DETERMINATION OF NEUTRON FLUX DISTRIBUTION BY USING ANISN, A ONE-DIMENSIONAL DISCRETE S_n ORDINATES TRANSPORT CODE WITH ANISOTROPIC SCATTERING

by

Susanta K. Ghorai

Associate Professor of Physics

Alabama State University

Montgomery, Alabama 36195

ABSTRACT

The purpose of this project was to use a one-dimensional discrete ordinates transport code called ANISN in order to determine the energy-angle-spatial distribution of neutrons in a 6-feet cube rock box which houses a D-T neutron generator at its center. The project was two-fold. The first phase of the project involved adaptation of the ANISN code written for an IBM 360/75/91 computer to the UNIVAC system at JSC. The second phase of the project was to use the code with proper geometry, source function and rock material composition in order to determine the neutron flux distribution around the rock box when a 14.1 MeV neutron generator placed at its center is activated.

Advisor: Dr. James E. Keith

INTRODUCTION

Accurate determination of neutron flux distribution as a function of energy, angle and space is highly important in situations such as neutron dosimetry work, shielding problems, and in situations which involve neutron exposure. Analytical method of determining energy-angle-spatial distribution of neutrons or photons involves solving the conservation equation known as the Boltzmann transport equation. Much of the stimulus for the development of transport theory came from problems connected with the design and operation of nuclear reactors. However, actual problems are usually highly complex which can be best handled through high speed computing machinges by using approximate numerical solution of the transport equation. The method of discrete ordinates has become a powerful tool for the numerical solution of the Boltzmann transport equation. Oak Ridge National Laboratory transport program called ANISN-ORNL (1) is a one dimensional discrete ordinates S_n transport code with general anisotropic scattering. In this project ANISN has been successfully adapted to the UNIVAC system of JSC and some progress has been made in analyzing the rock box problem.

ANISN AND ITS ADAPTATION

ANISN is a FORTRAN IV, version 13 program which uses the discrete ordinates or S_n method in solving one dimensional Boltzmann transport equation for slab, cylinder and spherical geometry. As a secondary calculation, the detailed flux generated as the solution may be used to perform group reduction of the cross sections. The discrete ordinates method has been reviewed by Carlson (2), Lee (3), Mynatt (4) and Lathrop (5). It is not the prupose of this report to discuss the discrete ordinates method or to describe the ANISN code. However, for facilitating the process of running the ANISN program,

some observations will be made here regarding the approximation features used in ANISN. Although the discrete ordinates method should solve the transport equation exactly in the limit of infinite computation time and infinitesimally fine mesh in all variables, in practice a number of approximations are essential. These include the approximation of continuous functions by discontinuous sets of approximations in energy, spatial and angular meshes and representation of the angular dependence of scattering by a small set of truncated Legendre polynomials.

a. Selection of Groups and P_ℓ

ANISN allows general anisotropic scattering through an ℓ-th order (P_ℓ) Legendre polynomial expansion of the scattering cross section. There are really two types of anisotropic scattering, first is the heavy nuclide elastic scattering of neutrons which at high energies is extremely anisotropic but the angle-energy correlation is unimportant; second is the elastic scattering of neutrons by hydrogen or the Compton scattering of gammas which has an important angle-energy correlation which becomes an angle-group correlation. The method used for anisotropic scattering in the discrete ordinates equations appears to work very well for both types of scattering (4). Low order approximations such as P_2 or P_3 are adequate for most practical problems (4).

The multigroup Legendre polynomial expansion method is used to prepare cross sections. A typical discrete ordinates transport calculation may use from 30 to 100 groups and a P_3 expansion (6). One group-to-group transfer table is required for each Legendre term, hence 4 for P_3 (P_0, P_1, P_2, P_3). Computer storage increases rapidly with the number of energy groups and tables. Bugle-80 which has been used in this project to provide cross sections for ANISN, provides 47 neutron and 20 gamma, P_3 cross sections for ANISN. An example of neutron group cross section is given in Table 1. This

table gives the P_0 through P_3 cross section tables for the first three neutron groups in iron. The format corresponds to the positions used in ANISN. Position 1 contains the absorption cross section. Position 2 contains $\nu\sigma_f$ (it is 0 in case of iron since there is no fission in iron). The total cross section appears in position 3. Position 4 contains the within-group scattering cross section $\sigma_{g\to g}$ where g is the group number. Position 5 contains the cross section for scattering from group (g-1) into group g. Position 6 contains the cross section for scattering from group (g-2) into group g, and so forth.

b. Selection of Angular Quadrature

The flux is anisotropic, and a reasonably large order of angular quadrature set (quadrature direction μ_m and quadrature weights w_m) is necessary (7). The most accurate quadrature set for integrating the Legendre polynomials for a given n is the Gauss-Legendre quadratures (μ_m at zeros of Legendre polynomials, m = 1, 2, 3,..., n+1). A relatively low-order quadrature, such as S_8 for P_3 cross sections, would be sufficient as far as inscattering source is concerned (6). However, in radiation transport, the angular flux density is usually very anisotropic and a high-order set may be needed to properly represent the angular distribution in the output (6).

