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Institut für Neutronenphysik und Reaktortechnik
Projekt Schneller Brüter

Fine Group Calculations for Reactivity Coefficients of Structural Materials in Fast Reactors

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by

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A B S T R A C T

The comparison of calculated and measured reactivity coefficients of individual isotopes or elements may provide a fairly detailed check on the correctness of the important nuclear data for these materials. In order to be able to draw firm conclusions in this direction, one must be sure that other possible sources of error besides the data uncertainties can be excluded or at least neglected.

The present work mainly deals with one specific source of error namely with the influence of the energy resolution used in the multigroup formalism on calculated central reactivity coefficients of some isotopes and elements, particularly of predominantly scattering materials in fast reactors. For the calculations we assumed that first order perturbation theory can be applied. The results are based on fundamental mode diffusion calculations for the homogeneous composition. As starting point we used the 2o8 group scheme which consists of 196 fine groups above 1 KeV. The transition to the coarse group energy scheme of, e.g., 26 groups was obtained by group collapsing. Besides the usual normal flux weighting we have also applied bilinear weighting which takes into account normal and adjoint fluxes.

The results of this work indicate that the usual 26 group calculations of reactivity coefficients especially for predominantly scattering materials may lead to appreciable deviations from more refined treatments with better energy resolution. It is shown that these deviations are essentially due to discrepancies in the adjoint flux obtained with flux weighted coarse group constants. Bilinear weighting for the preparation of coarse group constants (e.g. for 26 groups) advoids the difficulties mentioned before.

K U R Z F A S S U N G

Die Güte wichtiger nuklearer Daten einzelner Isotope oder Elemente kann durch den Vergleich gemessener und gerechneter Reaktivitätskoeffizienten dieser Materialien überprüft werden. Diese Überprüfung kann nur dann zuverlässige Schlußfolgerungen liefern, wenn gewährleistet ist, daß alle anderen möglichen Fehlerquellen außer den Unsicherheiten in den nuklearen Daten ausgeschlossen oder vernachlässigt werden können.

Als eine mögliche Fehlerquelle wird in der vorliegenden Arbeit der Einfluß der Energie-Auflösung in dem allgemein üblichen Multigruppen - Formalismus untersucht. Dabei werden hauptsächlich Reaktivitätskoeffizienten von Streumaterialien in schnellen Reaktoren betrachtet. Bei den Berechnungen wird die Anwendbarkeit von Störungstheorie 1. Ordnung vorausgesetzt. Die Untersuchungen werden auf der Grundlage von nulldimensionalen Diffusionsrechnungen für eine homogene Mischung durchgeführt. Die Ausgangsresultate, die hier als Bezugsgröße dienen, werden in einem 2o8-Gruppen-Schema ermittelt, bei dem der Energiebereich zwischen 1 KeV und 1o,5 MeV in 196 Feingruppen aufgeteilt ist. Durch Zusammenfassung von Gruppen (Kondensation) gelangt man zu gröberen Gruppeneinteilungen, d.h. geringerer Energie-Auflösung.

Bei der Kondensation wurde neben der üblichen Wichtung mit dem normalen (realen) Neutronenfluß auch die bilineare Wichtung betrachtet, die den normalen und den adjungierten Fluß verwendet.

Die Ergebnisse der vorliegenden Arbeit zeigen, daß die gebräuchlichen 26-Gruppen-Rechnungen bei der Bestimmung von Reaktivitätskoeffizienten, insbesondere für Streumaterialien zu erheblichen Abweichungen führen können verglichen mit genaueren Bestimmungsverfahren mit besserer Energie-Auflösung. Diese Abweichungen sind in erster Linie auf Abweichungen zurückzuführen, die im adjungierten Neutronenfluß auftreten, wenn zur Berechnung flußgewichtete Gruppenkonstanten benutzt werden. Diese Schwierigkeiten können vermieden werden, wenn die bilineare Wichtung zur Bestimmung der Gruppenkonstanten insbesondere bei weniger guter Energie-Auflösung z.B. 26 Gruppen angewendet wird.

Contents

1. Introduction

The comparison of calculated and measured criticality parameters of fast zero-power reactors provides an overall check on the correctness of the nuclear data used in the calculations under the implied assumption that the accuracy of the measurements as well as that of the methods of calculation is sufficiently high. The corresponding comparison of reactivity coefficients of individual isotopes or elements provides a more detailed check on the correctness of the important nuclear data for these materials. There are several possible reasons and explanations for discrepancies between calculated and measured reactivity coefficients, e.g.:

a) The delayed neutron parameters
b) Sample size effects
c) Mutual interaction of the sample and the surrounding reactor region
d) Heterogeneity effects caused by the heterogeneous arrangement present in the region surrounding the sample
e) The space dependence of the real and adjoint neutron flux
f) The energy dependence of the real and adjoint neutron flux
g) The cross sections for the specific material considered

In order to draw firm conclusions on the last item, i.e. the correctness of the cross sections of the specific material studied, one must be sure that errors caused by any of the other items a) to f) can be excluded or at least neglected.

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The delayed-neutron parameters of the fuel isotopes are necessary in order to compare, on an absolute scale, the calculated reactivity coefficients with the corresponding measured quantities. Therefore these parameters - especially those of U 238 and Pu 239 - are a likely source of error if discrepancies in the absolute magnitude of reactivity coefficients are observed between theoretical and experimental results as indicated, e.g., by LITTLE and HARDIE /1/ or BÖHME et al. /2/. Sometimes one tries to avoid this difficulty of absolute values in the following way: for a series of calculated reactivity coefficients for the same reactor one normalizes all calculated values to that one obtained for a reference material, e.g. U 235, and performs the analogue procedure for the experimental results too, so that only normalized reactivity coefficients are to be compared. In the present work we are only comparing various theoretical results with eachother but not with experimental results. Therefore we may disregard in the following the effect of item (a). The items (b) to (d) are to some extend related to the methods of calculations, which should be able to take into account the experimental arrangement in an appropriate manner. The studies of FISCHER/3/, OOSTERKAMP /4/ and HEINDLER/4a/ besides many others are examples for the efforts to describe adequately the effects of sample size, heterogeneity, space- and energy-dependent resonance self-shielding and mutual interaction of the sample and its surrounding. Furthermore the work of OOSTERKAMP /4/ shows that specially deviced experimental set-ups may lead to less complicated models for the calculations. In the present work items (b) to (d) will not be considered. We will assume in the following that first order perturbation theory is applicable.

