	PHOSPHORUS		0
16	SULPHUR		0
17	CHLORINE		0
18			2
19	POTASSIUM		0
20	CALCIUM		0
21	SCANDIUM		0
22	TITANIUM		0
23	VANADIUM		0
24	CHROMIUM		0
25	MANGANESE		0
26	IRON	Metal has 0.0848 Fe/CC, density 7.86	0
27	COBALT		0
28	NICKEL	Metal has 0.0913 Ni/CC, density 8.90	0
29	COPPER	Metal has 0.0848 Cu/CC, density 8.94	0
30			2
31	XE-131	Xenon 131 Isotope	0
32	MO-95	Molybdenum 95 Isotope	0
33	CD-113	Cadmium 113 Isotope	0
34	SLAG 1	Fission product slag, abs, cross section= 44 barns thermal	0
35	SLAG 2	Long-lived slag, 4.5 barns thermal absorption	0
36			2
37			2

38			2
39	YTTRIUM		0
40	ZIRCONIUM	Metal has 0.0424 Zr/CC, density 6.4	0
41	NIOBIUM		0
42	MOLYBDENUM		0
43	TC-99	Technetium 99	0
44			2
45	RHODIUM		0
46			2
47			2
48	CADMIUM		0
49	INDIUM		0
50			2
51			2
52			2
53			2
54	XENON-135		0
55	CESIUM		0
56	BARIUM		0
57	1/V ABSORBER	Sigma abs. varies as 1/V, with 1.0 barns at 2200 M/sec	0
58	CONST.SCATTER	Constant 1.0 barns sigma-s and sigma transport, all groups	0
59	IMPORTANCE	NU-sigma fission for U-235 scaled to give 1.0 for sum	-2
60			2
61	PM-147		0
62	SAMARIUM		0
63	EUROPIUM		0
64	GADOLIUM		0
65			2
66	DYSPROSIUM		0
67	*ALLOY 212B	7.87 g/CC, 0.9866 FE, 0.0016 C, 0.009 MN, 0.002 SI	1
68	*ALLOY 302B	7.87 g/CC, 0.9778 FE, 0.0013 C, 0.0132 MN, 0.0052 MO	1
69	*CR-MO-STEEL	7.87 g/CC, .9597 FE, .0225 CR, .0045 MN, 0.01 MO, .0025 SI	1
70	*W-MO-RE	15.43 g/CC, 0.3 MO, 0.3 RE, 0.4 W	1
71			2
72	HAFNIUM	Metal has 0.0449 HF/CC, density 13.3	0
73	TANTALUM	Metal has 0.0553 TA/CC, density 16.6	0
74	TUNGSTEN	Metal has 0.0632 W/CC, density 19.3	0
75	RHENIUM (RE)	Metal has 0.0664 RE/CC, density 20.53	0
76	H ATOM ZRH	As bound in ZRH molecule	0
77			2
78	PLATINUM	Metal has 0.0660 PT/CC, density 21.37	0
79	GOLD	Metal has 0.0591 AU/CC, density 19.32	0
80	MERCURY	Liquid metal has 0.0407 HG/CC, density 13.55	0
81			2
82	LEAD	Metal has 0.0330 PB/CC, density 11.35	0

83	BISMUTH	Metal has 0.0281 BI/CC, density 9.747	0
84	SM-149		0
85	SM-151		0
86	SM-152		0
87	EU-153		0
88	GD-155		0
89	GD-157		0
90	THORIUM	Metal has 0.0293 TH/CC, density 11.3	-2
91			2
92	NAT. U-ATOM	Metal has 0.04783 U/CC, density 18.9, dioxide 0.0223 MO/CC	-2
93	U-233		-2
94	U-234		-2
95	U-235	Nu=2.40+0.1 E (MeV)	-2
96	U-236		-2
97			2
98	U-238		-2
99	*ORALOY	18.7 g/CC, .932(U-235), .01(U-236), .004(U-234),.0542(U-238)	-1
100	*WATER	Density 1.0 g/CC. with scatter transfer matrix	1
101	HYDROGEN GAS	Half the cross section of H2	0
102	DEUTERIUM	Heavy hydrogen atom as bound in heavy water	0
103	LITHIUM-6	Lithium 6 isotope	0
104	*BE (N,2N)	Beryllium metal, density 1.85, with (N,2N) reaction	-1
105	BORON-10	2200 m/sec absorption cross section = 4030 barns	0
106	*B4C (NAT)	Natural boron carbide, density = 2.59	1
107			2
108	*THERMOFLEX	Insulation density=0.224, 0.50 oxygen, 0.26 Al, 0.23 Si	1
109	PU-239		-2
110	PU-240		-2
111	PU-241		-2
112	PU-242		-2
113	*AL2-03	Aluminum oxide, density 3.97	1
114	*BEO	Beryllium oxide, density 3.01	-1
115	*SIO	Silicon dioxide, density 2.65	1
116	*NICHROME	Density 8.44,.786 Ni,.1985 Cr,.07 Fe, .025 Ti, .005 Mn, .01 Nb	1
117	*INCONEL-X	Density 8.30, 0.73 Ni, .15 Cr, .07 Fe, .025 Ti, .005 Mn, .01 Nb	1
118	*INCONEL	Density 8.43, 0.72 Ni, 0.165 Cr, 0.0985 Fe, 0.01 Mn, 0.005 Cu	1
119	*INCALLOY	Density 8.02, 0.4345 Fe, 0.325 Ni, 0.21 Cr, 0.008 Ti, 0.015 Mn	1
120	*FERCAL	Density 7.20, 0.70 Fe, 0.25 Cr, 0.05 Al	1
121	*303-STAINLS ST	Density 7.98, 0.7142 Fe, 0.18 Cr, 0.09 Ni, 0.0008 C, 0.005 Si	1
122	*304-STAINLS ST	Density 7.98, 0.7046 Fe, 0.19 Cr, 0.09 Ni, 0.01 Mn, 0.005 Si	1
123	*310-STAINLS ST	Density 7.92, 0.5262 Fe, 0.250 Cr, 0.205 Ni, 0.01 Mn, .0075 Si	1
124	*348-STAINLS ST	Density 7.98, 0.6985 Fe, 0.18 Cr, 0.11 Ni, 0.01 Mn, 0.001 Nb, 0.0005 T	1
125	*ZIRCALLOY-2	Density 6.55, 0.015 Sn, 0.0012 Fe, 0.0009 Cr, 0.0005 Ni	1

