IRANLIB (Improved Range of ANISN/PC Library): P-3 Coupled Neutron-Gamma Cross-Section Libraries in ISOTXS Format to be used by ANISN/PC (CCC-0514/02)

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ABSTRACT

IRAN.LIB is a Coupled Neutron-Gamma library which was developed to be used by the ANISN/PC (CCC-0514/02). The library was developed mainly for shielding calculations and it contains 33 elements mostly used as shielding materials, such as concrete. IRAN.LIB is a set of six libraries, each having the same elements but different number of energy groups. In order to use IRAN.LIB by ANISN/PC, this code must be modified.

INTRODUCTION

ANISN Code was originally developed by Engle at Oak Ridge National Laboratory in 1965[2]. The code solves one-dimensional transport equation for neutron or gamma-ray in spherical, cylindrical or slab geometry with general anisotropic scattering.

Since 1965, several versions of ANISN Code were developed and most of them are distributed by Nuclear Energy Agency Data Bank (NEA Data Bank) in Europe, and by Radiation Shielding Information Centre (RSIC) in the U.S.A.. Among several versions there are:

i) ANISN - ORNL (CCC-0254)
ii) ANISN - E (CCC-0082)
iii) ANISN - W (CCC-0255)
iiii) ANISN - JR (CCC-0082)

In March 1985, Pearsons & Nigg adapted ANISN - W for personal microcomputer (CCC-255-PC), and after that a new version developed by Pearsons [8] from Idaho National Engineering Laboratory, CCC-0514-ANISN/PC, was released and is currently distributed by NEA Data Bank or RSIC (Radiation Shielding Information Center). In the Code package, besides the executable and source files (ANISN.EXE and ANISN.FOR), it is distributed an interactive input generator (APE32.EXE) and a P-3, 21 group photon cross section master library in CCCC ASCII ISOTXS format (FLUNGP.LIB) in which particular materials can be selected by using an editing utility Program (LMOD.EXE). FLUNGP enables the user to solve some shielding problems for a given gamma-ray source using a personal microcomputer (PC).[6]

However, if one needs to solve a realistic shielding problem for either a neutron or gamma source it will be necessary to generate the cross sections using a system such as AMPX-II[4] together with the VITAMIN-4C [9] master library, on a mainframe and then copy the generated cross-section file onto the ANISN/PC (array 14 **). This procedure is not only time consuming but is a limitation on the use of ANISN/PC since it will require the use of a big mainframe, which is not available for some users, mainly in the under developing countries.

In order to overcome the above mentioned problems, we have developed a P-3, coupled neutron-gamma cross section library called **IRAN.LIB** (Improved Range of ANISN/PC Library). This library contains the cross sections for 33 elements which are mainly encountered in the shielding materials such as concrete, borated polyethylene, etc.. Therefore IRAN.LIB is most suitable for neutron-gamma shielding calculations.

The cross sections were taken from VITAMIN-4C master library using the AMPX-II system and ENDF/B-IV [3], ENDF/B-V [5], and JENDL/3 [10] master libraries using the NJOY [7] Code.

Due to the limitation of personal microcomputer, it may not be possible to solve a very large problem by PC. The number of energy groups is one of the parameters which greatly effects the size of a problem. This fact forced us to develope a set of libraries called IRAN1.LIB (40 groups), IRAN2.LIB (35 groups), IRAN3.LIB (25 groups), IRAN4.LIB (13 groups), IRAN5.LIB (9 groups) and IRAN6.LIB (6 groups); being each one used according to the size of the problem. An assessment of the accuracy of these libraries are discussed in a latter section.

Also since in ANISN/PC the cross sections sets to be read from a file (ANISNC4.LIB) in array 13 $$ is in CCC ISOTXS format, the libraries had been written in the same way.

Since ANISN/PC [8] is based on 25 groups of energy, then in order that IRAN.LIB to be used by ANISN/PC as master library, this code was modified to adapt it for using 40 groups of energy.

LIBRARY DESCRIPTION AND USES

VITAMIN.4C, as the main master library was used to generate cross sections using several modules of AMPX-II Code on the IBM 4381. The block diagram to develope IRAN.LIB is shown in Fig. 1.

The AJAX module extracts the neutron

cross sections of desired elements from the library. CHOX module serves to combine master neutron, gamma production and gamma interaction master libraries into a coupled neutron-gamma library. The MALOCS module collapses the cross section into given energy groups, and NITAWL module writes the collapsed cross sections in ANISN format. A Computer program, CONVERT, was written to convert the cross section from ANISN format to ISOTXS(1) format.