The space dependence of the real and adjoint neutron flux is influenced by the method of calculation e.g. diffusion - or transport - theory and by the diffusion - or transport - properties of the composition. Errors in the space dependence of the reactivity coefficient of a specific material may therefore be caused by the errors just mentioned or by errors in the cross sections of this specific material. In this work we do not study space dependent problems; only fundamental mode calculations are performed and results for central reactivity coefficients are derived.

The present work is mainly concerned with item (f), the energy dependence of the real and adjoint neutron flux. Generally, the energy scale is divided into a number of energy groups and the equation governing the energy distribution of the neutron flux is solved in the multigroup formalism. It is evident that a good resolution for the energy dependence of the neutron flux calls for a large number of energy groups. In the following the influence of the energy resolution on calculated central reactivity coefficients of some isotopes and elements will be studied using the multigroup formalism. This can be considered as an extension of an earlier work /5/ /6/; but in the present work we use for the first time a more narrow energy resolution i.e. a larger number of energy groups. Since we are interested mainly in energy dependent effects we confine ourselves to fundamental mode calculations, which are suffient for this purpose. It is well known (see e.g. /6/, /7/ and /7a/) that the reactivity coefficients of predominantly scattering materials are fairly sensitive to the number of energy groups. Therefore in the present study we have mainly in view the reactivity coefficients of these materials.

The main purpose of this study is to get some experience for the possible range of uncertainty which may be inherent to the methods of calculation usually applied for the determination of the reactivity coefficients of predominantly scattering materials. This experience is necessary for a judgement of the reliability of the conclusions drawn from discrepancies between experimental results and those obtained by the usual multigroup calculations.

Especially the conclusions with respect to item (g), the accuracy of the cross sections or group constants for these specific materials, are heavily dependent on the reliability of the calculated reactivity coefficients.

2. Comments on the Formalism

We are considering the fundamental mode eigenvalue equation for the diffusion approximation in the multigroup formalism:

$$(1)\quad D^i \cdot B^2 \cdot \phi_i + \Sigma^i_{rem} \cdot \phi_i = \sum_{j<i} \Sigma^{j\to i} \cdot \phi_j + \frac{1}{k} \cdot \chi^i \cdot \sum_j (\nu\Sigma_f)^j \cdot \phi_j$$

All symbols in this equation have their usual meaning. The buckling B^2 is considered to be independent of the group number which begins with i=1 at the highest neutron energy. Since we are dealing here only with fast reactors, the scattering term includes only the sum of down - scattering terms. If we are considering first order perturbation theory for a critical reactor (k =1) we obtain the following expression for the criticality perturbation caused by an overall change of the composition in the whole reactor system.

$$(2)\quad \delta k_{IRC} = \frac{1}{F} \cdot \Bigg\{ \sum_i \left[\phi_i^+ \cdot \chi^i \right] \cdot \sum_j \left[(\delta \nu \Sigma_f)^j \cdot \phi_j \right] \sum_i \sum_{j<i} \left[\phi_i^+ \cdot \delta \Sigma^{j \to i} \cdot \phi_j \right] - \sum_i \left[\phi_i^+ \cdot \delta \Sigma^i_{rem} \cdot \phi_i \right] - \sum_i \left[\phi_i^+ \cdot \delta D^i \cdot B^2 \cdot \phi_i \right] \Bigg\}$$

In equation (2), ϕ^+ is the adjoint neutron flux, i.e. the solution of that equation which is adjoint to equation (1). The normalization integral F is defined as

$$(3)\quad F = \sum_i \left[\phi_i^+ \chi^i \right] \cdot \sum_j \left[(\nu \Sigma_f)^j \phi_j \right]$$

The integral reactivity coefficient δk_{IRC}, given in equation (2), corresponds to an overall perturbation of the whole system. It is fairly easy to see that omitting the last term, the diffusion part, in equation (2) leads to a reactivity coefficient given in equation (4), which is proportional to the central reactivity coefficient CRC of a perturbation in a reactor for which the energy distribution of the normal and adjoint neutron flux in the core center can be described by equation (1) and its adjoint, respectively.

$$(4)\quad \delta k_{CRC} = \frac{1}{F} \cdot \Bigg\{ \sum_i \left[\phi_i^+ \cdot \chi^i \right] \cdot \sum_j \left[(\delta \nu \Sigma_f)^j \cdot \phi_j \right] \sum_i \sum_{j<i} \left[\phi_i^+ \cdot \delta \Sigma^{j \to i} \cdot \phi_j \right] - \sum_i \left[\phi_i^+ \cdot \delta \Sigma^i_{rem} \cdot \phi_i \right] \Bigg\}$$

The last two terms of equation (4) can be rearranged to give

(4 a)
$$\delta k_{CRC} = \frac{1}{F} \cdot \left\{ \sum_i \left[\phi_i^+ \cdot \chi^i \right] \cdot \sum_j \left[(\delta \nu \Sigma_f)^j \cdot \phi_j \right] \right.$$
$$+ \sum_i \sum_{j<i} \left[(\phi_i^+ - \phi_j^+) \cdot \delta \Sigma^{j \to i} \cdot \phi_j \right]$$
$$\left. - \sum_i \left[\phi_i^+ \cdot \delta \Sigma_a^i \cdot \phi_i \right] \right\}$$

This formula shows more clearly that the moderation - or degradation - term - the double sum in (4 a) - is fairly sensitive to the slope of energy distribution of the adjoint neutron flux.

CRCs are measured frequently in critical fast zero power reactors to determine the material worths of small samples inserted in the core center. Therefore, we will consider in the following only the theoretical results for the CRC of some isotopes and elements, i.e. quantities which can be determined by the application of formula (4) or (4 a), respectively.