2.2.1 Cross Section Correction Factor

With built-in cross section, all derived from ENDF data, the user still has the option of modifying any cross section of a mixture, in any group, by use of the "Cell Correction Factor" option. An example is to account for thermal flux depression (or resonance self-shielding, see section 2.3), in which the flux in a fuel element may be significantly lower than the moderator. One may either increase the moderator cross section accordingly (increase the moderator interaction rate, or the equivalent of a flux increase), or reduce the fuel cross section accordingly (vice versa reduces the fuel interaction rate, or the equivalent of a flux decrease). *

With this option, the user can insert hand-calculated cell correction factor. Or, alternatively, the user could perform first a separate "cell" calculation, then use those results to obtain "Cell Correction Factors" for the subsequent whole reactor calculation. The "Cell Correction Factor" would be Φ(mod.average)/Φ(fuel.average), or the reciprocal, depending on section by the user as for the moderator or fuel, respectively. In the case of developing hand-calculation, one might use a conventional treatment of the type in Glasstone & Sesonske, 2nd Edition (1963, ref.8 page 190 to 194) to calculate the thermal flux depression factor. This factor can then be inserted as a cell correction factor for the thermal (group 19) cross section of the moderator (factor >1.0) or in the fuel (factor <1.0).

---

* It has been customary to consider the moderator flux and cross section as the base and correct fuel. However, there is fundamentally no difference in overall result whichever material receives the correction.

2.3 Resonance Absorption

The resonance cross sections in the library are for infinite dilution, i.e. the direct integrals without self-shielding. For elements with a single major resonance with a given energy group, the formula:

$$\frac{RI_{\infty}}{RI_{eff}} = \sqrt{1 + \frac{\sigma_r \left(\frac{\Gamma_{\gamma}}{\Gamma}\right)}{\frac{S}{4VN}}} \qquad \text{Equation 1}$$

where:

RI_{∞} and RI_{eff} are the infinite dilution and effective resonance integrals, respectively

σ_r is peak cross section of the resonance

Γ_{γ} and Γ are the (n,γ) and total widths, respectively

The group cross section is $\frac{RI}{\Delta U}$, where ΔU is the group lethargy width. The square root in the above expression thus represents the group cross section correction factor (for a single resonance in the group).

In the case of U-238 and U-235, there are many narrow resonances in a single energy group. Self-shielding factors for these two isotopes are shown in Table 3 and 4*, obtained from the table in ANL 5800, Reactor Physics Constants, P-526. The energy group structure in those tables is almost identical to the energy structure of this code, and the minor difference in the boundary between groups 14 and 15 will be of little consequence in computing self-shielding factors.

In the case of uranium, the NRIA approximation is assumed. An improved semi empirical formula for computing σ_p is given (4):

$$\sigma_p = \frac{f\,\sigma'}{1.27} + \frac{S}{4\,NV} * \frac{1-C}{1+0.1C}$$ Equation 2

where :

σ' is the potential scattering cross section per absorber atom

C is the "Dancoff correction factor" (5) for view-shielding of nearest neighbor rods

f is an empirical correction factor which is 0.700 for oxygen and 0.766 for carbon

Generally, above 167 eV, the resonances can usually be the assumed to be essentially non-shielded. However, in cases where the configuration is such that the higher energy groups should have self-shielding factors applied. The user is referred to the literature (fo instance, Levin).