Having obtained the cross sections in ISOTXS format, control parameters were added at top of the set of cross section of the individual isotope. Besides, control parameters were added at the top of the whole set of isotopes.

Since IRAN.LIB was developed mainly for the shielding purposes, the elements selected for the library are those, which are most encountered in the shielding materials. Some elements were not present in VITAMIN-4C master library, so we have used data from ENDF/B-IV, ENDF/B-V and JENDL/3 nuclear data files instead of VITAMIN.4C. Table 1 shows the elements contained in IRAN.LIB.

The principal cross sections contained in the library are as follows:

1 - transport cross section
2 - total cross section
3 - (n,γ) cross section
4 - fission cross section
5 - ν (average value of neutrons produced/fission)
6 - (n,α) cross section
7 - (n,p) cross section
8 - (n,2n) cross section
9 - (n,d) cross section
10 - (n,T) cross section
11 - absorption cross section

The maximum order of scattering in scattering matrix is L=3. Besides, no upscattering and full down scattering was considered.

To overcome the limitation on the size of a problem six libraries called IRAN1.LIB, IRAN2.LIB, IRAN3.LIB, IRAN4.LIB, IRAN5.LIB and IRAN6.LIB were developed, being each one used according to the size of a problem. The number of elements in all these libraries remains the same as shown in Table(1). Tables (2-1) through (2-6) show the energy group structure of the libraries, as the size of the libraries are shown in table (3). The lower limit for the last neutron group in all libraries is 10^{-5} eV.

TABLE 1: Elements contained in IRAN.LIB

MT No. in IRAN.LIB	ELEMENT	SOURCE OF MASTER LIB.	MT No. IN MASTER LIB.	REMARKS
1	H-1	VITAMIN-4C	1296	
2	H-2	VITAMIN-4C	1120	noγproduction data
3	LI-6	VITAMIN-4C	1271	
4	LI-7	VITAMIN-4C	1272	
5	BE-9	VITAMIN-4C	1289	
6	B-10	VITAMIN-4C	1273	
7	C-12	VITAMIN-4C	1274	
8	N-14	VITAMIN-4C	1275	
9	O-16	VITAMIN-4C	1276	
10	NA	VITAMIN-4C	1156	
11	MG	VITAMIN-4C	1280	
12	AL-27	VITAMIN-4C	1193	
13	SI	VITAMIN-4C	1194	
14	K	VITAMIN-4C	1150	
15	V	VITAMIN-4C	1196	noγproduction data
16	CR	VITAMIN-4C	1191	
17	MN-55	VITAMIN-4C	1197	
18	FE	VITAMIN-4C	1192	
19	NI	VITAMIN-4C	1190	
20	NB-93	VITAMIN-4C	1189	
21	PB	VITAMIN-4C	1288	
22	U-235	VITAMIN-4C	1261	
23	U-238	VITAMIN-4C	1262	
24	PU-239	VITAMIN-4C	1264	
25	BA-134	ENDF/BV	9684	
26	BA-135	ENDF/BV	9685	
27	BA-136	ENDF/BV	9687	
28	BA-137	ENDF/BV	9689	
29	BA-140	ENDF/BV	9683	
30	BI-209	JENDL/3	3831	
31	CA-NAT	JENDL/3	3200	
32	ZR-NAT	JENDL/3	3400	
33	CD-NAT	ENDF/BIV	1281	noγproduction data

Table 2-1 Energy Group Structure of IRAN1.LIB

NAME : IRAN1.LIB — NUMBER OF ENERGY GROUPS : 40

NEUTRON		GAMMA	
GROUP	UPPER ENERGY (EV)	GROUP	UPPER ENERGY (EV)
1	1.7333 E + 7	23	1.4000 E + 7
2	5.2205 E + 6	24	8. 000 E + 6
3	3.0119 E + 6	25	6. 500 E + 6
4	1.0026 E + 6	26	6. 0 E + 6
5	4.9787 E + 5	27	4. 0 E + 6
6	1.4996 E + 5	28	3. 0 E + 6
7	9.8037 E + 4	29	2. 6 E + 6
8	5.6565 E + 4	30	2. 0 E + 6
9	5.6565 E + 4	31	1. 66 E + 6
10	5.2475 E + 4	32	1. 32 E + 6
11	2.4788 E + 4	33	1. 00 E + 6
12	2.4176 E + 4	34	8. 00 E + 5
13	2.2487 E + 3	35	6. 00 E + 5
14	2.0347 E + 3	36	4. 00 E + 5
15	1.4800 E + 2	37	3. 00 E + 5
16	1.3007 E + 2	38	2. 00 E + 5
17	1.0130 E + 2	39	1. 00 E + 5
18	2.9023 E + 1	40	5. 00 E + 4
19	1.0677 E + 1		
20	3.0590 E + 00		
21	1.1254 E + 00		
22	4.1399 E - 01		