TABLE 1

IRON NEUTRON GROUP CROSS SECTION FOR FIRST THREE NEUTRON GROUPS (BARNS)

	Position		Group 1	Group 2	Group 3
P_0	1	σ_a	2.022-1	1.608-1	1.121-1
	2	$\nu\sigma_f$	0.0	0.0	0.0

	3	σ_{tot}	2.620		2.939		3.259
	4	$\sigma_{1\to1}$	1.267	$\sigma_{2\to2}$	1.546	$\sigma_{3\to3}$	1.784
	5		0.0	$\sigma_{1\to2}$	1.097-1	$\sigma_{2\to3}$	1.155-1
	6		0.0		0.0	$\sigma_{1\to3}$	2.100-2
P_1	1		0.0		0.0		0.0
	2		0.0		0.0		0.0
	3		0.0		0.0		0.0
	4	$\sigma_{1\to1}$	3.002	$\sigma_{2\to2}$	3.881	$\sigma_{3\to3}$	4.522
	5		0.0	$\sigma_{1\to2}$	1.356-2	$\sigma_{2\to3}$	2.748-2
	6		0.0		0.0	$\sigma_{1\to3}$	0.0
P_2	1		0.0		0.0		0.0
	2		0.0		0.0		0.0
	3		0.0		0.0		0.0
	4		4.250		5.550		6.531
	5		0.0		4.013		7.055-2
	6		0.0		0.0		0.0
P_3	1		0.0		0.0		0.0
	2		0.0		0.0		0.0
	3		0.0		0.0		0.0
	4		4.968		6.252		6.858
	5		0.0		3.535-2		3.979-2
	6		0.0		0.0		0.0

c. Selection of Spatial Mesh

Nested spherical shells or layers of different materials can be handled

by specifying a radius at the interface, and specifying the material in each layer or zone. The spacing Δr should be small in regions of large attenuation or curvature, such as near the origin in spherical and cylindrical geometry (6). On the other hand, small Δr implies very many space points in a thick shield, and some compromise may be necessary. Typical shielding problem in one dimension may use 100 to 300 radii. One rule of thumb is $\Delta r \leq 2\mu_{min}/\Sigma_{t_{max}}$ where μ_{min} is the smallest discrete cosine and $\Sigma_{t_{max}}$ is the largest total cross section in the multigroup set (6). Near the origin in curved geometry the angular flux density changes rapidly even without collisions, and a smaller Δr may be required.

Following comments in addition to the use of ANISN manual would be helpful in running ANISN code.

1. A better definition of some of the parameters and terms used in ANISN can be found in reference 8. However, one must be careful in using this reference, since it does not use the same array number as ANISN.

2. The ANISN manual (1) does not include an output. Reference 9 includes a sample output for a three-group ANISN problem.

3. Before using any cross section file from Bugle-80 tape, it is necessary to convert this file to binary form. Four Bugle files (nos. 4-7) are needed for this conversion. File 4 contains the IBM JCL cards for conversion, and file 6 contains the IBM DD cards. File 7 contains an input data card for the conversion program contained in file 5. Before a cross section file is converted to binary form, it must first be converted to field data, and all "&" signs must be changed to "+" signs. The conversion program can now be applied to make a binary cross section tape which can be used with ANISN.

4. The output should always be examined for possible lack of convergence

and for negative or oscillatory angular flux densities (6). The total flux should not contain any negative value. If there are any at all, they must be very few in numbers.

5. There are four ID numbers for cross section of each element or physical material in bugle-80. The first ID number refers to P_0 cross section set, the second one to P_1 set, the third one to P_2 set, and the fourth one to P_3 set. Each of these sets is counted as one material in the parameters MTP, MCR or MT in the 15$ array. However, in the 9$ array (material number by zone) only the P_0 material ID number of each element or physical material in a given zone is required.

