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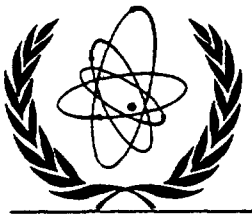

INTERNATIONAL ATOMIC ENERGY AGENCY

NUCLEAR DATA SERVICES

DOCUMENTATION SERIES OF THE IAEA NUCLEAR DATA SECTION

EURLIB-LWR-45/16 AND - 15/5, TWO BROAD GROUP LIBRARIES FOR LWR-SHIELDING PROBLEMS

WÜRENLINGEN, APRIL 1982

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Summary

Specifications of the broad group cross section libraries EURLIB-LWR-45/16 and -15/5 are given. They are based on EURLIB-III data and produced for LWR shielding problems. The elements considered are H, C_{12}, O, Na, AL, Si, Ca, Cr, Mn, Fe, Ni, Zr, U_{235}, U_{238}. The cross section libraries are available upon request from EIR, RSIC, NEA-CPL and IAEA-NDS.

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1. Introduction and summary

Broad group cross section libraries have only a restricted range of applications. They are particularly useful in project design work, 2-dimensional transport calculations and cross section adjustment. Two optimized broad group sets in 45/16 and 15/5 neutron/gamma groups were produced in applying the automatic collapsing scheme AGRUKO (1) to the radial PWR shielding design benchmark (2). The total number of groups and the group structure was selected by AGRUKO to respect required design accuracies for four of the most important response functions (6). The achieved accuracies (1) were for

- pressure vessel damage 5 and 20 %
- thermal activation in the inner shield 2 and 13 %
- gamma heating of the concrete shield 6 and 7 &
- external $\left\{\begin{matrix}\text{neutron}\\ \text{gamma}\end{matrix}\right\}$ dose rate $\left\{\begin{matrix}11 \text{ and } 68\ \%\\ 1 \text{ and } 52\ \%\end{matrix}\right.$

for the 45/16- and the 15/5-group structures respectively.

Additionally an iterative criterium was met to guarantee good convergences of inner interation schemes as used in ANISN (4) and DOT (5) codes. The number of inner interations were reduced roughly proportional to the number of groups compared to the original 100/20 EURLIB-groups calculations. This means, that the calculation time is reduced by a factor of two in applying the 45/16-group library and by a factor of 6 in applying the 15/5-group library (1).

The cross section data are produced for the 14 elements H, C_{12}, O, Na, Al, Si, Ca, Cr, Mn, Fe, Ni, Zr, U_{235}, U_{238}. The maximum legendre expansion is P_3, the moments are not multiplied by the factor $(2\ell+1)$. The weighting spectra of 100/20 and 45/16 are given in the library,

that the user can perform his own collapsing of the original EURLIB data set or response functions.

2. Availability

The cross section data described here are available upon request from

- Federal Institute of Reactor Research (EIR)
  5303 Würenlingen, Switzerland
- NEA-CPL, Saclay, France
- RSIC, Oak Ridge, Tennessee, USA
- IAEA-NDS, Vienna, Austria

3. Data basis

The data basis is the 100/20 fine group EURLIB-3 library (3), which was produced from ENDF/B-IV.

4. Weighting spectrum

For the condensation of the fine group cross section by AGRUKO suitable weighting spectra had to be chosen. The spectrum integrated over the thickness of the pressure vessel seemed to be the most typical for this problem type. The spectrum calculations and the AGRUKO collapsing proceedure were performed in a simplier version of the benchmark (1), which was simplified with respect to geometry and mesh spacing to reduce the computational effort:

- The geometry was changed from cylindrical to spherical.

- The numbers of spatial and angular mesh points where reduced from 202 to 28 and from S_8 to S_4 respectively. The P_1 approximation was limited to P_1.

This simplification is a general approach, because the effect on the weighting spectra and the collapsed cross sections is rather small. In any case this additional error, which is introduced into the collapsed cross sections by the simplified spectrum calculations, can be controled - among other errors - by the comparison of the results of the fine group EURLIB to the results of its collapsed version EURLIB-LWR for the complete benchmark. The results are very satisfactory and can be found in (1). They were sumarized above in chapter 1.

The simplified mesh distribution for the ANISN-spectrum calculations in AGRUKO is given in table 1.

The radial dimensions along a main axis, the material distribution and the material composition are the same as in the tables 1 and 2 of reference (1).

Table 1

Simplified local mesh distribution along a radial main axis of spherical geometry.

Zone and total number of intervals	Number of intervals	Thickness of intervals [cm]	Radius [cm]
Reactor core	-	-	103.5
	1	48	151.5
	1	17.2	168.7
	1	2.6	171.3
4	1	1.2	172.5
Core baffle			
1	1	2.5	175.0
1. Water layer			
	1	0.8	175.8
5	4	8.675	210.5
Core barrel			
1	1	8.0	218.5
2. Water layer			
4	4	7.875	250.0
Cladding			
1	1	0.6	250.6
Pressure vessel			
	1*)	0.3	250.9
4	3**)	8.233	275.6
Concrete shield			
	1*)	0.4	276.0
	1	3.4	279.4
	1	12.5	291.9
	1	22.5	314.4
	1	35.0	349.4
	1	55.0	404.4
	1	63.0	467.4
8	1*)	8.2	475.6

*) These intervals were defined as separated zones for zone integrated spectra output: In total 11 zones.

**) Zone for integrated weighting spectrum

The power distribution was collapsed from the original 30 core intervals to the 4 intervals of table 1:

Table 2

Power distribution in outer core regions along radial midplane axis.

Interval number	Radius [cm]	Interval centre	Power distribution factor
1	103.5	127.5	1.03
2	151.5	160.1	0.998
3	168.7	170.0	0.65
4	171.3	171.8	0.357
	172.5		

The power distribution factor is of no importance for the collapsing of the cross sections, except it gives the normalization of the zone intergrated weithting spectra. Corresponding to (1):

Power distribution factor 1 $\triangleq$ 92.23 $\frac{W}{cm^3}$ = 2.8775 · 10^{12} $\frac{MeV}{cm^3 sec}$,

which has still to be multiplied by the volume of the interesting zone: In our case the pressure vessel between radius 250.6 and 275.6 cm.

The neutron fission spectrum of U-235 of table 5 and of the total gamme yield per fission of table 6 of reference (1) have to be collapsed to the broad group structures, which are indicated in table 3.1 and 3.2. They are reproduced from (1). The precision desired was 0.0001 for the spectrum-calculation by ANISN.