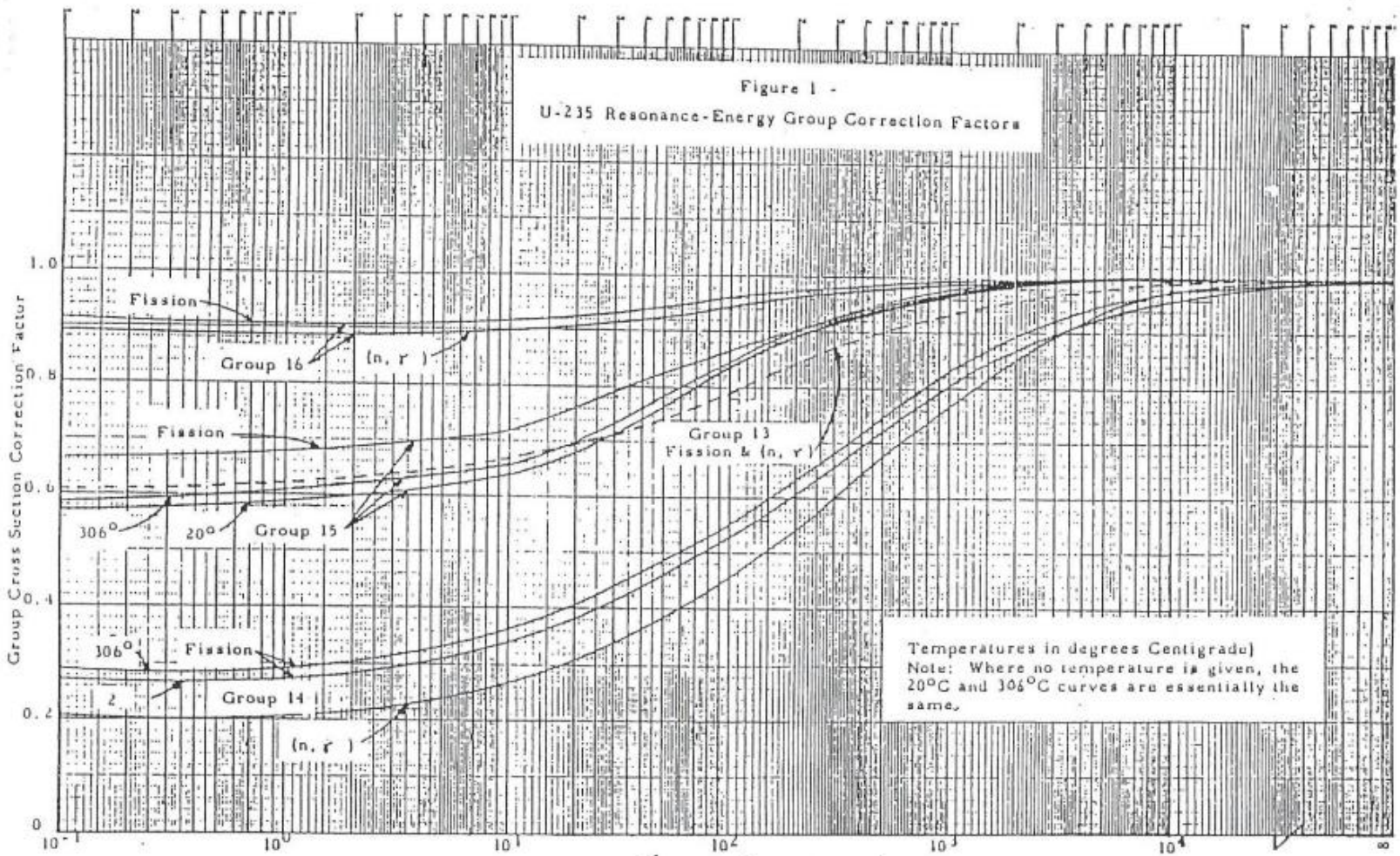
---

* Also listed in Table 3 and Table 4, the latter for 2038 ^{0}C

Table 3

Self-Shielding Corrections in Resonance-Energy Groups

20^0C U-235 (n,f)	Group	Group	Group	Group	Group
P	16	15	14	13	12
0.1	0.916	0.659	0.274	0.620	
10	0.925	0.713	0.342	0.670	
32	0.936	0.779	0.419	0.720	
100	0.961	0.864	0.533	0.790	
200	0.975	0.911	0.609	0.840	
400	0.985	0.948	0.693	0.890	
1,600	0.996	0.985	0.852	0.940	
10,000	0.999	0.998	0.966	0.990	
∞	1.000	1.000	1.000	1.000	
U-235 (n,ϒ)					
0.1	0.887	0.571	0.205	0.610	
10	0.898	0.641	0.267	0.670	
32	0.917	0.726	0.343	0.720	
100	0.945	0.835	0.469	0.790	
200	0.963	0.895	0.559	0.840	
400	0.978	0.938	0.659	0.880	
1,600	0.993	0.982	0.843	0.980	
10,000	0.999	0.996	0.965	0.990	
∞	1.000	1.000	1.000	1.000	
U-238 (n,ϒ)					
0.1	0.990	1.000	0.0099	0.0076	0.010
10	1.000	1.000	0.0271	0.0365	0.085
32	1.000	1.000	0.0361	0.0506	0.126
100	1.000	1.000	0.0688	0.1020	0.152
200	1.000	1.000	0.1110	0.1390	0.243
400	1.000	1.000	0.1620	0.1980	0.346
1,600	1.000	1.000	0.3690	0.3460	0.656
10,000	1.000	1.000	0.6920	0.6500	0.887
∞	1.000	1.000	1.0000	1.0000	1.000



$$\sigma_\rho = \frac{\Sigma_s}{N_u} + \frac{S}{4VN_u}(1-C)$$

For higher fuel temperatures, see ANL 5800, Reactor Physics Constants, page 526, or Tables 2 and 3

Table 4

Self-Shielding Corrections in Resonance-Energy Groups

$2038^0C = 3700^0F$

U-235 (n,f)	Group	Group	Group	Group	Group
P	16	15	14	13	12
0.1	0.919	0.683	0.378	0.620	
10	0.927	0.737	0.447	0.670	
32	0.942	0.801	0.527	0.720	
100	0.963	0.881	0.640	0.790	
200	0.976	0.923	0.714	0.840	
400	0.986	0.956	0.791	0.890	
1,600	0.997	0.987	0.915	0.940	
10,000	0.999	0.998	0.983	0.992	
∞	1.000	1.000	1.000	1.000	
U-235 (n,ϒ)					
0.1	0.893	0.640	0.310	0.610	
10	0.903	0.710	0.386	0.670	
32	0.921	0.788	0.474	0.720	
100	0.949	0.787	0.664	0.790	
200	0.966	0.923	0.699	0.840	
400	0.980	0.956	0.786	0.880	
1,600	0.994	0.999	0.918	0.990	
10,000	0.999	0.997	0.984	0.990	
∞	1.000	1.000	1.000	1.000	
U-238 (n,ϒ)					
0.1	0.990	0.996	0.0101	0.0105	0.010
10	1.000	1.000	0.0288	0.0468	0.141
32	1.000	1.000	0.0400	0.0687	0.220
100	1.000	1.000	0.0870	0.1534	0.266
200	1.000	1.000	0.1552	0.2110	0.410
400	1.000	1.000	0.2400	0.3080	0.542
1,600	1.000	1.000	0.5320	0.5075	0.813
10,000	1.000	1.000	0.8310	0.8030	0.948
∞	1.000	1.000	1.0000	1.0000	