ROCK BOX PROBLEM

The second phase of the project was to determine the neutron flux distribution around a 6-ft cube solid rock box which houses a D-T neutron generator at its center. This experimental arrangement was designed to conduct a combined pulsed neutron experiment and to study its application to nuclear waste disposal testing. When the generator is activated, it produces 5 microsecond pulses (1 to 10 pulses/s) of 14.1 MeV neutrons. The strength of the neutron source is less than 10^9 n/s. The rock has a bulk density of about 2 g/cm^3 and the composition shown in Table 2.

In order to use ANISN code to determine the energy-angle-spatial flux distribution around the rock box, the neutron source can be treated as a point source which can be approximated for ANISN by a small shell source at the center of a sphere of radius 90 cm. The problem of selecting a suitable set of approximation parameters to be used in ANISN code is acute in the calculation of fast neutron penetration to large depths (7). Following parameters have been worked out in the rock box analysis.

1. The finite-difference equations are solved subject to boundary conditions. The vacuum condition is usually specified at the outer boundary. The reflective condition is required at the "left" boundary (r = 0) in the sphere (6). Hence IBR = 0 and IBL = 1.

2. As discussed earlier, near the origin in spherical geometry, the angular flux changes rapidly even without collisions, and hence a smaller Δr is required. The intervals used in this problem for 4* array input are given as follows:

```
4**ß3Iß0.0ß4Iß0.001ß4Iß0.01ß4Iß0.1ß84Iß1.0ß39Iß50.0ß90.0
```

There are 144 intervals, and Δr is very small near the origin and it increases outwards.

3. An S_8-P_3 analysis is being applied. The neutrons are generated in the energy group 2. Because of the discretization of ANISN code in angle and space, with an isotropic source in spherical geometry, the source has to be placed in the last angle which, in this case, is the 9th angle. The shell source used in this analysis is given below in ANISN format.

```
col 1
    ↓
    18*
     9Rb0.0    col16
                  ↓
     8Rb0.0       1.5734+07
      Fb0.0
      T
```

The total shell source given in 18* array was derived as follows.

$$\text{Total shell source} = \sum_{i=1}^{\text{all intervals}} \sum_{j=1}^{\text{all angles}} \sum_{k=1}^{\text{all energy groups}} \left(\phi_{ijk} \cdot \omega_j |\mu_j| A_{i+1}\right)$$

Total shell source must be 1 neutron/s.

Since the source is in the first interval, 9th angle and group 2,

$i = 1$, $j = 9$ and $k = 2$

Hence total shell source = $\phi_{192} \cdot \omega_9 |\mu_9| \cdot A_2 = 1 \text{ n/s}$

From the output using the above 144 intervals we find that

$A_2 = 7.85398 \times 10^{-7} \text{cm}^2$

Also from the output we find from the Angular quadrature constants

$\omega_9 |\mu_9| = 8.09256 \times 10^{-2}$

Hence

$$\phi_{192} = \frac{1 \text{ n/s}}{\omega_9 |\mu_9| A_2} = 1.57335 \times 10^7 \text{ n/cm}^2\text{/s}$$

If the shell source = 1.57335×10^7 n/cm^2/s is used, it will give a total source strength of 1 n/s.

4. The composition of the rock box and the number densities (12*) in cross section mixing table are given in table 2. Note that the number densities are in units of 10^{24} atoms/cm^3.

TABLE 2

ROCK COMPOSITION AND NUMBER DENSITIES (12*)

(in 10^{24} atoms/cm^3)

Bugle-80 ID	Element	% by wt.	Number density (12*)
1-4	H	0.63	0.0075884
9-12	O	48.39	0.0364286
13-16	Cr	0.000003	0.069477×10^{-8}
21-24	Fe	2.46	0.0005305
45-48	Si	28.01	0.0120107
53-56	Na	1.35	0.0007073
57-60	Mg	0.54	0.0002674
61-64	A	5.08	0.0022673
69-72	K	2.62	0.0008071
73-76	Ca	10.87	0.0032667
129-132	Ti	0.11	0.0000277
137-140	Co	0.00000059	0.0120573
153-156	Ba	0.000282	2.4728378×10^{-8}

The first ten elements (H through Ca) are in bu.e file 1 and the last three elements (Ti, Co and Ba) are in bugle file 2.