Both weighting spectra in 100/20 and in 45/16 group are enclosed in the library tape. For any new compilation of EURLIB these spectra can be reused in a fist approach to collapse the data in the corresponding AGRUKO structure of 45/16 and 15/5 groups respectively. The sound and better approach will be to rerun AGRUKO, which will be disseminated too.

Tabel 3

GROUP STRUCTURES OF THE EURLIB-LWR-45/16 and 15/5 LIBRARIES OPTIMIZED FROM THE EURLIB - 100/20 LIBRARY

3.1 Neutron groups

Broad groups 45	Fine groups 100	Upper energy (eV)	Broad goups 15	Fine groups 100
1	1 - 7	1.4918 E 7	1	1 - 12
2	8 - 8	7.4082 E 6		
3	9 - 9	7.0469 E 6		
4	10 - 10	6.7032 E 6		
5	11 - 11	6.3763 E 6		
6	12 - 12	6.0653 E 6		
7	13 - 13	5.4881 E 6	2	13 - 17
8	14 - 14	4.9659 E 6		
9	15 - 15	4.7240 E 6		
10	16 - 17	4.4933 E 6		
11	18 - 18	3.6788 E 6	3	18 - 18
12	19 - 19	3.3287 E 6	4	19 - 23
13	20 - 21	3.0012 E 6		
14	22 - 22	2.4660 E 6		
15	23 - 23	2.3460 E 6		
16	24 - 24	2.2313 E 6	5	24 - 24
17	25 - 25	2.0190 E 6	6	25 - 25
18	26 - 26	1.8268 E 6		
19	27 - 27	1.6530 E 6		
20	28 - 28	1.4957 E 6		
21	29 - 29	1.3524 E 6	7	29 - 35
22	30 - 31	1.2246 E 6		
23	32 - 32	1.0026 E 6		
24	33 - 33	9.0718 E 5		
25	34 - 34	8.2085 E 5		
26	35 - 35	7.4274 E 5		
27	36 - 37	6.7206 E 5	8	36 - 41
28	38 - 39	5.5023 E 5		
29	40 - 41	4.5049 E 5		
30	42 - 43	3.6883 E 5	9	42 - 55
31	44 - 47	3.0197 E 5		
32	48 - 50	2.0242 E 5		
33	51 - 52	1.4996 E 5		
34	53 - 53	1.2277 E 5		
35	54 - 54	1.1109 E 5		
36	55 - 55	8.6517 E 4		
37	56 - 57	6.7379 E 4	10	56 - 57
38	58 - 67	4.0868 E 4	11	58 - 67
39	68 - 69	7.1017 E 3	12	68 - 73
40	70 - 73	4.3074 E 3		
41	74 - 77	1.5846 E 3	13	74 - 93
42	78 - 93	5.8295 E 2		
43	94 - 98	8.3153 E 0	14	94 - 99
44	99 - 99	6.2500 E-1		
45	100 - 100	4.1399 E-1	15	100 - 100
		0.0		

3.2 Gamma groups

Broad groups 16	Fine groups 20	Upper energy (MeV)	Broad groups 5	Fine groups 20
1	1 - 4	14.0	1	1 - 5
2	5 - 5	6.5		
3	6 - 6	5.0		
4	7 - 7	4.0		
5	8 - 8	3.0		
6	9 - 9	2.5	2	6 - 6
7	10 - 10	2.0	3	7 - 14
8	11 - 11	1.66		
9	12 - 12	1.33		
10	13 - 13	1.0		
11	14 - 14	0.8		
12	15 - 15	0.6	4	15 - 16
13	16 - 16	0.4		
14	17 - 17	0.3	5	17 - 20
15	18 - 18	0.2		
16	19 - 20	0.1		
		0.02		

5. Content of the library tape

Tape content: The tape contents 4 files

1. file: EURLIB-LWR-15/5 library
   microscopic cross sections

2. file: Flux integral (pressure vessel integrated
   spectrum) in 45/16 groups

3. file: EURLIB-LWR-45/16 library
   microscopic cross sections

4. file: Flux integral (pressure vessel integrated
   spectrum) in ~~15/5~~ 100/20 groups

Tape characteristics: 9 tracks
EBCDIC, DTF-IV format
1600 CPI
Unlabelled

Reference list

(1) V. Herrnberger and S. Padiyath,
Optimized Broad Energy Group Structures for Radiation Transport in Air and in LWR-Shields, EIR-Bericht Nr. 443, October 1981.

(2) G. Hehn and J. Korban,
Reactor Shield Benchmark No. 2, ESIS-Newsletter, Special Issue No. 4, January 1976.

(3) E. Caglioti et. al.
Generation and Testing of the Shielding Library EURLIB for Fission and Fusion Technology, Proceedings of the Vth International Conference on Reactor Shielding, April 1977, Knoxville, USA.

(4) W. Engle, Jr.,
A Users Manual for ANISN, A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering, K-1693, Computing Technology Center, Union Carbide Corporation, Oak Ridge, TN (1967).

(5) W.A. Rhoades and F.R. Mynatt,
The DOT III Two-Dimensional Discrete Ordinates Transport Code, ORNL/TM-4280, Oak Ridge National Laboratory (1973).

(6) V. Herrnberger,
New Requirements Needed for Target Accuracies in Radiation Shielding? ESIS Newsletter, No. 40, January 1982.

EIR - Bericht Nr. 443

OPTIMIZED BROAD ENERGY GROUP STRUCTURES FOR RADIATION TRANSPORT IN AIR AND IN LWR - SHIELDS

V. Herrnberger, S. Padiyath

Würenlingen, October 1981

Abstract

Basic ideas of the automatic group collapsing scheme AGRUKO are briefly described. The errors introduced by the collapsing process are controlled by criteria, which are constructed by the sensitivity profiles and the required target accuracies of the specific shielding type configurations. The group widths are optimized to reduce the calculation time with respect to the fine group calculations.

Optimized group structures were generated for two rather different shielding benchmarks: Neutron and gamma transport in a LWR-shield and in air using a fusion source respectively. In the case of the LWR-shield the 100/20 groups EURLIB-3 structure was collapsed to 45/16 and 15/5 groups. In the case of the "air" problem the original 22/18 groups were collapsed to 4/8 groups. The accuracies achieved were in general within the required accuracies for the targets thermal flux (activation), radiation damage, radiation heating and dose rates.

Because the broad group structures were optimized in view of basic physical and numerical principles, they are nearly free from arbitrary assumptions as constant lethargy width e.g. Therefore they may be recommended for further use in the field of more complex transport calculations or cross section adjustment procedures.