3. Details of Calculation

The basic calculations have been done in the 2o8-group structure /9/, which below 1 KeV has the usual Russian ABBN group structure; above 1 KeV each ABBN group is subdivided into 14 fine groups of equal lethargy-width. Since we wanted to get an impression of how accurate the corresponding result in the usual 26-group ABBN structure can be determined, we performed a group collapsing from the 2o8-group to the 26-group structure. For the reason of comparison we collapsed also to some intermediate group structures containing 11o, 61 and 4o groups, respectively. In each case the last 12 groups- below 1 KeV - remained unchanged. This means that we collapsed 2, 4, 7 and 14 fine groups, respectively, to one coarse group; the last step leading to the usual ABBN structure. For collapsing we used in all cases the results of 2o8 group calculations.

We used three different procedures for group collapsing which were already applied in the preceding work /5/ /6/:

(P1): Usual flux weighting, i.e. using only ϕ_{2o8} as weighting function

(P2): Bilinear weighting, i.e. using ϕ_{2o8} and ϕ^{+}_{2o8} as weighting functions

(P3): Combined weighting; i.e. using ϕ_{2o8} for collapsing group constants subsequently used in a few-group calculation for the real flux ϕ_{FG}, using ϕ^{+}_{2o8} for collapsing group constants subsequently used in a few-group calculation for the adjoint flux ϕ^{+}_{FG}, and using bilinear weighting for collapsing group constant differences ($\delta\Sigma_{FG}$) subsequently used in a few-group perturbation calculation, where we used also ϕ_{FG} and ϕ^{+}_{FG} determined in the way just mentioned.

The formulae used for the different group collapsing schemes are the usual ones. They are given, e.g., in the work of PITTERLE /1o/.

For the fundamental mode model applied here the two procedures (P2) and (P3) lead to identical results for the few-group CRCs as is shown in the Appendix and as could also be demonstrated in the calculations except for small purely numerical effects. Furthermore these identical results obtained with both procedures are also in agreement with the corresponding results obtained in the original 2o8-group structure. This fact which is proved in the Appendix too, could also be verified in the numerical results. The small differences of less than at most 2 % which we found in reality are probably due to numerical effects: the moderation - or degration - term in (4 a) is especially sensitive to the limited accuracy of the computer because of the large number of addition operations involved in the double sum particularly with 2o8 groups.

In all three collapsing procedures (P1) - (P3) we use the results of the many-group calculations for the specific problem i.e. ϕ_{2o8} and ϕ^{+}_{2o8}, respectively. We are therefore sure that e.g. in (P1) we are using the correct many-group flux for group collapsing. This gives us an idea of the reliability of the few-group results, e.g. for reactivity coefficients, provided the correct many-group weighting function is exactly known. In reality the few-group constants (e.g. for 26 groups) are prepared for a specific class of reactors, e.g. those using oxide fuel, stainless steel as cladding and structural material and sodium as coolant. For the preparation of these few-group constants a certain weighting function has to be applied. The origin of this weighting function is generally outside the scope of few-group reactor calculations.

Sometimes it is based on a more or less sophisticated decision, e.g. fission spectrum in the high energy range and 1/E - dependence below that range as has been done for the Russian ABBN set. Another possibility consists in using some simplified analytical models for determining the energy distribution as e.g. those mentioned by STACEY /11/ or to use the result of a fundamental mode calculation using an ultrafine-group structure as e.g. provided by MC^2 /12/.

In any case the weighting function can at best be correct for only one specific composition. For each of different compositions the application of the set of group constants is due to some doubt, because for a rigorous treatment new group constants should be used which were generated with a new appropriate weighting function. This procedure is generally not applied because it is rather inconvenient; only for special cases a new weighting function is adopted. For this reason the results for any few-group reactor calculation depend to some extent on the weighting function used for the preparation of the few-group constants. In order to study the effect on the calculated reactivity coefficients we applied for the group collapsing some alternative weighting functions besides the neutron flux which was determined in a many-group calculation for the specific composition considered. In accordance with the usual procedure we used a collision density F as basic function and derived the weighting flux:

$$\phi = F/\Sigma_t$$

where Σ_t is the total macroscopic cross section of the specific composition in a many-group representation.

In this way the resonance behaviour of the correct neutron flux can, at least partially, be approximated.

The results for two collision densities will be discussed in the following: the first one is representative for the central zone of the German prototype fast sodium cooled power reactor and will be labelled SNR-collision density; the second one is similar to the Russian ABBN weighting function and is composed of a fission spectrum above 2.5 MeV and a 1/E - spectrum below 2.5 MeV and will be named χ + 1/E in the following. Both collision densities are given in Fig. 1 as a function of lethargy.

4. Results

Our studies are done for two examples of critical fast zero power reactors: SNEAK-3A2 and ZPR III-48. The first one has already been considered in the preceding work /5/ and /6/. The second one is a well known critical assembly for which many evaluations have been published and which was the basis of an international intercomparison /8/. The atomic number densities used in the calculations are given in table 1. For the buckling we used for both assemblies $B^2 = 25.549 \cdot 10^{-4}$ cm^{-2} which was originally derived for SNEAK-3A2 but is also an acceptable guess for ZPR III-48.

Table 1 Data for SNEAK-3A2 and ZPR III-48 (atomic number densities in $10^{22}/ cm^3$)

	SNEAK-3A2	ZPR III-48
Al	1.2910	0.0109
C	0.0932	2.0767
Cr	0.3647	0.2681
Fe	1.2204	0.9985
H	0.1792	-
Mg	0.0064	-
Mo	0.0039	0.0206
Na	-	0.6231
Ni	0.1854	0.1330
O	1.4529	-
Pu 239	-	0.1645
Pu 240	-	0.0106
Pu 241	-	0.0011
Pu 242	-	0.0004
Si	0.0188	-
Ti	0.0040	-
U 235	0.2031	0.0016
U 238	0.8104	0.7427