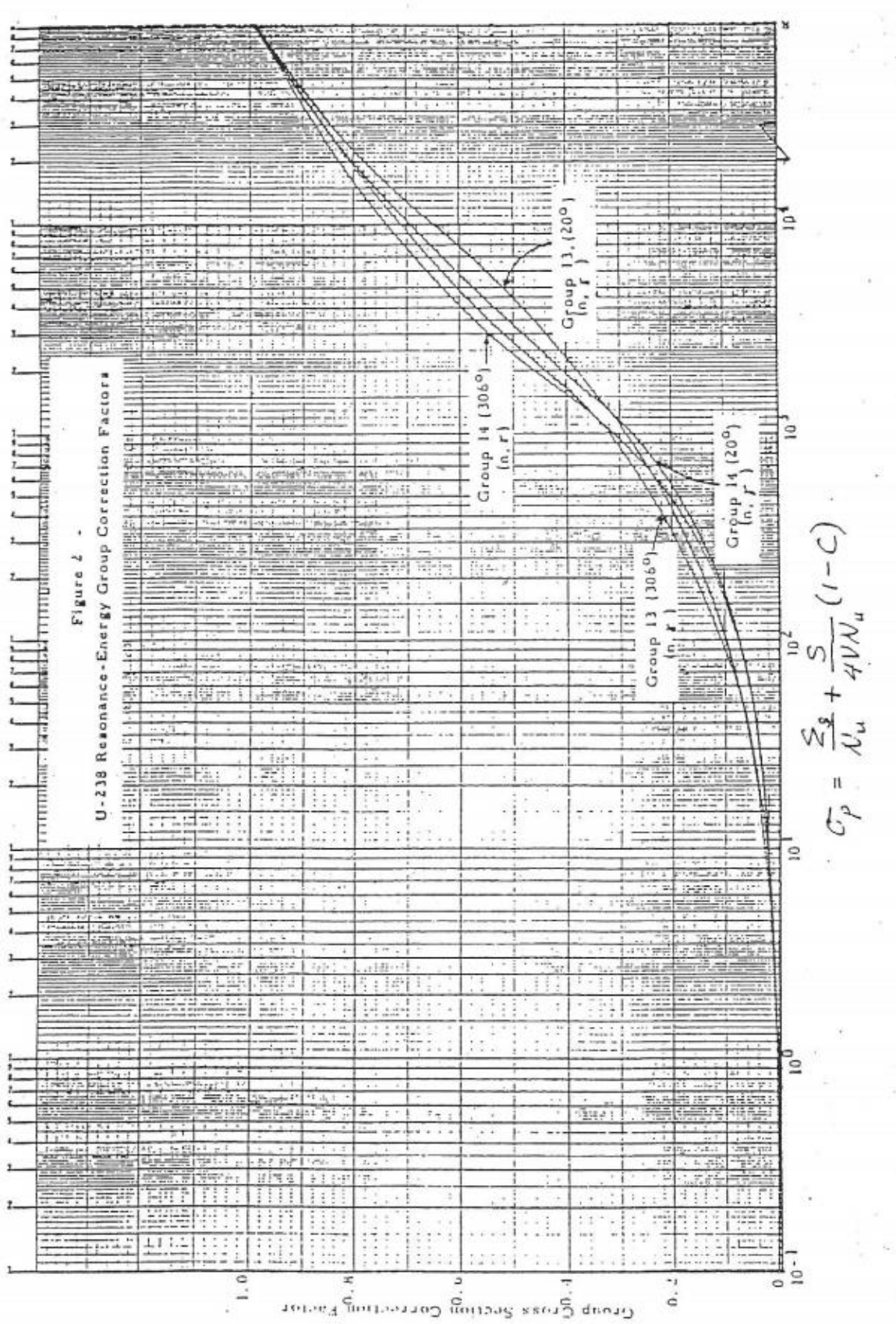


Figure 2 -
U-238 Resonance-Energy Group Correction Factors
Group 14 (306°) (n, r)
Group 13, (20°) (n, r)
Group 13 (306°) (n, r)
Group 14 (20°) (n, r)
Group Cross Section Correction Factor
1.0
0.9
0.8
0.7
10^{4}
10^{3}
10^{2}
10
10^{0}
10^{-1}
$C_p = \frac{\Sigma_s}{\nu_u} + \frac{S}{4\nu N_u}(1-C)$

2.4 Behren's Correction

This correction is for use in those regions in which the diffusion of neutrons in one coordinate direction may be substantially different than in other. Examples are the vertical arrangement of gas-cooled fuel elements in a water or graphite moderated system. (The treatment was originally developed for the British Calder Hall reactors, and later modified aircraft Nuclear Propulsion reactor designs in the U.S.) The vertical steaming of neutrons will substantially enhance this diffusion coefficient, which in turn will be larger than the orthogonal (radial) diffusion coefficient.

The corrected diffusion coefficient is defined as:

$$D_{corr} = D_0(1 + \epsilon) \qquad \text{Equation 3}$$

The correction term ϵ is calculated using the following formulae, depending on the option chosen for BARON.

a. For options 1 and 2 in the input format the form derived by Behren's (6) is used.

$$\epsilon = \frac{1}{(1+\Phi)^2}\left[\frac{\Phi D}{\lambda}\left(AQ + \frac{1}{\exp\left(\frac{D}{\lambda\Phi}\right) - 1}\right) - \Phi^2\right] \qquad \text{Equation 4}$$

where A = 0.5 for the radial direction.
= 1.0 for the axial direction, the direction of orientation of the fuel elements or other channels
= 0.667 if the average or isotropic correction is to be used.