Zusammenfassung

Die zugrundeliegenden Ideen des automatischen Gruppenkondensationsverfahren AGRUKO werden skiziert. Alle Fehler, die durch den Kondensationsprozess bedingt sind, werden durch verschiedene Kriterien kontrolliert, welche von den Sensitivitätsprofilen und den gewünschten Genauigkeiten auf den Zielgrössen spezifischer Schildkonfigurationen abhängen. Die Gruppenbreite wird ausserdem optimiert, um die Rechenzeit im Vergleich zu den Feingruppenrechnungen zu reduzieren. Optimalisierte, für Neutronen/Gamma gekoppelte Gruppenstrukturen wurden für zwei recht unterschiedliche Abschirmungsprobleme (benchmarks) erzeugt: Neutronen- und Gammatransport in einem LWR-Schild und in Luft. Beim letzteren Problem war die Strahlenquelle eine vom Fusionstyp. Im Falle des LWR-Schildes wurde die 100/20-EURLIB-3-Gruppenstruktur auf 45/16 und 15/5 Gruppen kondensiert. Im Falle des "Luftproblemes" wurden die ursprünglich 22/18 Gruppen auf 4/8 Gruppen kondensiert. Die erreichten Genauigkeiten lagen im Allgemeinen innerhalb den gewünschten Genauigkeiten für die 4 Zielgrössen thermischer Fluss (massgebend für Aktivierung), Strahlenschaden, Wärmeentwicklung und Dosisleistungen.

Die abgeleiteten, breiten Gruppenstrukturen sind nahezu frei von irgendwelchen Annahmen, wie z.B. konstanter Lethargiebreite pro Gruppe, weil sie auf Grund physikalischer und numerischer Prinzipien optimalisiert wurden. Darum können diese Strukturen für zwei Anwendungsbereiche empfohlen werden, die besonders auf eine möglichst kleine Gruppenzahl angewiesen sind: Mehrdimensionale Transportrechnungen und Adjustrierung von Wirkungsquerschnitten.

Content page

1. Introduction and problem description

Broad energy group cross section libraries are currently employed in tackling energy dependent transport problems in the fields of shield design, benchmark experiment interpretation and adjusting cross sections to experimental results. Their main goals are to restrict computer storage and costs to reasonable limits, without introducing intolerable errors into the results.

To achieve these goals the proper and optimized selection of group boundaries and weighting spectra in the condensation procedure is the central point. In general the selection of the weighting spectra is not difficult, because they are defined by the problems to be solved.

The selection of a proper group boundary structure is less evident. Depending on the user's physical feeling or the possibilities of the data processing codes, more or less important resonance and anti-resonance details of the cross-sections are taken into account. The structure is verified a posteriori, if the errors introduced into the results are tolerable. Then the structure has to be modified eventually.

This approach by trial and error is perhaps sufficient in simple cases with one detector response, but not in real cases with complicated particle transport environments and more than one detector type and position.

More systematic approaches which are able to tackle real cases and to avoid as far as possible arbitrary assumptions were proposed by (1), (2) and one of the authors (3), (4) in which our approach is discussed in any detail. Here after its short descriptions we will give our main results in

form of several group structures and the accuracies which were achieved by them in the case of two benchmark problems. The results are quite satisfactory, so that their further application may be recommended. They were presented in (11) first, and summarized in (12).

2. Outline of the collapsing scheme AGRUKO

The scheme reduces the number of groups f≤F to a number of broad groups b≤B, needed to solve a specific problem with the following constraints (4):

1st: The change in detector response R (their sensitivity to energy group condensations) should remain within given experiment or design margins $(\frac{\delta R}{R})_a$ (error criterion):

$$\left| \frac{R^{(b)} - R^{(f)}}{R^{(f)}} \right| \lesssim \left| \left(\frac{\delta R}{R} \right)_a \right| \qquad (1)$$

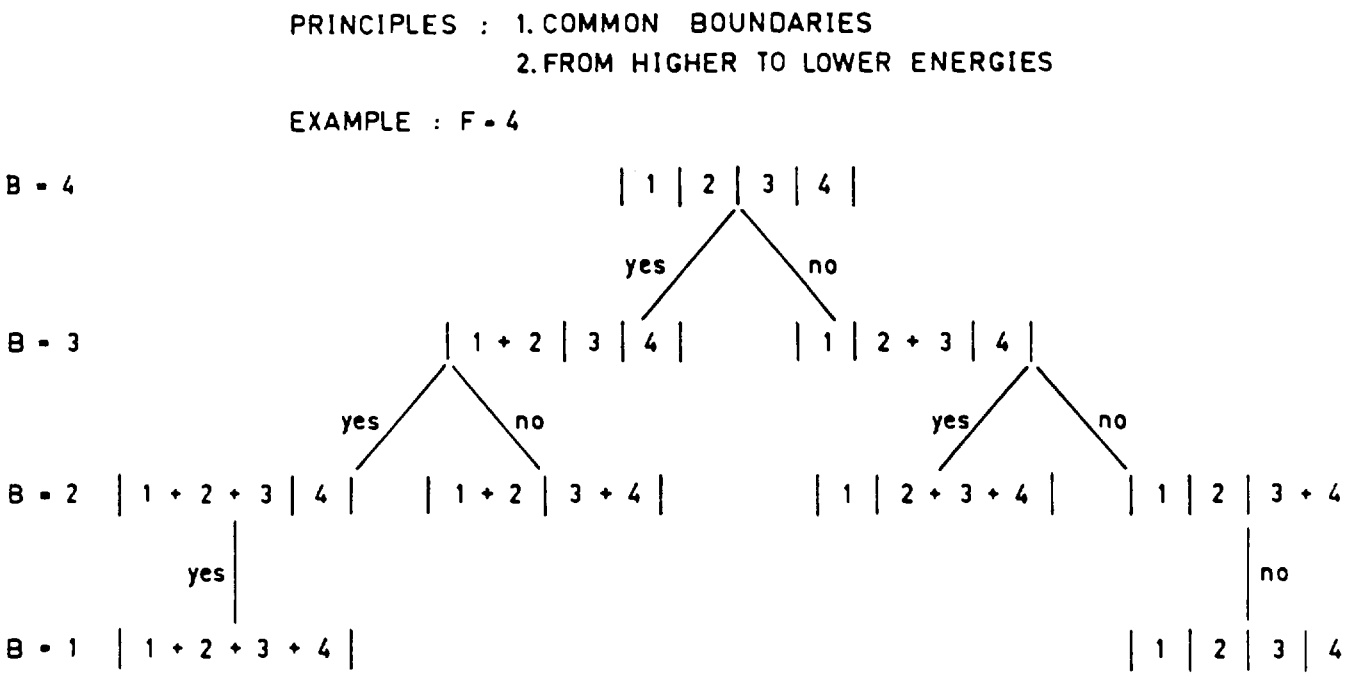
where the index b or f stays for the group structures, in which the response R is calculated.