Table 2 Central Reactivity Coefficients for SNEAK-3A2

	Number of energy groups	Material										
		Al	C	Fe	H	Mo	Ni	O	U 235	U 238		
CRC per atom normalized to U 235	2o8	-o.216	+o.589	-1.16o	+13.53	-8.528	-1.8o8	+o.327	1oo.	-8.o72		
Contribution of the degradation term to the total CRC	2o8	+o.oo5	+1.232	+o.157	+1.o41	-o.o24	-o.o58	+1.474	-o.oo4	+o.o57		
Weighting function for group collapsing with flux-weighting		Few group CRCs normalized to the corresponding 2o8-group results									$\frac{k_{eff}}{k_{eff\ 2o8}}$	$\frac{l}{l_{2o8}}$
ϕ_{2o8}	11o	o.9944	o.9826	o.995o	o.9991	1.oo24	o.9927	o.9842	1.ooo1	1.oo1o	1.oooo1	o.9999
ϕ_{2o8}	61	o.96o8	o.9446	o.9894	o.9953	1.oo1o	1.oo81	o.9725	1.ooo5	1.oo27	1.oooo1	o.9994
ϕ_{2o8}	4o	o.8624	o.8415	o.977o	o.9866	1.oo13	o.998o	o.9695	1.ooo8	1.oo68	1.oooo2	o.9991
ϕ_{2o8}	26	1.o2o8	o.7216	o.9755	o.9834	1.oo52	1.o58o	1.211o	1.oo2o	1.o212	1.oooo1	o.9976
SNR-collision density/$\Sigma_{t\ 2o8}$	26	o.8729	o.7347	o.9619	o.9722	1.ooo2	1.o1o8	o.9851	1.oo18	1.o326	1.oo24o	1.oo39
$(\chi\ (E) + C/E)/\Sigma_{t\ 2o8}$	26	o.8o66	o.7997	o.96o1	o.9371	o.9961	o.9866	1.o728	o.9961	o.9842	1.oo529	1.oo38

Table 3 Central Reactivity Coefficients for ZPR III-48

	Number of energy groups	Material									
		Al	B1o	B11	C	Cr	Fe	Na	Ni		
CRC per atom normalized to B 1o	2o8	5.66	1ooo.	2.o7	1.27	8.35	11.17	2.81	14.67		
Contribution of the degradation term to the total CRC	2o8	o.7116	o.oo28	o.7134	o.4116	o.5285	o.3541	o.3873	o.o511		
Weighting function for group collapsing		Few-group CRCs normalized to the corresponding 2o8-group results								$\frac{k_{eff}}{k_{eff\ 2o8}}$	$\frac{1}{1_{2o8}}$
ϕ_{2o8}	11o	1.oo87	o.9997	1.o222	1.o361	o.9967	o.9966	1.oo42	o.993o	1.oooo1	o.9997
ϕ_{2o8}	61	o.9845	o.998o	1.o658	1.1363	1.oo27	o.9835	o.9983	1.o324	1.oooo2	o.998o
ϕ_{2o8}	4o	1.o18o	o.996o	1.1348	1.3o55	1.o217	o.9823	o.9242	1.o258	1.oooo2	o.9959
ϕ_{2o8}	26	1.o311	o.9872	1.1251	1.4262	o.9755	o.9958	o.96o4	1.o66o	1.oooo1	o.9895
SNR-collision density/ $\Sigma_{t\ 2o8}$	26	1.o473	o.9873	1.2711	1.5445	1.oo39	o.96oo	1.o781	o.9965	o.99828	o.9864
$(\chi(E) + C/E)/\Sigma_{t\ 2o8}$	26	o.9215	1.oo85	o.7o36	o.5484	o.9598	o.952o	o.7o31	o.9427	1.oo881	1.o14o

In table 2 and table 3 the important results of the present study are given. The magnitude of the CRCs of the various materials can be found in the first line. The values are normalized to U 235 or B 1o, respectively. The CRCs of these materials are fairly large and remain nearly unchanged upon group collapsing irrespective of the weighting-spectrum and collapsing procedure used. For each material the contribution of the degradation term to the total CRC is shown in the second line. As expected the degradation component is small for the predominantly fissioning or absorbing materials. For Al in table 2 and Ni in table 3 it is small because of compensating contributions of different signs and approximately equal absolute magnitude which appear in summing up the contributions of all energy groups.

Using flux weighting, as is done in the next four lines in table 2 and table 3, the deviation between the calculated few-group results for the CRCs and the corresponding original 2o8-group result generally increases with decreasing total number of energy groups used in the few-group calculations.

Using the two other weighting functions for collapsing to 26 groups, the deviation of the few-group results from the corresponding many-group result is qualitatively the same as that obtained when using the exact flux as weighting function for collapsing to 26 groups. This means that the overall shape of the weighting function has not a too pronounced effect on the calculated few-group CRCs.Much more important is the common fact that flux weighting is used for all three cases shown in the last three lines of tables 2 and 3. Bilinear weighting with exact normal and adjoint fluxes, of course, would give 26 group results in agreement with the 2o8 group results as mentioned before and as is shown in the Appendix.

From the results presented in tables 2 and 3 some conclusions can be derived on the reliability or uncertainty which may be expected from few-group (e.g. 26) perturbation calculations for the CRC of a predominantly scattering material using few-group constants prepared by normal flux weighting.

Typical degree of uncertainty attributed to usual few-group CRCs

Material	Al	B11	C	Cr	Fe	Na	Ni	O
Uncertainty	± 2o%	± 3o%	± 5o%	± 5%	± 5%	± 3o%	± 1o%	± 2o%

These uncertainty ranges provide a certain guess for the possible error of theoretical CRCs obtained in 26 group calculations using group constants determined with flux-weighting or flux-collapsing. For structural materials as chromium, iron, or nickel the indicated uncertainty is probably small compared to uncertainties contributed by other effects, as e.g. nuclear data uncertainties or sample size- or heterogeneity-effects. For the predominantly scattering materials, as Al, B11, C, Na or O, the uncertainty of 2o - 5o % caused by the too low number of energy groups for the calculations with usually used flux-weighted group-constants is quite remarkable. In the interpretation of experiments and the discussion of discrepancies between theory and experiment for CRCs of predominantly scattering materials one should be aware of the possibility of such a considerable source of uncertainty.