D $= D_0 e^{-\Sigma_a D_0}$ the effective hydraulic diameter. The effective hydraulic diameter is herein defined by this formula with D_0 being the actual

diameter, which is multiplied by the factor exp(-$\sum_a D$), $\sum_a$ representing the cross section for absorption of any fuel or other materials in the "void diameter," i.e. the non-diffusing diameter (D_0 is input DEFF).

Φ $= \frac{Volume\ of\ Void}{Volume\ of\ Material}$ average over the cell or the region. Φ is input RMOD.

λ $= (\sum_{tr} + \sum_a)$ cell ave.* (volume of cell)/(volume of moderator)
The input $RMOD = \frac{Volume\ of\ Cell}{Volume\ of\ Moderator}$ i.e. the reciprocal of the moderator volume fraction

Q = a shape of factor, as derived by Behren's, $\mu = \frac{inner\ void\ dia.}{outer\ void\ dia.}$

μ	0.0	0.2	0.6	0.8	1.0
Q	1.00	1.12	1.20	1.34	∞

The model employed is flexible, subject to the user's convenience within the above description limitations.

b. For options 4 and 5 in the input format, a modified form used in NMPO, Evendale since 1958 is calculated:

$$\epsilon = \frac{e^{-x}}{1 + \frac{V_f}{V_m}} \left[1 + 2\left(\frac{V_f}{V_m}\right) + \left(\frac{V_f}{V_m}\right) * \frac{Y}{e^Y - 1} + AY\right] - e^{-x} \qquad \text{Equation 5}$$

where:

V_f = volume of fuel
V_m = volume of moderator
Y $= (V_f/V_{cell}) * (\sum_s + \sum_a)$ for the moderator
X $= \sum_a * (distance\ across\ moderator)$
Where $\sum_a$ is for the fuel only
A = 1, 2/3, 0.5 for axial, isotropic, and radial coefficient, respectively.
The model for these equations is an inner cylinder of moderator surrounded by an annulus of fuel and void, which in turn is surrounded by an annulus of moderator.

If the Behren's correction for the diffusion coefficient is to be used, a distinction between fuel and moderator is necessary. "Moderator" is assumed to be a continuous medium, except for full length holes that contain the "fuel". This interpretation is that needed in applying the Behren's correction. For instance, structural material that is in the moderator should be designated as "Moderator", but if it is part of the fuel element structure or cladding, it should be designated as "fuel".

2.5 Diffusion Coefficient Correction Factor

Diffusion theory implicitly limits the angular dependence of the flux to first order terms. Therefore, in regions of high absorption (relative to scattering) or in void regions, the diffusion theory approximation is incorrect. A method of accounting for the first case, high absorption, is to modify the diffusion coefficient to give a flux spatial dependence more closely resembling the results of transport theory.

In the asymptotic mode*, the transport P_3 solution gives:

$$\frac{K}{\sum_{tot}} = \tanh\left(\frac{K}{\sum_s}\right) \qquad \text{Equation 6}$$

Where:

$K^2 = \frac{\sum_a}{D}$ (See, for instance, Weinberg & Wigner, The Physics of Chain Reactors, P-238)

This transcendental equation can be approximated by

$$K = \sqrt{3\sum_t\sum_a}\left[1 - \frac{2}{5} * \frac{\sum_a}{\sum_s}\right] \qquad \text{Equation 7}$$

The correction factor

$$\left[1 - C\frac{2}{5} * \frac{\sum_a}{\sum_s}\right]$$

is available in the DISNEL code as a division factor for the diffusion coefficient. The value of C is input for DCORR, columns 71 to 75 of line #5. If left blank, the value will automatically be zero and the diffusion coefficient will not be altered from the normal definition; If a value of 1.0 is inputted, then one obtains the approximate "asymptotic" solution. The user can select my value for C that he wishes. However, one should be cautioned that this expression with C=1 is asymptotic diffusion theory only in an infinite medium with no sources. Thus, it is not a complete panacea for the deficiencies of diffusion theory.

More rigorously, the transport solution given is only valid in the asymptotic flux. Unfortunately, such an asymptotic flux rarely ever exists where this approximation is most needed. However, if K^2=-B^2, where B^2 is buckling, then the equation can be applied anywhere that B^2 (or alternately K^2) is known. Indeed, such a scheme could be employed (and has been in some codes), by which one uses the regular diffusion coefficient expression, D=1/3 λ_{tr} to obtain an initial solution. The values of B^2 are then computed in discrete sub-regions across the reactor, and these employed to solve the above transcendental equation to obtain new diffusion coefficient from which a new flux solution is obtained. Iterations would continue this way until the flux stabilizes.

2.6 Cross Matched Cylindrical Calculation

For each energy group, the average value of $\nabla^2\Phi$ is computed across the average core regions (LCORE) and set equal to $-B^2\Phi$, where B^2 is the buckling. This value of

the buckling is then multiplied by D and added to the absorption cross section in order to account for the transverse leakage in all regions of the subsequent calculation (radial if the just-finished calculation was axial, etc.). However, if $B^2$is negative (a leakage of neutrons into the region), the absolute value of DB^2that is combined with $\sum_a$ is not allowed to exceed $0.5\sum_a$ for that region. The remaining portion of the $DB^2$is inserted into the source term if it is a core region and ignored if it is a non-core region. (This avoids the possibility of zero effective absorption, and a potential singlative condition)

For this cross matched cylindrical calculation, the number of buckling iterations to be performed is specified by the user. In principal, at least three iterations are needed to converge on K-effective to within 1%.

2.7 Power and Flux Calculation

To obtain flux per megawatt, following equation can be used.

$$Flux\ per\ MW = \frac{(Conv\ Factor) * (Printed\ fluxes)}{A}$$

where:

1. Conv factor = 2.43*(3.1*10^{16}) fission/sec/MW
2. A = cross section area of core for kind = 1 (slab)
3. A = length of core for kind = 2 (cyl-rad)
4. A = 1 for kind = 4 (sphere)

For kind = 3, use (2) and (3) for appropriate cross matching case.