2nd: A strong reduction in calculational effort, e.g. measured in number of iterations I_b should result (Iteration criterion):

$$\sum_{b=1}^{B} I_b \ll \sum_{f=1}^{F} I_f \qquad (2)$$

The design margins were evaluated elsewhere (5). The number of broad groups B collapsed from F and their group boundary structure will depend upon the design margins, the iterative

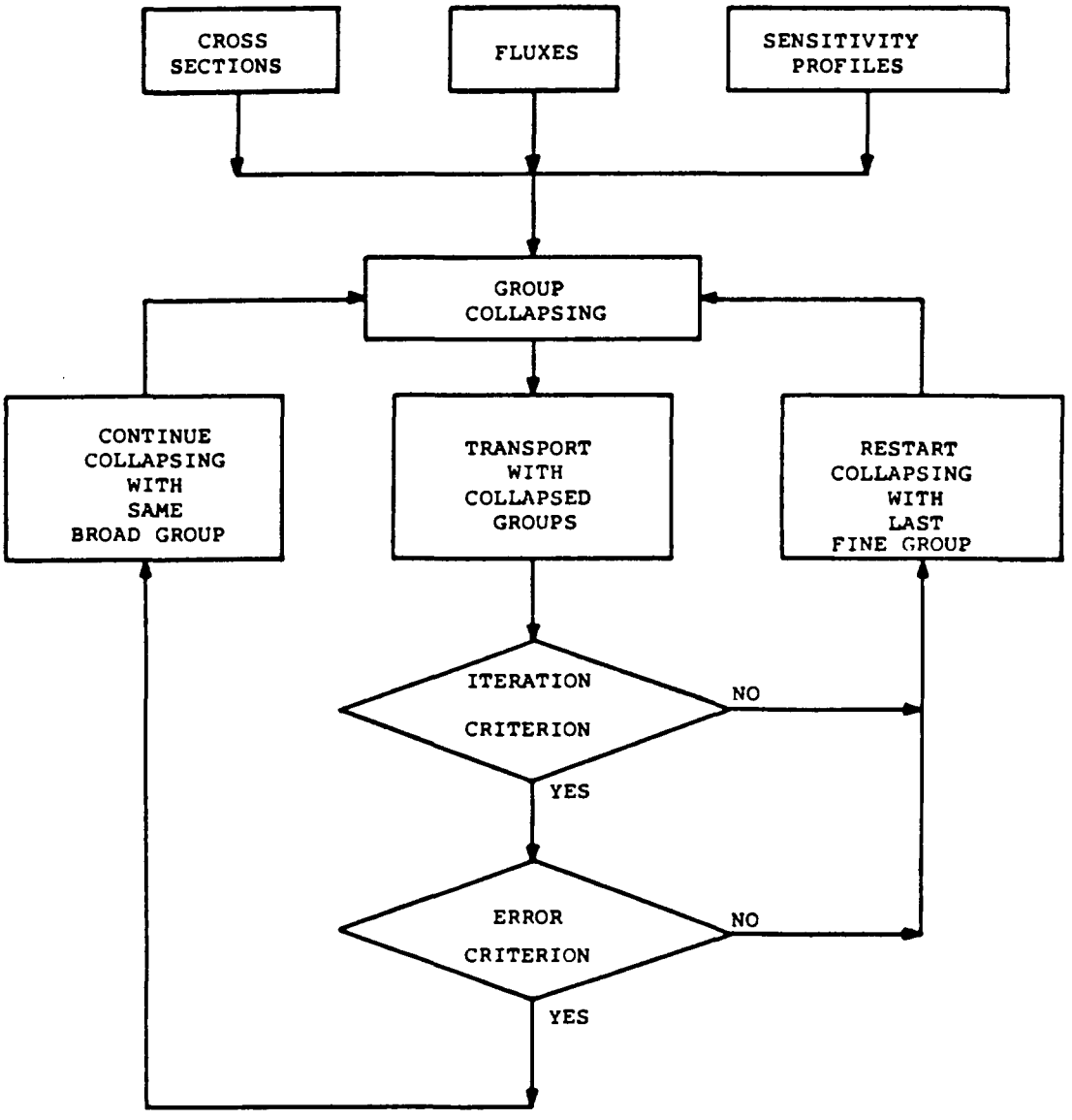
Fig. 1 GROUP BOUNDARY SELECTION.



efficiency of the transport method and the method of fine group collapsing. The method chosen begins with the highest energy group and works down progressively to the lowest one (figure 1). For the group collapsing groupwise iteration and error criteria have to be fulfilled, which were deduced from the criteria (1) and (2). The groupwise error criterion takes into account the importance of the groups by their sensitivity profiles P_f, P_b or groupwise detector responses: A low error is allowed for collapsing groups of high importance and vice versa. This distribution of importance is defined by a so called distribution function, which assumes different functional relationship between groupwise error margin and sensitivity profile. Appendix 1 shows possible "Ansätze", which are available in AGRUKO. Their mathematical form can be briefly characterized by the form of the assumed distribution function with regard to the sensitivity profiles:
General Criterion 1: Monotonic decreasing
Criterion 2: Inverse proportionality of broad group profiles
Criterion 3: Inverse proportionality of fine group profiles
Criterion 4: Square root inverse proportionality
Criterion 5: Double square root inverse proportionality
Our study has begun with criterion 2, which appeared to be rather strong: The number of groups were reduced only by a factor of two and the accuracy achieved was far below the required target accuracies. Therefore weaker functional relationships were introduced which improved remarkably the effectivness of the procedure.
The groupwise iteration criterion guarantees a reduction of the calculational effort roughly proportional to the final number of collapsed groups.
Figure 2 gives an overview of the logical flow in AGRUKO and shows the central role of the error and iteration criteria. Neutron and gamma cross sections are condensed separately.

Fig. 2

Flow chart of AGRUKO



3. Examples of collapsed energy group structures

Two typical shielding benchmark problems were chosen, to check the collapsing procedure particularly with regard to the different error criteria to find the most useful criterion on the one hand and to generate collapsed group cross sections with it, on the other hand, which can be recommended for further use in design and cross section adjustment work.