The reason for obtaining rather poor results in these cases is caused by the fact that the few-group adjoint flux can not be sufficiently well represented when its determination is based on flux-weighted few-group constants. This disadvantage can be eliminated by using bilinear weighted few-group constants as has already been found in the preceding work /6/. Fig. 2 shows the adjoint flux for the assembly ZPR III-48 in the energy range above 1 keV. In addition to the many-group representation, two few-group representations are given. That one obtained by using bilinear weighted few-group constants corresponds exactly to the values derived from the many-group representation by averaging within the few-group structure, whereas the other one, obtained by using flux weighted few-group constants, deviates to a considerable extent from these average values, especially in the energy range below 4oo keV as can be seen from Fig. 2. The differences are generally less

than about 5 %. In accordance with this, the differences in the 26 group results for the neutron lifetime and for the reactivity coefficients of fissile and absorber materials when determined with flux weighted constants are generally less than 2 % compared to the corresponding 2o8 group results.

In order to explain the much larger differences in the reactivity coefficients of scattering materials we have shown in Fig. 3 the differences in the 26 group adjoint neutron flux between adjacent energy groups (i.e. $\Delta\phi_I^+ = \phi_{I+1}^+ - \phi_I^+$). These differences are important for the contribution of the moderation term to the reactivity coeffient as can be seen from Eq. (4a). In addition to the exact values ($\Delta\phi_I^+$, exact = $\Delta\phi_I^+$, bilinear weighted group constants) obtained from the adjoint flux determined with bilinear weighted constants we have also shown in Fig. 4 the deviations from these exact values which are due to using the adjoint flux from calculations with flux weighted constants. These deviations D_I^+ (i.e. $D_I^+ = \Delta\phi_I^+$, bilinear weighted group constants - $\Delta\phi_I^+$, flux weighted group constants) are rather large compared to the basic values $\Delta\phi_I^+$ itself. Especially in the groups below about 1 MeV the absolute magnitude of the deviations is frequently half as large as the absolute magnitude of the basic values. Therefore, it is not surprising that the moderation term and consequently also the reactivity coefficients of predominantly scattering materials can only be determined within 5o % uncertainty if flux weighted few-group constants are applied in the corresponding calculations. One possible way to avoid this difficulty or at least to reduce its importance could probably consist in using fairly accurate approximations for the weighting functions each time when few group constants for a specific reactor configuration have to be established. In this respect the continuous slowing down theory of STACEY /11/ and particularly the approximations given by DUNN and BECKER /13/ in the form of analytic representations for the fast reactor normal and adjoint flux are helpful indications in which way it may be possible to obtain sufficiently accurate approximations for the energy-dependent weighting functions without consuming too much computer time.

Attention should also be given to another fact which can be deduced from the results of the present study: If the CRC of a material has a negative sign then the reactivity coefficient of an extended sample or the reactivity effect in an off-center position may have even a larger relative uncertainty than indicated before, because of the positive contribution of the diffusion term which can be omitted in our calculations of CRCs. In particular, the correct spatial position of the change of sign of the space dependency of the reactivity coefficient may be affected by this increased uncertainty-range. For fast power reactors this fact may be important for the precise determination of the spatial area in which the sodium void coefficient has a positive sign.

As already discussed by PITTERLE /1o/, bilinear averaging should be preferred to flux averaging also in those cases where the weighting functions are not known exactly. This suggestion has been checked in the present work for a few test cases using as weighting functions the normal and adjoint fluxes of the SNR composition. In addition to the collision density weighting F_{SNR}/Σ_{tot}, where Σ_{tot} is the fine group representation of the total cross section of the specific mixture considered, we have tried for group collapsing to 26 groups in a few cases two different weightings: using ϕ_{SNR} and using both ϕ^{+}_{SNR} and ϕ_{SNR}; i.e. flux weighting with the fine group fluxes for the SNR-composition and bilinear weighting using fine group fluxes and adjoints for the SNR-composition. In almost all cases studied the results for k_{eff}, l and CRCs obtained with the F_{SNR}/Σ_{tot} weighting have been found to be slightly superior to the results obtained with the two other weighting functions. The results with these two latter weighting functions have been found fairly similar. It was particularly interesting for us to note that using approximate weighting functions practically no improvement could be obtained when using bilinear weighting (i.e. ϕ^{+}_{SNR} and ϕ_{SNR}) instead of flux-weighting (i.e. ϕ_{SNR}) for the quantities considered here namely k_{eff}, l and CRCs.

This somewhat surprising fact is illustrated in the following table 4

Table 4 — 26 group results obtained by group collapsing, normalized to the corresponding basic 2o8 group results.

weighting functions	ASSEMBLY						
	SNEAK 3A2				ZPR III-48		
	Quantity				Quantity		
	k_{eff}	1	CRC(C12)	CRC(O16)	k_{eff}	1	CRC(C12)
F_{SNR}/Σ_t	1.oo24	1.oo39	o.7347	o.9851	o.9983	o.9864	1.5445
ϕ_{SNR}	1.oo16	o.9945	o.6344	1.1163	o.998o	o.966o	1.5767
$\phi_{SNR'}^{+}/\phi_{SNR}$	1.oo58	o.9946	o.6498	1.1847	o.998o	o.97o6	1.4258

The reason for obtaining essentially no improvement upon using bilinear weighting instead of flux weighting when the weighting functions are only approximately known is that the approximate adjoint flux is in our case fairly dissimilar to the correct adjoint flux if one considers its fine-group energy dependence within one coarse group of the 26 group structure (the global energy dependence of both, of course, shows some similarity).

This means that using an adjoint flux which is a too crude approximation to the correct one, one can not expect any considerable improvement compared to taking an adjoint flux equal to unity which is equivalent to the usual flux weighting.