Table 2-2 : Energy Group Structure of IRAN2.LIB

NAME: IRAN2.LIB — NUMBER OF ENERGY GROUPS: 35

NEUTRON		GAMMA	
GROUP	UPPER ENERGY (EV)	GROUP	UPPER ENERGY (EV)
1	1.7333 E + 7	18	1.4 E + 7
2	1.4918 E + 7	19	1.0 E + 7
3	3.0119 E + 6	20	8.0 E + 6
4	1.4277 E + 6	21	7.0 E + 6
5	9.0718 E + 5	22	6.0 E + 6
6	4.0762 E + 5	23	5.0 E + 6
7	1.1109 E + 5	24	4.0 E + 6
8	1.5034 E + 4	25	3.0 E + 6
9	3.0354 E + 3	26	2.5 E + 6
10	5.8295 E + 2	27	2.0 E + 6
11	1.013 E + 2	28	1.5 E + 6
12	2.9203 E + 1	29	1.0 E + 6
13	1.0677 E + 1	30	7.0 E + 5
14	3.0590 E + 00	31	4.5 E + 5
15	1.1254 E + 00	32	3.0 E + 5
16	4.1399 E - 01	33	1.5 E + 5
17	1.000 E - 01	34	6.0 E + 4
		35	3.0 E + 3

Table 2-3 : Energy Group Structure of IRAN3.LIB

NAME: IRAN3.LIB		NUMBER OF ENERGY GROUPS: 25	
NEUTRON		GAMMA	
GROUP	UPPER ENERGY (EV)	GROUP	UPPER ENERGY (EV)
1	1.7333 E + 7	8	1.4 E + 7
2	5.2205 E + 6	9	8.0 E + 6
3	1.0026 E + 6	10	6.0 E + 6
4	4.9787 E + 5	11	4.0 E + 6
5	9.8037 E + 4	12	3.0 E + 6
6	9.1188 E + 3	13	2.5 E + 6
7	5.3156 E - 1	14	2.0 E + 6
		15	1.5 E + 6
		16	1.0 E + 6
		17	7.0 E + 5
		18	4.5 E + 5
		19	3.0 E + 5
		20	1.5 E + 5
		21	1.0 E + 5
		22	7.5 E + 4
		23	4.5 E + 4
		24	3.00 E + 4
		25	2.00 E + 4

Table 2-4 : Energy Group Structure of IRAN4.LIB

NAME: IRAN4.LIB		NUMBER OF ENERGY GROUPS: 13	
NEUTRON		GAMMA	
GROUP	UPPER ENERGY (EV)	GROUP	UPPER ENERGY(EV)
1	1.7333 E + 7	8	1.4 E + 7
2	5.2206 E + 6	9	1.0 E + 7
3	1.0026 E + 6	10	5.0 E + 6
4	4.9787 E + 5	11	2.0 E + 6
5	9.8037 E + 4	12	1.0 E + 6
6	9.1188 E + 3	13	5.0 E + 5
7	5.3156 E - 1		

Table 2-5 : Energy Group Structure of IRAN5.LIB

NAME: IRAN5.LIB		NUMBER OF ENERGY GROUPS: 9	
NEUTRON		GAMMA	
GROUP	UPPER ENERGY (EV)	GROUP	UPPER ENERGY (EV)
1	1.7333 E + 7	6	1.4 E + 7
2	1.4918 E + 7	7	4.0 E + 6
3	8.2085 E + 5	8	2.5 E + 6
4	5.5308 E + 3	9	1.00 E + 6
5	6.8256 E - 1		

Table 2-6 : Energy Group Structure of IRAN6.LIB

NAME: IRAN6.LIB		NUMBER OF ENERGY GROUPS: 6	
NEUTRON		GAMMA	
GROUP	UPPER ENERGY (EV)	GROUP	UPPER ENERGY (EV)
1	1.7333 E + 7	3	1.4 E + 7
2	6.8256 E - 1	4	4.0 E + 6
		5	2.5 E + 6
		6	1.00 E + 6