3.1. Neutron and gamma transport in air

This example is a fusion type source in air (7). The dose rate is measured at a distance of two thousand meters, which was selected as detector position. The effect of different criteria was examined for a "required design accuracy", RDA, of 50 % on the neutron dose rate. The reference case uses the highest number of spatial mesh and a 22/18 (n/γ)-coupled cross section library. Table 1 shows the result of the study. The definitions of the columns are:

TYPE : type of transport calculation, direct (D) or adjoint (A).
APP. : transport approximation
IM : number of spatial mesh points
IGM : number of groups
CRIT. : criterion used: P, with sensitivity profile or A, with groupwise relative detector response
%-DEV.COND: % deviation of broad group from fine group results for low IM (=9)
%-DEV.REF.: as above but for the reference case with high IM (=169)

Criteria P/2, A/3 and P/3 are rather strong, because the collapsed group cross sections show an accuracy of 10-80 x

TABLE 1

COMPARISON OF FINE/BROAD GROUP RESULTS

Neutron transport in air, RDA = 50 %

TYPE	APP.	IM	IGM	CRIT.	%-DEV. COND.	%-DEV. REF.
D	S40P3	9	22	-	-	(100x)
A	"	"	"	-	-	(60x)
D	"	169	"	-	-	[0.72]
A	"	9/169	"	-	-	∿ 3.
D	"	9/169	1	A/3+4 P/4	28	-96.
"	"	9/169	3	P/3	4.9	-41.
"	"	9/169	4	A/2	2.9	-26.
"	"	9/169	10	P/2	0.69	- 6.5

below the required one. The application of the weaker criteria P/4, A/4 (A/3 shows the same effect) results in a complete condensation of all 22 groups into a single one. The accuracy was only a factor 2 below the required one. On the other hand when looking at the reference case the deviations are much greater and only A/2 seemed to have a reasonable safety margin of a factor 2 with regard to the required 50 % deviation. The results calculated by collapsed group cross sections seem to be less sensitive to lower spatial mesh than those obtained from fine group cross sections. In consequence criterion A/2 was used for the coupled n,γ- case.

The detailed results of AGRUKO are given in table 2 and 3. The new group structures for neutron and gamma cross sections, the relative deviation, the permissible deviation and the failed criterion per group as the total deviation are given.

It is very interesting to see that the gamma groups are much less collapsed for the same required accuracy. This fact shows their relative importance in this type of transport problem, which was already reflected in the unusually high fine number of γ groups compared to that of the neutron groups (18:22). The %-deviation from the reference case was less than 1 % for the γ-dose rate.

3.2. Neutron transport in a PWR shield

In a first step the displacement rate at the inner side of a PWR pressure vessel was selected as target (8) to check the error criteria. The EURLIB-3 library with 100/20 n/γ-groups was used as fine group data base. Only the most efficient criterion 3, 4 and 5 were applied and the RDA were varied. The results for criterion P/4 are shown in table 4.

TABLE 2

AIR, S40/P3, 9 INT. CONDENSATION FROM 22 GR. WITH RELATIVE ACTIVITY: NEUTRONS

NUMBER OF TARGETS = 1
TARGET = DOSE RATE
RDA % = 50
CRITERION = 2
INTERVAL NO. = 8
FINE GROUP TARGET RESPONSE = 7.1E-15

BROAD GROUPS	FINE GROUPS	RELATIVE DEVIATION	PERMISSIBLE DEVIATION	FAILED CRITERION
1	1 - 10	-40.1E-2	55.4E-2	FEH
2	11 - 12	-47.8E-2	65.9E-2	FEH
3	13 - 15	-33.3E-2	41.9E-2	FEH
4	16 - 22	-16.8E-1	14.6	NO

ITE = ITERATION CRITERION

FEH = ERROR CRITERION

THE TOTAL RELATIVE DEVIATION OF
4 GROUP CROSS SECTIONS = -2.9 %

TABLE 3

AIR, S40/P3, 9 INT. CONDENSATION FROM 18 GR. WITH RELATIVE ACTIVITY: GAMMAS

NUMBER OF TARGETS = 1
TARGET = DOSE RATE
RDA % = 50
CRITERION = 2
INTERVAL NO. = 8
FINE GROUP TARGET RESPONSE = 4.1E-16

BROAD GROUPS	FINE GROUPS	RELATIVE DEVIATION	PERMISSIBLE DEVIATION	FAILED CRITERION
1	23 - 23	-24.8E-2	97.5E-2	ITE
2	24 - 24	-36.7E-1	49.4E-2	ITE
3	25 - 25	-90.0E-2	15.9E-2	FEH
4	26 - 26	-22.3E-2	48.5E-2	ITE
5	27 - 27	27.9E-2	49.1E-2	ITE
6	28 - 31	-22.9E-2	30.1E-2	FEH
7	32 - 38	-16.4E-2	50.3E-2	FEH
8	39 - 40	-69.7E-3	98.6E-1	NO

ITE = ITERATION CRITERION

FEH = ERROR CRITERION

THE TOTAL RELATIVE DEVIATION OF
8 GROUP CROSS SECTIONS = -2.5 %

TABLE 4

LWR - BENCHMARK, CRIT. P/4

TYPE	APP.	IM	IGM	RDA[%]	%-DEV. COND.	%-DEV. REF.
D	S4P1	20	100	-	-	52.
A	"	"	"	-	-	196.
D	S8P3	146	"	-	-	[0.264]
"	S4P1/S8P3	20/146	42	10	3.41	-15.3
"	S4P1/S8P3	20/146	36	30	6.9	9.2
"	S4P1/S8P3	20/146	17	100	-0.71	1.5
"	S4P1/S8P3	20/146	21	300	41.9	54.2

The reference case was S8/P3, IM=146, IGM=100. Between 10 % - 100 % RDA the collapsing process gives satisfying results. The number of groups are reduced with reducing accuracy. The %-deviation shows some fluctuation, because error compensation gets more important with lower numbers of groups. For extremly "low" RDA of about 300 % a reversed tendency appears in the sense, that the number of groups increase slightly, but the %-DEV. increases remarkably.

The overall result of the check of the criteria 3, 4 and 5 was, that as in table 1 the P/4 is the more efficient one with regard to the reduction of the number of groups. A/4 is less efficient but it does not show the reversed tendency for very low required accuracies. The criterion P/5 collapsed to 21 groups and 10.7 % - DEV. COND. and the criterion A/5 to 25 groups and 1.9 % - DEV. COND. for RDA = 100 %. Therefore criterion 5 cannot be considered as to be clearly better than criterion 4.