User must account for peak to average in the other (orthogonal) direction. Also the above conversion factor is for thermal U-235 reactors with Nu=2.43. The conversion factor is altered proportionally with larger or smaller Nu.

2.8 Adjoint Flux Calculations

In a critical reactor, we will define the adjoint flux.

$$\Phi(r_0) \sim \frac{\Delta\rho}{a\Phi(r_0)} \qquad \text{Equation 8}$$

where: $\Delta\rho$ = reactivity change

$a\Phi(r_0)$=the absorption rate at r_0

It is simply proportional to the changes in reactivity per neutron absorbed at r_0 per second. In this sense, then, the adjoint flux is a measure of how effective an absorber inserted at a position r_0 is in changing the reactivity of the core. Evidently if the adjoint flux is large at r, the core multiplication will be quite sensitive to be absorption of neutrons at that point . Hence the adjoint flux is sometimes referred to as the neutron importance or the importance function. We can see this from a somewhat different perspective if we consider the flux induced in a subcritical reactor by an arbitrary source. We will define the adjoint flux Φ^+ :

$$\Phi^+(r_0) = \int_V d^3r \sum_d(r)\Phi(r) \qquad \text{Equation 9}$$

where: d=space distance

The adjoint flux is simply the response of a detector in the core to a unit point source inserted at a position. Once again we find that $\Phi^+(r_0)$ is a measure of the importance of a neutron event (in this case, the production, rather that the absorption, of a

neutron) at a point in contributing to the response of a detector with cross section $\sum_d(r)$ (as opposed to reactivity).

2.8.1 Perturbation Theory

A first-order perturbation is defined as a small change in one of the variables of a system, a change that is small enough that the order variables are not affected. For instance, if the fuel loading of a system is altered slightly, the reactor flux not to be expected to change sufficiently so that the relative amounts of flux in the various energy groups would be altered. If the perturbation were large enough to alter the fluxes significantly, then second order perturbation theory would need to be applied, i.e. the first order perturbation of the fuel loading altered the overall multiplication factor (to first order) but the effect was sufficient to also alter the fluxes so that the multiplication factor was affected to second order. The following treatment is first order perturbation theory, i.e. the perturbations are sufficiently small so that changes in the flux shapes and group balance are essentially insignificant. Consider a multi-group formulation for diffusion theory as the general case. Each group equation can be represented as:

$$\sum_{j=1}^{n} M_{ij}\Phi_j = \frac{1}{v_i}\frac{\delta\Phi_j}{\delta t} \qquad \text{Equation 10}$$

which can be abbreviated in matrix notation to the multi-group equitation:

$$M\Phi = \frac{\delta\Phi}{\delta t} \qquad \text{Equation 11}$$

The equitation in matrix form

$$M\Phi = \omega\Phi \qquad \text{Equation 12}$$

Temporarily, let us consider this set of equations as just single group equitation for a bare reactor, the slab case. The solutions for the flux will be:

$\sin(\frac{\pi}{H}X)$ and $\cos(\frac{\pi}{H}X)$

for the fundamental mode and for all the modes:

$\sin(n\frac{\pi}{H}X)$ and $\cos(n\frac{\pi}{H}X)$

where n takes various integral values from 1 to infinity. However, any and all of these "eigenfunctions" are said to form an orthogonal set, a property defined as

$$\int \Phi_m \Phi_n dv = c \quad if\ m = n\ and\ both\ are\ sines\ or\ cos$$

$$\int \Phi_m \Phi_n dv = 0 \quad if\ m \neq n\ or\ one\ is\ a\ sine\ and\ the\ orther\ a\ cos \qquad \text{Equation 13}$$

The integral is taken over the entire reactor space. These functions (the sines or the cosines) are also said to be self-adjoint, another way of defining the above property. But now consider the case of a reflected reactor that requires either a single or multigroup treatment. The eigenfunctions are no longer simple functions over the entire reactor and are not self adjoint. For now, we shall define the matrix operator that gives this set of adjoint functions as $M*$ and the functions as Φ^* and:

$$M^*\Phi^* = \omega\Phi^* \qquad \text{Equation 14}$$

Where the M^* is the same as the obtained with the direct equation. Therefore, since as a result of the adjoint property,

$$\int \Phi^*\, \Phi\, dv = \int \Phi\, \Phi^*\, dv \qquad \text{Equation 15}$$

When taken over the entire reactor.

Hence,

$$\int \Phi^*\, M\, \Phi\, dv = \int \Phi\, M^*\, \Phi^*\, dv \qquad \text{Equation 16}$$

Now suppose a small perturbation is inserted into the system, and the right hand side of the above equation 15 and 16 is used to describe the reactor before the perturbation, i.e. the initial conditions, while the left hand side describes the condition after the perturbation that altered the operator M to become M+P, with P representing that altered perturbation. The eigenvalue ω will now become ω', but the fluxes will not be significantly altered if the perturbation is small. Subtracting the equation for the initial conditions from the equation for the perturbed conditions gives:

$$\omega' = \frac{\int \Phi^*\, P\, \Phi\, dv}{\int \Phi^*\, \Phi\, dv} \quad (assuming\ \omega = 0) \qquad \text{Equation 17}$$

One needs to insert the value of the perturbation operator P and solve the integrals to obtain the value of the reciprocal prompt reactor period, ω, assuming that the delayed neutrons are ignored and the initial period was infinite.

2.9 Other Options

Several other options are available to user, such as specifying detailed group-dependent buckling and albedo factor at boundaries. The user is referred to the input manual section for further information.