5. Cross section mixing table (10$, 11$, 12*) for the rock box composition with thirteen elements has been prepared as shown in table 3. In this table the first 10 elements are in Bugle file 1 and the last three are in

Bugle file 2. Table 3 shows how the cross sections of the thirteen elements could be combined to form those of the mixture (the rock). When the cross sections are read from Bugle binary tape, the materials are identified by integers 1,2,3,....,52 (52 materials read in 15$ array) according to the order in which they were read from the tape. Positions 1 through 4 in table 3 cause the block of locations reserved for materials 1,2,3 and 4 to be replaced by zeros. Position 5 through 52 cause materials 5 through 52 to be multiplied by their respective number densities in column 12* and combined to form four new macroscopic materials, material numbers 1 through 4.

TABLE 3

CROSS SECTION MIXING TABLE FOR ROCK BOX

Position	Element ID	10$	11$	12*
1		1	0	0.0075884
2	H-1	2	0	"
3	'-4	3	0	"
4		4	0	"
5		1	5	0.0364286
6	0-16	2	6	"
7	9-12	3	7	"

8		4	8	"
9		1	9	6.9477-10
10	Cr	2	10	"
11	13-16	3	11	"
12		4	12	"
13		1	13	0.0005305
14	Fe	2	14	"
15	21-24	3	15	"
16		4	16	"
17		1	17	0.0120107
18	Si	2	18	"
19	45-48	3	19	"
20		4	20	"
21	Na	1	21	0.0007073
22	53-56	2	22	"
23		3	23	"
24		4	24	"
25		1	25	0.0002674

26	MG	2	26	"
27	57-60	3	27	"
28		4	28	"
29		1	29	0.0022673
30	Al	2	30	"
31	61-64	3	31	"
32		4	32	"
33		1	33	0.0008071
34	K	2	34	"
35	69-72	3	35	"
36		4	36	"
37		1	37	0.0032667
38	Ca	2	38	"
39	73-76	3	39	"
40		4	40	"
41		1	41	0.0000277
42	Ti	2	42	"
43	129-132	3	43	"
44		4	44	"

45		1	45	1.2057-10
46	Co	2	46	
47	137-140	3	47	
48		4	48	
49		1	49	2.4728-8
50	Ba	2	50	"
51	153-156	3	51	"
52		4	52	"

In this case

MS = 52

MCR = 0

MTP = 52

MT = 52

and material number 1 is entered into 9$ array.

There are different possible ways a mixing table can be prepared. Some are more efficient than others. For example, reference 8 gives an illustration of a mixing table which is composed differently than table 3.

CONCLUSIONS

At the time of wrting, all the input data for the rock box problem have

been worked out, and the binary tapes for Bugle files 1 and 2 have been prepared. Computer runs have been made with all the input data as discussed above, except that in spheric l geometry the concrete problem has been executed instead of the mixture. A stepwise approach will be taken to use the mixture. At first, runs will be made with first two elements of the mixture, next with five elements, next with ten elements, and lastly with all the thirteen elements. In this approach it will be easier to apply corrections, if needed, to the program input. There is also a possibility of reaching the storage limit of the computer.

Before using all the thirteen elements, some "runstream" cards need to be changed and some added in order that ANISN can read the binary tapes of Bugle files 1 and 2 in one run. Another approach would be to combine these two binary tapes into one.

FUTURE PROJECT

Experience in other places working with ANISN has shown that when as few as 2 or 3 elements are used in a mixture, it is possible that the resulting input cross-section matrix will exceed the storage capacity of the computer (10). When this occurs, two approaches may be attempted (10).

1. First, attempt may be made to increase the dimension in the statement COMMON/BULKBU/I, J. A(45000) in the main routine from 45000 to the maximum permissible number. It will also be necessary to change the statement J = 45000 in the main routine (10).

2. Secondly, use can be made of the routine LIM1 (given in ANISN manual) to prepare a group independent cross section tape for ANISN. When this tape is used, rather than storing the entire matrix for the mixture, only the cross-section data for a single group are stored in the memory while the calculations for this group is performed. Data for the next group are then read from the group independent tape replacing the data of the previous group, and the calculations for this group are performed. The process continues for all groups.

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LIST OF TAPES

ANISN X08628 (6-22-83)

Bugle ..... X23300 (7-21-83, created from a new tape from Oak Ridge)

Binary Tapes Created

Bugle file 1....X19289 (7-26-83)

Bugle file 2....X20761 (7-29-83)

Bugle file 3....X07033 (7-29-83)

Bugle files 1, 2, & 3....X21958 (7-29-83)

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ADDENDUM

After the report was completed, a successful ANISN run was made with a two-components mixture using the first two elements, H and O of the mixing table 3. But when the third element, Cr of table 3 was added, ANISN would not run because the resulting cross section matrix for a three-elements mixture exceeded the allowed computer storage space.