In Fig. 5 are compared the adjoint fluxes obtained for the central zone of the SNR and for the assembly ZPR III-48. In each of the 14 coarse groups the adjoints are normalized to unity so that the different energy dependence within one coarse group becomes evident, especially the discrepant behaviour in the coarse groups 6 - 1o, i.e. in the energy range 2o keV- 1 MeV which is most important in fast reactor calculations. Fig. 6 shows the analogous comparison between the adjoint fluxes for the central zone of the SNR and for SNEAK-3A2. Both figures demonstrate that with respect to collapsing to coarse groups, ϕ^+ (SNR) is fairly dissimilar to both ϕ^+ (ZPR III-48) and ϕ^+ (SNEAK-3A2). This is in accordance with the results presented in Table 4 that practically no improvement could be obtained by using the approximate weighting function ϕ^+ (SNR) for collapsing of group constants subsequently used for the calculation of ZPR III-48 and SNEAK-3A2, respectively.

One may expect that the superiority of bilinear weighting compared to normal flux weighting becomes more apparent if the number of energy groups in the few-group scheme is further reduced, i.e., using less than 26 coarse groups. Fig. 7 shows that above about 1 MeV the global behaviour of the three adjoints is fairly similar whereas below 1 MeV the energy dependence is quite different. Therefore we tried to collapse the energy range above o.8 MeV into one coarse group. Together with the normal ABBN group structure below o.8 MeV this leads to a total of 22 groups.

Table 5 22 group results obtained by group collapsing normalized to the corresponding basic results.

weighting function	ASSEMBLY						
	SNEAK-3A2				ZPR III-48		
	Quantity				Quantity		
	k_{eff}	l	CRC (C12)	CRC (O16)	k_{eff}	l	CRC (C12)
ϕ_{SNR}	1.0004	0.9994	0.5601	0.7665	0.9972	0.9700	2.0201
$\phi_{SNR}, \phi^{+}_{SNR}$	1.0057	0.9973	0.6616	1.2261	0.9977	0.9728	1.4815

The results presented in Table 5 indicate that in this case bilinear weighting indeed is superior to the normal flux weighting. The 22 group results with bilinear weighting in this case show approximately the same deviations from the 2o8-group results as those obtained for the 26 group results presented in Table 4 whereas with normal flux weighting the 22 group results, as could be expected, show larger deviations from the corresponding 26 group results, which leads to an increasing disagreement with the original 2o8 group results for the reactivity coefficients.

These results underline the condition that the approximate adjoint weighting functions have to be fairly similar to the correct adjoint weighting functions in order to obtain improved results with bilinear weighting when approximate weighting functions are used.

We have also studied the merits of the combined weighting, which is also sometimes called consistent weighting (see e.g.

GREENSPAN /14/). Table 6 shows the results for some fairly sensitive quantities obtained by collapsing from 2o8 to 26 groups. As before, we have used the approximate weighting functions for the SNR composition. No major improvements can be found compared to both normal flux- and bilinear- weighting. This result is not in agreement with that one obtained by GREENSPAN. The reason is probably that, contrary to GREENSPAN, we have used rather crude approximations for the weighting functions which are fairly dissimilar to the correct weighting functions for the two compositions studied. Especially the adjoint fluxes show a remarkably different energy dependence below about 1 MeV as discussed before. This is, e.g., illustrated by the fact that using ϕ^{+}_{SNR} as weighting function for adjoint weighting within the procedure of combined weighting we obtained rather poor results for the criticality in the subsequent 26-group calculations for the coarse-group adjoint flux: for SNEAK-3A2 we are off by about 1.4 %, for ZPR III-48 by about o.3 %. Both deviations are larger than the corresponding values with flux- and bilinear weighting.

Table 6 26 group results obtained by flux-, bilinear- and combined-weighting, normalized to the corresponding basic 2o8-group results.

weighting	A S S E M B L Y						
	SNEAK-3A2				ZPR III-48		
	k_{eff}	1	CRC (C12)	CRC (O16)	k_{eff}	1	CRC (C12)
Flux	1.oo16	o.9945	o.6344	1.1163	o.998o	o.966o	1.5767
BILINEAR	1.oo58	o.9946	o.6498	1.1847	o.998o	o.97o6	1.4258
COMBINED		o.9844	o.5611	o.9557		o.97o1	1.3956

5. Summary

The results of this work indicate that the usual 26 group calculational procedure for determining reactivity coefficients in fast reactors may lead to appreciable deviations from more refined treatments with better energy resolution. This statement especially holds for predominantly scattering materials such as structural materials or the coolant material sodium. Deviations of 3o - 4o % have been obtained for C12 if the appropriate normal flux weighting is used to prepare the group constants for the 26-group scheme. It has been shown that these deviations are essentially due to discrepancies in the adjoint flux obtained with flux weighted coarse group constants.

In those cases where the appropriate weighting flux is not known precisely and an approximate weighting flux has to be used instead of the correct one, the deviation may become even larger. The central sodium void coefficient may become inaccurate by about 3o % in that case.

If the appropriate normal and adjoint weighting functions are available, bilinear weighting turns out to become highly preferable compared to normal flux weighting.

If the normal and adjoint weighting functions are not known accurately and some approximate functions must be taken instead of the correct ones, bilinear weighting does not generally lead to improved results. Only if the approximate adjoint function is fairly similar to the correct one, some improvement may be expected by using bilinear weighting.

The same statements apply to a modified weighting procedure, called combined or consistent weighting, which has the additional drawback, compared to flux- or bilinear-weighting, that three different sets of coarse group constants have to be established and handled for the coarse group calculations.

As a conclusion of the present work we have found that one has to be cautious in the interpretation of calculated results for reactivity coefficients of predominantly scattering materials in fast reactors and eventual discrepancies to corresponding experimental results because the usual 26 group calculational procedure may not in all cases be considered to be sufficiently reliable as has been shown in the preceding chapters.

6. Appendix

Comparison of the collapsing procedures (P2) and (P3) and comparison of the derived few-group results with the corresponding many-group results in the case of fundamental mode calculations.

The following considerations and conclusions can partially be found in the work of PITTERLE /1o/ too. They are included here for the sake of a complete and comprehensive presentation. We start from equation (A1) and its adjoint (A 1a) which are considered as many-group (MG) representation for the following.