3. User's Instruction

3.1 Input Format

"Input Data Lines" refers to each line entry, 80 characters or less on the monitor, equally spaced. (Use Notepad or Wordpad)

Line	Space	Variable	Format		Remarks
0	1		0		Baseline Printer Reset
1	1	Page-Control	1		
	2	NSPECT	I – 1		Type of spectrum
				1 to 6	Each of the six principal delayed neutron groups
				7	Prompt neutrons only
				8	Po-Be spectrum
				9 or blank	**Standard prompt plus delayed spectrum**

Note: This is on the front line, and permits the user to select a normal fission neutron spectrum, or any one of the delayed or the prompt neutron spectrum. There is also an option to use a polonium-beryllium neutron source spectrum, which could also be used as a driver for certain fixed source calculations.

	3 – 4	NDATA	I – 2	1	Use cross section file
				2	Use cross section file & NELEMTS (new elements)
				3	Read NELEMTS only
				0 or blank	If no new mixtures must be calculated for this case
	5 – 8				Blank
	9 – 80	Case ID	Alphanumeric		Anything (Title) may be written

(Skip to line #8 if NDATA is 0 or blank)

2	1 – 5	NCALC	I – 5		Number of mixture compositions to be calculated. Must be no larger than 20 and no more than 10, may

Line	Space	Variable	Format		Remarks
					have hydrogen or deuterium (or water)
	10	LIST	I – 1	0	Gives no listing of mixed cross section
				1	Gives listing
	15	LIBRY	I – 1	0	Gives no library listing
				1	Gives an index only
				2	Gives all the library cross section
	18 – 20	NELEMTS	I – 3		Number of library elements to be read. Not needed if cross section file is used and no new elements are to be read
	25	NTRAN	I – 2		Number of scatter-transfer matrices to be read, (new elements)
	30	ILINE	I – 1	0 or blank	No printing of input cross sections on line.
				1	Print input cross sections

3 and 4 type lines as needed, containing the new cross section data. Title line plus 12 (16 for elements with production cross section) lines of data for each element. Elements need not be in order.

The first 18 groups are read sequentially, followed by a reference 0.042 eV cross section (never used), then by 6 thermal cross sections, sequentially for 3000, 2500, 2000, 1500, 1000, 500, and 68 ^{0}F.

These are read in as follows:

Title line for this new element

- I3 Identification number
- I2 Alphanumeric description
- 4x and an indicator (in columns 79 and 80), INDIC, which is -1 if there are production cross section for this element

26	Scatter cross sections in 13F6.2 format (2 lines)
26	$\xi \sum_S$ cross sections in 8x9F8.4 format (3 lines)
26	"Transport" $\sum_S(1-\mu_0)$ in 8x9F8.4 format (3 lines)
26	Absorption cross sections in 7E11.5 format (4 lines)
	If INDIC = -1, then
26	Production cross sections ($\nu\sum_F$) in 7E11.5 format (4 lines)

If a scatter transfer matrix is required, follow the cross sections with this matrix in 10E8.4 format, with each line representing the down scatter from a group to the next 10 lower groups.

Line	Space	Variable	Format		Remarks
Specifications of compositions (NCALC)					
5	1 – 5	IDENT	I – 5		An arbitrary identification number for this composition
	6 – 10	NFUEL	I – 5		Number of fuel materials (contain production cross sections)
	11 – 15	NMOD	I – 5		Number of non-fuel (moderator) materials (no production cross section)

Note: NFUEL plus NMOD totals the number of type 5 lines that will follow. Whether these are designed as fuel or moderator is important only if Behrens corrections are being made.

Note: BARON corrects the diffusion coefficient for streaming in channels of gas cooled reactors

16 – 20	BARON	I – 5		Type of Behren's correction
			1	anisotropic (Kunze model)
			2	isotropic (Kunze model)
			3	none
			4	anisotropic (Evandale)
			5	isotropic (Evandale)
21 – 30	TEMP (F)	F10.0		Material temperature used (or determination of thermal Maxwell-Boltzman averaged cross section. Temp. +3000F)

Line	Space	Variable	Format	Remarks
	31 – 40	RMOD	F10.0	If Baron=1 or 2, moderator fraction If Baron=4 or 5, fuel inner diameter If Baron=3, not used
	51 – 60	RVOID	F10.0	If Baron=1 or 2, void fraction compared to material, (Vol void)/(Vol material) If Baron=4 or 5, cell diameter If Baron=3, not used
	61 – 70	Que	F10.0	If Baron=1 or 2, correction factor Q If Baron=3,4 or 5, not used
	71 – 75	DCORR	F5.0	Diffusion coefficient correction factor
	76 – 80	NEW	I – 20	If NEW=2, Volume fractions, cell correction factors, materials are same as last region. Lines #6 and #7 are not used. If NEW=0, continue with Line #7 If NEW=1, one new element is to be added
6	1 – 5	Mop	I – 5	Type of material If Mop=1, material is in fuel section of cell If Mop=0, material is in moderator section of cell
	6 – 10	ELE	I – 5	Material code (from library listing)
	11 – 20	ATOM	E10.3	Volume fraction (* indicator) or atom fraction (no * indicator) for ELE in this region

Line	Space	Variable	Format	Remarks
	21 – 25	NCELLA	I – 5	Cell correction index. The first group working down in energy (up in number) that will have a cell correction other than 1.0 Entries must be provided for that energy group and all other to group 19
7	1 – 80	CELL NCELLA	8F10.0	Cell correction factor for group through thermal. As many lines as necessary with 8 factors/line. Not used if NCELLA>19 or 0

Lines 6 and 7 (if used) are repeated for each material contained in region.

Lines 5 through 7 (if used) are repeated for each distinct region. Maximum of 10 deuterium or hydrogen scattering matrices.

Lines 2 through 7 (if used) are repeated each time nuclear data tape is read.