Table 3 : Size of the Libraries

NAME	SIZE	
	LENGHT (LINES)	BYTES
IRAN1.LIB	17503	1,541,475
IRAN2.LIB	16165	1,208,740
IRAN3.LIB	8835	593,558
IRAN4.LIB	2955	228,506
IRAN5.LIB	1732	137,354
IRAN6.LIB	1037	88,254
TOTAL	48227	3,797,887

In order IRAN.LIB libraries to be used by ANISN/PC, this code must be modified for the maximum number of energy groups ,that is, for 40 groups. The modifications are as follows:
(1) all the variables having dimension 25 in routine S966 must be changed to 40 (e.g. SIGF(25) will be SIGF(40)).
(2) the scattering matrix SCAT(25,25,7,3) in routine S966 must be changed to SCAT(79,40,4,1). Also the maximum order of scattering must be changed from 7 to 4. In the same routine the neutron velocity VEL(30) must be changed to VEL(40).

SAMPLE PROBLEMS

In order to assess the accuracy of IRAN.LIB in solving shielding problems we solved two sample problems.

Neutron and secondary gamma-ray fluence through a slab of borated polyethylene. This problem was published by the Benchmark Problem Group of the ANS-6 Standard Committee for testing computational methods and data in radiation transport. In particular this problem is the number 6 of the Shielding Benchmark Problem(submitted by Burgart) and its objective is to calculate the neutron and gamma ray spectra which is transmitted through a slab of borated polyethylene for a fission spectrum neutron beam incident on the face (Figure 2). The published results of the benchmark were obtained using basic neutron and gamma cross sections from ENDF/B.II, manipulated by SUPERTOG and MUG to run the transport codes (ANISN and DOT) in 22-18 coupled neutron-gamma with P-3 scattering coefficients (S-32,62 mesh points)[11].

We solved the same problem using IRAN.LIB libraries and modified ANISN/PC. In table (4) the calculated particle fluence is shown. The latter is defined as angular flux multiplied by its respective cosine (=0.9861) and divided by $4\pi R^2$ (R=10000cm) and summed over all the respective groups of energy for neutrons and gamma rays. As a comparison the benchmark results are also shown. It is noted that our results are in a good agreement with the benchmark results, even considering that any special treatment was given for the the cross sections (not collapsing) and that we have used S-12, whereas the published results used S-32. Also, as an integral check the total flux integrated over the volume for the upper energy of about 5 Mev and divided by the group width (E = 5 Mev) was calculated to be 2.46E-06 ,whereas the published result was 2.62E-06.

Finally in table (5) we report the "absorption", "albedo" and "transmission" of neutrons and gamma obtained by IRAN.LIB libraries in order to have a comparison among them.

Table 4: Particle fluence* for 15.24 cm slab(μ =0.9861)

		NEUTRON	GAMMA
published results	ANISN	3.57E-10	8.80E-10
ORNL-RSIC-25	DOT	3.54E-10	8.49E-10
(ANS-SD-9)			
IRAN1.LIB/ANISN-PC(modified)		3.55E-10	8.20E-10

(*) by particle fluence it is understood

$$\frac{1}{4\pi R^2}\sum_{g}\phi_g(x,\mu)\mu$$

Table 5: Comparison of the results obtained by IRAN.LIB libraries

	absorption*		albedo		transmission	
	neutron	gamma	neutron	gamma	neutron	gamma
IRAN1.LIB	7.11E-1	3.71E-2	2.05E-1	3.62E-1	8.39E-2	2.68E-1
IRAN2.LIB	6.96E-1	2.29E-2	2.01E-1	3.63E-1	1.03E-1	2.73E-1
IRAN3.LIB	7.45E-1	2.29E-2	1.74E-1	3.91E-1	8.08E-2	2.85E-1
IRAN4.LIB	7.45E-1	1.67E-1	1.74E-1	3.25E-1	8.08E-2	2.06E-1
IRAN5.LIB	7.22E-1	8.77E-2	1.68E-1	3.59E-1	1.08E-1	2.47E-1
IRAN6.LIB	8.09E-1	8.63E-2	1.89E-1	4.79E-1	2.55E-4	1.92E-1

* note that for neutron: abs.+albedo+transm.=source(=1)