In a second step the whole PWR-benchmark was treated and the 100/20 groups were collapsed in two sets of 45/16 and 15/5 groups respectively. Three detectors (targets) were used, the displacement rate at the inner side of the pressure vessel as above, the γ-heating (energy deposition) at the inner side of the concrete shield and the dose rate at the outer side of the concrete shield. The required design accuracies were 20 %, 40 % (30 %) and 100 % for each n- and γ-dose rate respectively. The criterion A/4 was applied for two reasons: First, for its uniform tendency in the collapsing procedure. Second, for the reduction of calculational effort (no additional adjoint S_n- and sensitivity profile calculations for the other detectors are necessary). The resulting group structures are shown in tables 5-8. Table 5 and 6 give the example of the dose rate at the outer concrete shield for the 45 neutron and 16 gamma groups. Table 7 and 8 show the examples of the two targets displacement rate and γ-heating for the 15 neutron and 5 gamma groups. The effect of the error

compensation can be seen: The high relative deviation of the last (thermal) neutron group, which cannot be controlled by this type of a non iterative collapsing scheme, is largely compensated by those of the higher groups. Only one spectrum for the condensation was chosen in order to restrict the cross sections to one set per material zone. The spectrum in the pressure vessel seemed to be one of the most typical of the shield system. The 15/5 structure was obtained by repeated collapsing of the 45/16 groups using mostly the same RDA, which was the most difficult task. It turned out, that a direct condensation of the 100/20 group scheme to very few groups (<20) led to uncontrollable large errors in the γ-responses and to convergence problems in the keV-neutron-energy region of the cross sections ($1\text{-}10^2$ keV) within the pressure vessel of the reference case (with high angular and spatial mesh). Therefore the condensation was performed stepwise from 45/16 to 21/4 and to 13/3 n/γ-groups.

To reduce divergence problems due to large group widths the iteration criterion was changed to

$$I_{b+f} < a \cdot I_b \quad ,$$

where (b+f) means the condensation of broad group with the next fine group f and a is an experimental parameter depending upon the numerical iteration scheme of the transport code.

a=0,8 was too strong, because more than 70 % of the group limits were defined by the iteration criterion. a=1,2 seemed to be reasonable, but didn't solve (as a=1,0) completely the convergence problems. In consequence the original 21 group structure of 3 groups had to be maintained for group 10 of the 13 group structure (table 7).

TABLE 5

LWR, S4/P1, 28 INT. CONDENSATION OF 100 GR. WITH RELATIVE ACTIVITY: NEUTRONS

NUMBER OF TARGETS = 3
TARGET = DOSE RATE
RDA % = 100
CRITERION = 4
INTERVAL NO. = 28
FINE GROUP TARGET RESPONSE = 7.5E+01

BROAD GROUPS	FINE GROUPS	RELATIVE DEVIATION	PERMISSIBLE DEVIATION	FAILED CRITERION
1	1 - 7	-73.6E-4	22.5	FEH
2	8 - 8	74.6E-5	26.4E-1	FEH
3	9 - 9	10.6E-4	20.0E-1	FEH
4	10 - 10	15.8E-4	15.2E-1	FEH
5	11 - 11	18.2E-4	14.3E-1	FEH
6	12 - 12	29.2E-4	11.8E-1	FEH
7	13 - 13	39.7E-4	10.2E-1	FEH
8	14 - 14	24.4E-4	13.2E-1	FEH
9	15 - 15	23.1E-4	13.5E-1	FEH
10	16 - 17	-41.9E-4	22.1E-1	FEH
11	18 - 18	23.8E-4	12.5E-1	FEH
12	19 - 19	41.4E-4	91.4E-2	FEH
13	20 - 21	33.5E-3	12.9E-1	FEH
14	22 - 22	10.9E-3	51.4E-2	FEH
15	23 - 23	91.9E-4	53.9E-2	FEH
16	24 - 24	96.2E-4	47.6E-2	FEH
17	25 - 25	64.5E-4	58.8E-2	FEH
18	26 - 26	95.9E-4	46.9E-2	FEH
19	27 - 27	81.3E-4	50.3E-2	FEH
20	28 - 28	91.9E-4	47.4E-2	FEH
21	29 - 29	79.54-4	50.8E-2	FEH
22	30 - 31	-93.4E-3	11.3E-1	FEH
23	32 - 32	-12.6E-3	66.8E-2	FEH
24	33 - 33	-82.2E-5	53.1E-2	FEH
25	34 - 34	-28.5E-4	45.0E-2	FEH
26	35 - 35	-85.4E-5	43.7E-2	FEH
27	36 - 37	97.9E-3	86.6E-2	FEH
28	38 - 39	-17.5E-2	10.6E-1	FEH
29	40 - 41	-16.4E-3	15.0E-1	FEH
30	42 - 43	22.6E-4	13.3E-1	FEH
31	44 - 47	-14.8E-3	29.2E-1	ITE
32	48 - 50	32.1E-3	23.6E-1	ITE
33	51 - 52	21.2E-4	16.4E-1	ITE
34	53 - 53	-80.8E-5	85.5E-2	FEH
35	54 - 54	-18.1E-4	59.6E-2	FEH
36	55 - 55	-76.9E-5	61.8E-2	FEH
37	56 - 57	45.9E-3	14.0E-1	ITE
38	58 - 67	96.9E-2	13.2	ITE
39	68 - 69	-95.3E-4	22.5E-1	ITE
40	70 - 73	81.1E-3	41.4E-1	ITE
41	74 - 77	86.4E-3	37.2E-1	ITE
42	78 - 93	18.9E-1	11.4	ITE
43	94 - 98	16.1E-1	18.4E-1	ITE
44	99 - 99	73.2E-3	39.1E-2	FEH
45	100 - 100	20.6E-1	34.0E-3	NO

ITE = ITERATION CRITERION
FEH = ERROR CRITERION
THE TOTAL RELATIVE DEVIATION OF
45 GROUP CROSS SECTIONS = 6.74 %

TABLE 6

LWR, S4/P1, 28 INT. CONDENSATION FROM 20 GR. WITH RELATIVE ACTIVITY: GAMMAS

NUMBER OF TARGETS = 3
TARGET = DOSE RATE
RDA % = 100
CRITERION = 4
INTERVAL NO. = 28
FINE GROUP TARGET RESPONSE = 4.4E+1

BROAD GROUPS	FINE GROUPS	RELATIVE DEVIATION	PERMISSIBLE DEVIATION	FAILED CRITERION
1	101 - 104	-14.3	96.8	FEH
2	105 - 105	-47.2E-1	63.5E-3	FEH
3	106 - 106	-28.9E-1	77.0E-3	FEH
4	107 - 107	-26.9E-1	78.8E-3	FEH
5	108 - 108	-13.3E-1	11.7E-2	FEH
6	109 - 109	-14.1E-1	10.2E-2	FEH
7	110 - 110	-10.2E-1	11.5E-2	FEH
8	111 - 111	-95.2E-2	13.2E-2	FEH
9	112 - 112	-10.0E-1	12.9E-2	FEH
10	113 - 113	-65.4E-2	16.1E-2	FEH
11	114 - 114	-71.4E-2	15.4E-2	FEH
12	115 - 115	-81.1E-2	14.3E-2	FEH
13	116 - 116	-48.7E-2	18.4E-2	FEH
14	117 - 117	-54.8E-2	17.1E-2	FEH
15	118 - 118	-63.8E-2	15.8E-2	FEH
16	119 - 120	-68.1E-3	14.0E-1	NO