(A1)

$$D^i \cdot B^2 \cdot \phi_i + \Sigma_t^i \cdot \phi_i = \sum_j \Sigma^{j\to i} \cdot \phi_j + \frac{1}{k} \cdot \chi^i \cdot \sum_j (\nu\Sigma_f)^j \cdot \phi_j$$

(A1a)

$$D^i \cdot B^2 \cdot \phi_i^+ + \Sigma_t^i \cdot \phi_i^+ = \sum_j \Sigma^{i\to j} \cdot \phi_j^+ + \frac{1}{k} \cdot (\nu\Sigma_f)^i \cdot \sum_j \chi^j \cdot \phi_j^+$$

These forms are more general than equation (1) and can be handled easier in the following, because the in-group scattering is included on both sides of the equation but has been omitted in order to obtain equation (1). By collapsing to fewer groups we obtain the analogous few-group (FG) representation:

(A2)

$$D^I \cdot B^2 \cdot \phi_I + \Sigma_t^I \cdot \phi_I = \sum_J \Sigma^{J\to I} \cdot \phi_J + \frac{1}{k_{FG}} \cdot \chi^I \cdot \sum_J (\nu\Sigma_f)^J \cdot \phi_J$$

(A2a)

$$D^{+I} \cdot B^2 \cdot \phi_I^+ + \Sigma_t^{+I} \cdot \phi_I^+ = \sum_J \Sigma^{+I\to J} \cdot \phi_J^+ + \frac{1}{k_{FG}^+} \cdot (\nu\Sigma_f)^{+I} \cdot \sum_J \chi^{+J} \cdot \phi_J^+$$

We assume for the following that the number of coarse groups is larger than one because for only one coarse group it is no longer meaningful to speak of a few-group formalism. This case would correspond to the case of mono-energetic neutrons, so that some of the following considerations especially with respect to degradation - or moderation effects are no longer applicable as is e.g. mentioned in /7a/.

The criticality values in (A2) and (A2a) have been given an index to indicate that they are representative of the FG result. Furthermore they are distinguisted from each other, because it is not evident a priori that they should be identical. The same applies to the FG constants.

Using the MG fluxes and adjoints we define the following usual FG quantities which are correct in the sense that they correspond to the correct integral and average values, respectively, of the MG results.

(A3)

$$\tilde{\phi}_I = \sum_{i \varepsilon I} \phi_i ;$$

(A3a)

$$\tilde{\phi}_I^+ = \sum_{i \varepsilon I} \phi_i^+ \cdot \Delta u_i \; / \sum_{i \varepsilon I} \Delta u_i$$

(The summation is extended over all groups i which are collapsed into the coarse group I; Δu_i is the lethargy width of group i)

Using the collapsing procedure (P2) with bilinear weighting we obtain the following definitions of the FG constants (see also e.g. /1o/):

$$
(A4)\begin{cases}
D^I = D^{+I} = \sum\limits_{i\varepsilon I} \phi_i^+ \cdot D^i \cdot \phi_i \;/\; \tilde{\phi}_I^+ \cdot \tilde{\phi}_I \\
\Sigma_t^I = \Sigma_t^{+I} = \sum\limits_{i\varepsilon I} \phi_i^+ \cdot \Sigma_t^i \cdot \phi_i \;/\; \tilde{\phi}_I^+ \cdot \tilde{\phi}_I \\
\chi^I = \chi^{+I} = \sum\limits_{i\varepsilon I} \chi^i \cdot \phi_i^+ \;/\; \tilde{\phi}_I^+ \\
(\nu\Sigma_f)^I = (\nu\Sigma_f)^{+I} = \sum\limits_{i\varepsilon I} (\nu\Sigma_f)^i \cdot \phi_i \;/\; \tilde{\phi}_I \\
\Sigma^{J\to I} = \Sigma^{+J\to I} = \sum\limits_{j\varepsilon J} \sum\limits_{i\varepsilon I} \phi_i^+ \cdot \Sigma^{j\to i} \cdot \phi_j \;/\; \tilde{\phi}_I^+ \cdot \tilde{\phi}_J
\end{cases}
$$

Inserting these definitions into (A2) and (A2a) it can be easily verified that these eigenvalue-equations are satisfied if

$$
(A5)\begin{cases}
k_{FG} = k_{FG}^+ = k \\
\text{and} \\
\phi_I = \tilde{\phi}_I \text{ and } \phi_I^+ = \tilde{\phi}_I^+
\end{cases}
$$

This means that for the fundamental mode problem the collapsing procedure (P2) with the above mentioned definitions (A4) of the FG constants leads to solutions of the FG equations which produce:

a) an eigenvalue identical to that of the MG equation.
b) neutron fluxes and adjoints which agree with those collapsed from the original MG solutions.

This equivalence of both collapsing procedures of course is only valid, if the exact solutions in the MG-representation have been determined in advance and are then used as weighting functions for group collapsing.

Using the collapsing procedure (P2) for the generation of the FG constants it is fairly easy to see that the FG reactivity coefficients defined in an analogous manner to equations (2) to (4a) are in exact agreement with the corresponding quantities obtained in the original MG representation: because of the definitions given in (A4) and the equivalence established in (A5), each term in the FG-representation of the reactivity coefficient is in exact agreement with the corresponding term in the MG-representation. Therefore, as should be demonstrated, the FG-reactivity coefficient is equal to the corresponding MG-reactivity coefficient provided the collapsing procedure (P2) is applied for the generation of the FG-constants.

It is also fairly easy to show that for the fundamental mode problem both collapsing procedures (P2) and (P3) lead to identical results for the FG-reactivity coefficients:

The collapsing procedure for the group constant differences ($\delta \Sigma_{FG}$) in the FG-representation is identical in both cases. The flux weighting for the FG-constants used for the calculation of the FG-neutron flux ϕ_{FG} corresponds to taking $\phi_i^+ = 1$ in (A4) and (A3a). As is plausible from physical reasons, and can be shown easily in a rigorous manner, the flux determined as solution of the FG-equation using the FG-constants derived in the above mentioned collapsing procedure is equal to the corresponding result obtained upon collapsing the original MG solution for the neutron flux. It should be pointed out, however, that the FG-constants obtained by flux-weighting are definitely different from those obtained by the bilinear weighting procedure (P2) and furthermore, although the FG-flux agrees with that obtained using bilinear weighting,

the corresponding FG-adjoint generally is definitely different in the two cases. Therefore the adjoint obtained upon using flux-weighted FG-constants in the adjoint FG equation does no longer agree with the average of the corresponding MG result as defined in (A3a).