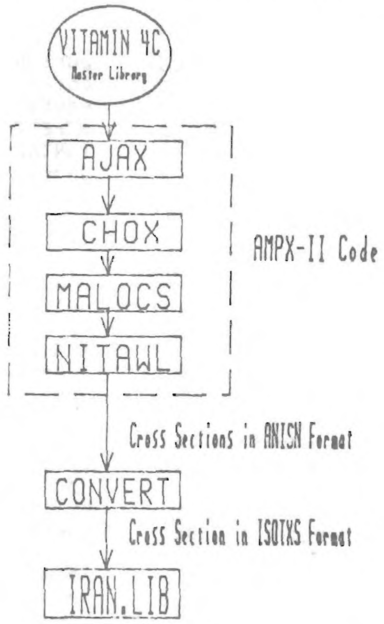
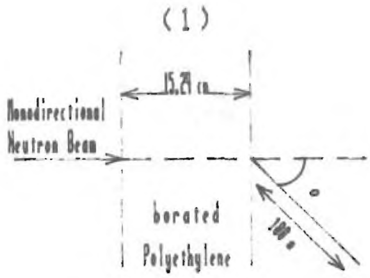


Figure 1:Codes Network to Construct IRAN.LIB

<u>Point Fission source with water-lead spherical shield</u>. This problem is only an illustration of a typical shielding problem which can be solved by ANISN/PC using IRAN.LIB. In Figure (2) the schematic diagram of this sample problem is shown, and in table (6) we have shown the results for the "total absorption fraction " in water and lead and the leakage from the entire media. The problem was solved using S-8 and 31 mesh intervals. The total radius of the system is 30 cm.

Table 6: Comparison of the results of sample problem 2 among IRAN.LIB libraries

	absorption H2O		absorption Pb		leakage system	
	neutron	gamma	neutron	gamma	neutron	gamma
IRAN1.LIB	7.14E-1	1.35E-2	5.90E-2	1.09E+0	2.37E-1	4.57E-3
IRAN2.LIB	7.11E-1	1.25E-2	5.54E-2	1.09E+0	2.51E-1	6.02E-3
IRAN3.LIB	7.05E-1	1.13E-2	5.84E-2	1.04E+0	2.40E-1	5.86E-3
IRAN4.LIB	7.05E-1	6.78E-2	5.84E-2	1.12E+0	2.40E-1	6.45E-3
IRAN5.LIB	6.85E-1	7.25E-2	5.70E-2	1.33E+0	3.10E-1	8.92E-3
IRAN6.LIB	8.60E-1	9.15E-2	4.12E-2	9.50E-1	1.03E-1	1.79E-3



Elements	Atomic Concentration (atoms/barn.cm)
C-12	0.037873
H	0.075746
B-10	0.0010019

Elements	Atomic Concentration (atoms/barn.cm)
H	0.0669
O	0.03345
Pb	0.03283

Figure 2: Sample Problems 1 and 2

CONCLUSION

From the results obtained, it is noticed that IRAN.LIB can provide reasonable results when comparing with the "benchmark results", even though we did not put the coupled multigroup cross sections into any special treatment.

However, if one wishes to have a better set of cross sections it is advised to run ANISN/PC once, and then collapses the input cross sections using the flux weight option(IFG=1 in array 15$) and arrays 27$ and 28$ to obtain a better set of cross sections in any desirable group structure and then to run ANISN/PC again using the collapsed cross sections.

It is also noticed that IRAN1.LIB up to IRAN5.LIB give consistent results and not IRAN6.LIB, then the latter should be used only for training activity. There is some discrepancy in the result of gamma absorption using IRAN4.LIB, and by the time of writing this paper we could not resolve it.

Finally, we believe that IRAN.LIB libraries can be of value to the user which has no access to a mainframe or processing coupled multigroup cross sections using such codes as AMPX-II and master library VITAMIN-4C. A copy of the set of IRAN.LIB libraries can be obtained directly either from M.K. Marashi or J.R. Maiorino by sending diskette with a capability to record the size described in table (3). Also the authors intent to send these libraries to be distributed by Nuclear Energy Agency Data Bank, and by Radiation Shielding Information Centre.

ACKNOWLEGEMENTS

The authors wish to express their gratitude to Mr. Alfredo Y. Abe for his help in the use of compilers and linkers.

Special thanks, from M.K. Marashi, is due to Dr. M.F.L'Annunziata, The Head of Fellowship and Training Section of IAEA for his consideration in prolongation of fellowship period which turned this project into reallity.

We also would like to thank the operating staff at CPD(Computer Centre) specially Miss Emilia K. Nakamura and Miss Maria do Carmo Costa Falcao for their great help in running the computer programs and codes. Great help of Miss Sandra Lopes da Silva in typing the manuscripts is gratefully appreciated.

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