ITE = ITERATION CRITERION

FEH = ERROR CRITERION

THE TOTAL RELATIVE DEVIATION OF
16 GROUP CROSS SECTIONS = -34.3 %

TABLE 7

LWR, S4/P1, 28 INT. CONDENSATION FROM 45 GR. WITH RELATIVE ACTIVITY: NEUTRONS

NUMBER OF TARGETS = 3
TARGET = DISPLACEMENT RATE
RDA % = 20
CRITERION = 4
INTERVAL NO. = 17
FINE GROUP TARGET RESPONSE = 5.3E+12

BROAD GROUPS	FINE GROUPS	RELATIVE DEVIATION	PERMISSIBLE DEVIATION	FAILED CRITERION
1	1 - 6	22.1E-7	31.1E-2	FEH
2	7 - 10	57.7E-2	11.3E-1	FEH
3	11 - 11	55.1E-3	56.4E-2	FEH
4	12 - 15	14.5E-2	36.1E-2	FEH
5	16 - 16	46.2E-3	50.4E-2	FEH
6	17 - 20	-53.7E-2	86.9E-2	ITE
7	21 - 26	-18.6E-1	29.1E-1	FEH
8	27 - 29	-24.8E-2	32.9E-2	FEH
9	30 - 36	44.4E-2	12.0E-1	FEH
10	37 - 37			
11	38 - 38	74.3E-2*	33.1E-1*	FEH*
12	39 - 40			
13	41 - 42	17.2E-3*	40.5E-1*	FEH*
14	43 - 44	66.1E-4*	41.7E-1*	FEH*
15	45 - 45	-25.2E-1*	30.4E-2*	NO

ITE = ITERATION CRITERION
FEH = ERROR CRITERION

THE TOTAL RELATIVE DEVIATION OF
13 GROUP CROSS SECTIONS = -3.1%

* VALID FOR THE 13 GROUP STRUCTURE. THE TENTH GROUP WAS SUBDIVIDED INTO 3 GROUPS

TABLE 8

LWR, S4/P1, 28 INT. CONDENSATION FROM 16 GR. WITH RELATIVE ACTIVITY: GAMMAS

NUMBER OF TARGETS = 3
TARGET = GAMMA HEATING
RDA % = 30
CRITERION = 4
INTERVAL NO. = 21
FINE GROUP TARGET RESPONSE = 2.9E-4

BROAD GROUPS	FINE GROUPS	RELATIVE DEVIATION	PERMISSIBLE DEVIATION	FAILED CRITERION
1	46 - 47	-82.5E-2	21.2E-1	FEH
2	48 - 48	-15.5E-1	14.0E-1	FEH
3	49 - 56	-87.6E-1	13.4	FEH
4	57 - 58	-10.6E-1	44.8E-1	ITE
5	59 - 61	11.0E-1	86.0E-1	NO

ITE = ITERATION CRITERION

FEH = ERROR CRITERION

THE TOTAL RELATIVE DEVIATION OF
5 GROUP CROSS SECTIONS = -11.1 %

TABLE 9

ACCURACIES OF COLLAPSED GROUP STRUCTURES, IF APPLIED TO THE SIMPLIFIED PWR-BENCHMARK

(S4/P1, IM=28)

POSITION	TARGET TYPE	IGM	RDA %	%-DEV. COND.
INNER SIDE PRESSURE VESSEL	DISPLACEMENT RATE	45 15	20 20	-0.4 -3* (Table 7)
INNER SIDE CONCRETE SHIELD	γ-HEATING	45/16 15/5	40 30	-27 -11 (Table 8)
OUTER SIDE CONCRETE SHIELD	n/γ-DOSE RATE	45/16 15/5	100/100 100/100	7/-34 (Tables 5/6) -3*/3

* VALID FOR THE 13 GROUP STRUCTURE.
THE TENTH GROUP WAS SUBDIVIDED
INTO 3 GROUPS, WHICH DEFINE THE 15 GROUPS.

The resulting 15 groups were used to collapse the 16 γ-groups (table 6) to the 5 γ-groups (table 8), which showed reasonable errors in the reference case.

Table 9 shows the accuracies achieved by the two structures during the condensation which was performed in a S_4P_1 approximation with IM=28. The results are very satisfying for all of the three targets in three different positions: The accuracies (%-DEV.), which were achieved stay within the required ones (RDA).

In tables 10.1 and 10.2 the two structures for the PWR-benchmark are summarized and set into perspective to the original 100/20-EURLIB group structure. The tables clearly show the need for a high resolution in the upper energy region for neutrons and in the lower energy region for gammas. This fact may be an indication, that the structure of the original 100/20 EURLIB groups is still unsufficient.

The same suggestion was made by (9). (10) recommends a much finer structure for CTR/LMFBR-type problems (VITAMIN-library).

The application of the PWR group structure to BWR-shielding problems should give comparable results, because no basic differences exist in between both shield configurations.

Table 11 illustrates the %-deviation from the 100/20 fine group reference (REF) calculations (in a S_8P_3 approximation with IM=202 intervals) for the above mentioned targets. Thermal fluxes are included, because they are mostly significant for capture γ-production or activation. The accuracies and the gain in computing effort stay in general fairly within the required ones. The only exception is the displacement

rate. The optimized 45/16- and 15/5 - group structures can be applied to similar LWR - shielding problems. They show sufficient advantages to be recommended for their further use in design calculations or cross section adjustement.

4. Conclusions

The generated broad group structures for the particle transport in air and in a PWR shield are very satisfying. They guarantee the required design accuracies of the different detector responses and they reduce the calculational effort roughly proportional to the number of groups. Up to now the use of group dependent relative detector responses instead of sensitivity profiles leads to satisfactory results. Condensation to very few groups is still difficult, as to guarantee convergence of the iterative transport methods. The approach cannot yet be done in a completely straight forward way.

TABLE 10

GROUP STRUCTURES OF THE EURLIB-LWR-45/16 and 15/5 LIBRARIES OPTIMIZED FROM THE EURLIB - 100/20 LIBRARY.