*Notes: "Cell correction factors" are herein defined to be the self-shielding factors for the absorption cross sections in each energy group. The same factors are applied to the fission cross sections. In the case of fissile material elements, self-shielding factors for fission and absorption will differ slightly, and the user must determine which he wishes to be calculated more accurately, fission or capture (absorption-fission), and choose his correction factors accordingly.

Specification of the reactor geometry and dimensions

8	1 – 5	KIND	I – 5		Geometry option
				1	Slab only
				2	Cylindrical-radial only
				3	Cylindrical-axial and radial cross match
				4	Spherical-radial only

Note: Only one diffusion iteration will be performed for KIND=1, 2, or 4

Line	Space	Variable	Format	Remarks
	6 – 10	$NREG_1$	I – 5	Number of axial regions for this case (≤20)
	11 – 15	$NREG_2$	I – 5	Number of radial regions for this case (≤20)
	16 – 20	$NREG_3$	I – 5	Specification of initial boundary conditions (axial) 1: $\Phi\|_{z=z_0} = 0$; zero flux 2: $\frac{d\Phi}{dz}\|_{z=z_0} = 0$; zero slope 3 or 4: $[W\frac{d\Phi}{dz} + \Phi]_{z=z_0} = 0$; W is input for 3 W is calculated for 4, i.e., extrapolated zero flux 5: $\Phi\|_{z=z_0}$ =input
	21 – 25	$NEND_1$	I – 5	Specification of final boundary conditions (axial). Same option codes as for $NORG_1$ except for $z = z_{max}$
	26 – 30	$NORG_2$	I – 5	Specification of initial boundary conditions (radial). Same option codes as for $NORG_1$ except for $r = r_{max}$
	31 – 35	$NEND_2$	I – 5	Specification of final boundary conditions (radial). Same option codes as for $NORG_1$ except for $r = r_{max}$
	36 – 40	LCORE	I – 5	Identification of core region. Used to calculate core buckling
	41 – 45	ISORE	I – 5	Initial source guess 1: Fission densities assumed equal to 1.0 2: Source term calculated from last case fission densities

Note: Program will execute option 1 instead of 2 if NDATA = 0.

Line	Space	Variable	Format		Remarks
	46 – 50	ITRATE	I – 5		Maximum number of buckling iterations to be performed. Ignored for KIND = 1, 2, or 4
	51 – 55	IBAL	I – 5	≠0:	A neutron balance will be made and printed for each region
				=0:	No balance
	56 – 60	NFLUX	I – 5	0:	No flux point
				1:	Flux and adjoint printout (if adjoint asked for under JOINT)
				2:	Flux and adjoint punched line output
				3:	Printout and tape storage of flux and adjoint
	61 – 65	JOINT	I – 5	0:	No adjoint flux calculation (direct only)
				1:	Direct and adjoint flux calculation
				2:	Adjoint flux calculation only
	66 – 70	KTER	I – 5		Maximum number of diffusion calculation iterations. Automatically set = 20 is not specified
9	1 – 10	RAD_1	F10.0		Starting axial dimension
	11 – 20	RAD_2	F10.0		Starting radial dimension
	21 – 30	BUCK	F10.0		Starting value for core transverse buckling. Also see BUKLE (line 10, Col. 21) and BUCKL (line 15, etc.)
	31 – 40	CONVK	F10.0		Effective multiplication factor convergence criterion; absolute change between two

Line	Space	Variable	Format	Remarks
				successive diffusion iterations.
	41 – 50	CONVB	F10.0	Buckling convergence criterion. Relative (fractional) change between two successive buckling iterations. (Radial and axial)
	51 – 60	ACC	F10.0	Source (fission density) convergence (extrapolation) factor used to speed up convergence. 0.0 is recommended, i.e. (no extrapolation)
	61 – 70	CHKTME	F10.0	Time limit on buckling iterations. Set=1 minute if not specified
10	1 – 5	$IREG_i$	I – 5	Region composition identification (one region must be LCORE and must be included in one of the IDENT, line 5)
	6 – 10	$NVALS_i$	I – 5	Number of intevals in region $IREG_i$
	11 – 20	$WIDTH_i$	F10.0	Width of region $IREG_I$
	21 – 30	$BUKLE_i$	F10.0	Transverse buckling for region $NREG_i$

Note: Two regions may be specified per line – second region starting in column 31. All axial regions are specified (if used), then all radial regions (if used). First radial region must start a new line.

Note: If BUCK (line 9) = 0.0, the calculated core bucklings are used for all regions in cross matched cylindrical calculations.

Note: The total number of intervals must be < 1000 for each dimension.

Line	Space	Variable	Format	Remarks

Note: These are not needed unless user desired to specify a different type of boundary condition.

11	1 – 80	WO_1	8F10.0	If $NORG_1 = 3$, flux extrapolation factors at origin. (axial case) If $NORG_1 = 5$, values of flux at origin. This entry should always be positive (axial case) If $NORG_1 = 1$, 2, or 4, not Used
12	1 – 80	WE_1	8F10.0	If $NEND_1 = 3$, flux extrapolation factors at end. (axial case) If $NEND_1 = 5$, values of flux at end. This entry should always be positive (axial case) If $NEND_1 = 1$, 2, or 4, not used
13	1 – 80	WO_2	8F10.0	Same as line 11 except for radial case
14	1 – 80	WE_2	8F10.0	Same as line 12 except for radial case

Note: If the options requiring lines 11, 12, 13, and/or 14 are used, one value is needed for each energy group; e.g., line #10 actually consists of 3 data lines. The extrapolation factors are the W_i in the equation

$$\left[\Phi + W_i \frac{d\Phi}{dr}\right] = 0$$

16	1 – 80	$BUCKL_i$	8F10.0	If BUCK < 0.0 (negative and non-zero), lethargy dependent values of core buckling are read as input. Not used unless user desires to enter special buckling values for each lethargy (energy) group

APPENDIX A

References

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