10.1 Neutron groups

Broad groups 45	Fine groups 100	Upper energy (eV)	Broad groups 15	Fine groups 100
1	1 - 7	1.4918 E 7	1	1 - 12
2	8 - 8	7.4082 E 6		
3	9 - 9	7.0469 E 6		
4	10 - 10	6.7032 E 6		
5	11 - 11	6.3763 E 6		
6	12 - 12	6.0653 E 6		
7	13 - 13	5.4881 E 6	2	13 - 17
8	14 - 14	4.9659 E 6		
9	15 - 15	4.7240 E 6		
10	16 - 17	4.4933 E 6		
11	18 - 18	3.6788 E 6	3	18 - 18
12	19 - 19	3.3287 E 6	4	19 - 23
13	20 - 21	3.0112 E 6		
14	22 - 22	2.4660 E 6		
15	23 - 23	2.3460 E 6		
16	24 - 24	2.2313 E 6	5	24 - 24
17	25 - 25	2.0190 E 6	6	25 - 28
18	26 - 26	1.8268 E 6		
19	27 - 27	1.6530 E 6		
20	28 - 28	1.4957 E 6		
21	29 - 29	1.3524 E 6	7	29 - 35
22	30 - 31	1.2246 E 6		
23	32 - 32	1.0026 E 6		
24	33 - 33	9.0718 E 5		
25	34 - 34	8.2085 E 5		
26	35 - 35	7.4274 E 5		
27	36 - 37	6.7206 E 5	8	36 - 41
28	38 - 39	5.5023 E 5		
29	40 - 41	4.5049 E 5		
30	42 - 43	3.6883 E 5	9	42 - 55
31	44 - 47	3.0197 E 5		
32	48 - 50	2.0242 E 5		
33	51 - 52	1.4996 E 5		
34	53 - 53	1.2277 E 5		
35	54 - 54	1.1109 E 5		
36	55 - 55	8.6517 E 4		
37	56 - 57	6.7379 E 4	10	56 - 57
38	58 - 67	4.0868 E 4	11	58 - 67
39	68 - 69	7.1017 E 3	12	68 - 73
40	70 - 73	4.3074 E 3		
41	74 - 77	1.5846 E 3	13	74 - 93
42	78 - 93	5.8295 E 2		
43	94 - 98	8.3153 E 0	14	94 - 99
44	99 - 99	6.2500 E-1		
45	100 - 100	4.1399 E-1	15	100 - 100
		0.0		

10.2 Gamma groups

Broad groups 16	Fine groups 20	Upper energy (MeV)	Broad groups 5	Fine groups 20
1	1 - 4	14.0	1	1 - 5
2	5 - 5	6.5		
3	6 - 6	5.0		
4	7 - 7	4.0		
5	8 - 8	3.0		
6	9 - 9	2.5	2	6 - 6
7	10 - 10	2.0	3	7 - 14
8	11 - 11	1.66		
9	12 - 12	1.33		
10	13 - 13	1.0		
11	14 - 14	0.8		
12	15 - 15	0.6	4	15 - 16
13	16 - 16	0.4		
14	17 - 17	0.3	5	17 - 20
15	18 - 18	0.2		
16	19 - 20	0.1		
		0.02		

TABLE 11

ACCURACIES AND GAIN IN COMPUTING COSTS, IF THE COLLAPSED STRUCTURES APPLIED TO THE REFERENCE PWR-BENCHMARK (S8/P3, IM=202)

POSITION	TARGET	45/16 → STRUCTURES → 15/5			
		RDA [%]	DEV.REF [%]	RDA [%]	DEV.REF [%]
INNER SIDE PRESSURE VESSEL	DISPLACEMENT RATE	20	5	20	20
	THERMAL FLUX	-	2	-	2
INNER SIDE CONCRETE SHIELD	γ-HEATING	40	- 6	30	- 7
	THERMAL FLUX	-	- 0.3	-	13
OUTER SIDE CONCRETE SHIELD	DOSE RATE n	100	11	100	-68
	DOSE RATE γ	100	- 1	100	-52
	THERMAL FLUX	-	13	-	-66
	%-GAIN OF COMPUTING COSTS (CDC 6400/6500)	50	60	83	88

APPENDIX 1

GROUPWISE CRITERIA
==========

1. ITERATIONS

$$I_b < I_{b'} + I_P << \sum_{f \in b} I_f$$

2. ERRORS

CRITER. 1 (GENERAL)

$$\frac{\delta R_b}{R} = \left|\frac{\delta R}{R}\right|_a \cdot \underbrace{F(P_b)}$$

DISTRIBUTION FUNCTION WITH $F'(P_b) < o$

$$\frac{\delta R_b}{R} = \frac{R_b - \sum_{f \epsilon b} R_f}{R^{(f)}}$$

$$\left| \sum_{b=1}^{B} \frac{\delta R_b}{R} \right| < \left|\frac{\delta R}{R}\right|_a \Rightarrow \underbrace{\left| \sum_{b=1}^{B} F(P_b) \right|}_{C(f,b)} < 1$$

CRITER. 2

$$F(P_b) = C_2 \cdot P_b^{-1}$$

$$\left| C_2 \right| < \left| \sum_{b=1}^{B} P_b^{-1} \right|^{-1}$$

APPROXIMATION NEEDED:

$$P_b \approx \sum_{f \varepsilon b} P_f$$

LOWER LIMIT OF C_2:

$$\left| C_2^* \right| = \left| \sum_{b'=1}^{b} P_{b'}^{-1} + \sum_{f>b} P_f \right|^{-1} < \left| C_2 \right|$$

CRITER. 3

$$F(P_b) = C_3 \cdot \sum_{f \varepsilon b} P_f^{-1}$$

$$\left| C_3 \right| \leq \left| \sum_{f=1}^{F} P_f^{-1} \right|^{-1}$$

CRITER. 4

$$F(P_b) = C_4 \cdot \sum_{f \epsilon b} P_f \Big| \cdot P_f \Big|^{-3/2}$$

$$\Big| C_4 \Big| \leq \Big| \sum_{f=1}^{F} P_f \cdot \Big| P_f \Big|^{-3/2} \Big|^{-1}$$

CRITER. 5

$$F(P_b) = C_5 \cdot \sum_{f \epsilon b} P_f \cdot \Big| P_f \Big|^{-5/4}$$

$$\Big| C_5 \Big| \leq \Big| \sum_{f=1}^{F} P_f \cdot \Big| P_f \Big|^{-5/4} \Big|^{-1}$$

POSSIBLE SIMPLIFICATION:

$$P_f \approx \frac{R_f}{R^{(f)}}$$

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