The adjoint flux weighting is similar to the flux-weighting just mentioned and corresponds to taking $\phi_i = \Delta u_i$ in equations (A4) and (A3). In the same way as for the flux-weighting it can be shown that the FG adjoint flux obtained as solution of the FG adjoint equation using the FG-adjoint weighted constants is equal to the corresponding result obtained upon collapsing the MG result according to (A3a). In general the FG adjoint weighted constants are different from both the flux weighted and the bilinear weighted few-group constants. The FG flux obtained as solution of the normal FG equation using adjoint weighted FG-constants generally differs from the corresponding result (A3) of the MG representation.

Summarizing the results presented in the Appendix we have shown that for the fundamental mode problem:

a) the two collapsing procedures (P2) and (P3) lead to the same results with respect to the few-group results for the normal and adjoint neutron flux and for the reactivity coefficients
b) these few group results, just mentioned, are in exact agreement with those considered to be correct because they are derived directly from the corresponding many-group solution.
c) as could be expected the three different kinds of collapsing using normal flux, adjoint flux and bilinear weighting, respectively, yields different results for the few-group constants

d) the solution of the adjoint few-group equation with flux weighted constants does provide an adjoint flux which is not in agreement with the corresponding correct result obtained by collapsing the many-group adjoint flux
e) the analogous statement holds for the solution of the normal few-group equation with adjoint weighted constants which does not agree with the corresponding correct flux obtained by collapsing the corresponding many-group solution
f) the bilinear weighting, however, produces the correct normal and adjoint few-group fluxes.

It should be stressed, however, that bilinear weighting is not the appropriate procedure, if few-group reaction rates are to be determined accurately. This has already been reported, e.g., in /6/ and /10/. In this case, normal flux weighting of course will provide the best results. This statement is valid only for the collapsing procedures considered here. However, using specially suited adjoint functions as is done in generalized perturbation theory and in variational methods (see e.g. /15/), it is possible to achieve collapsing procedures which are superior to normal flux weighting for the special purpose of determining reaction rates or reaction rate ratios in few-group calculations.

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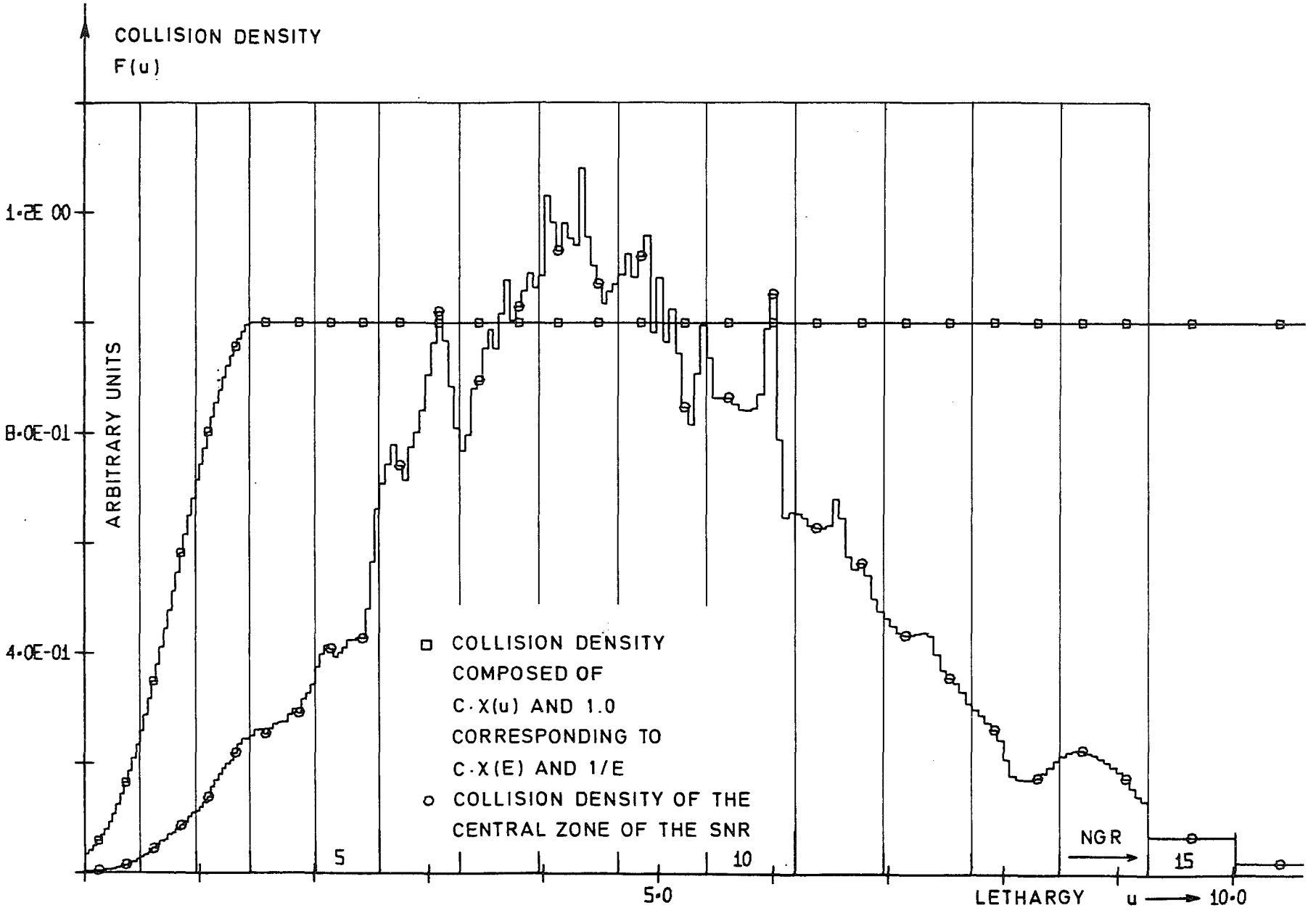

Fig.1: Comparison of different collision densities

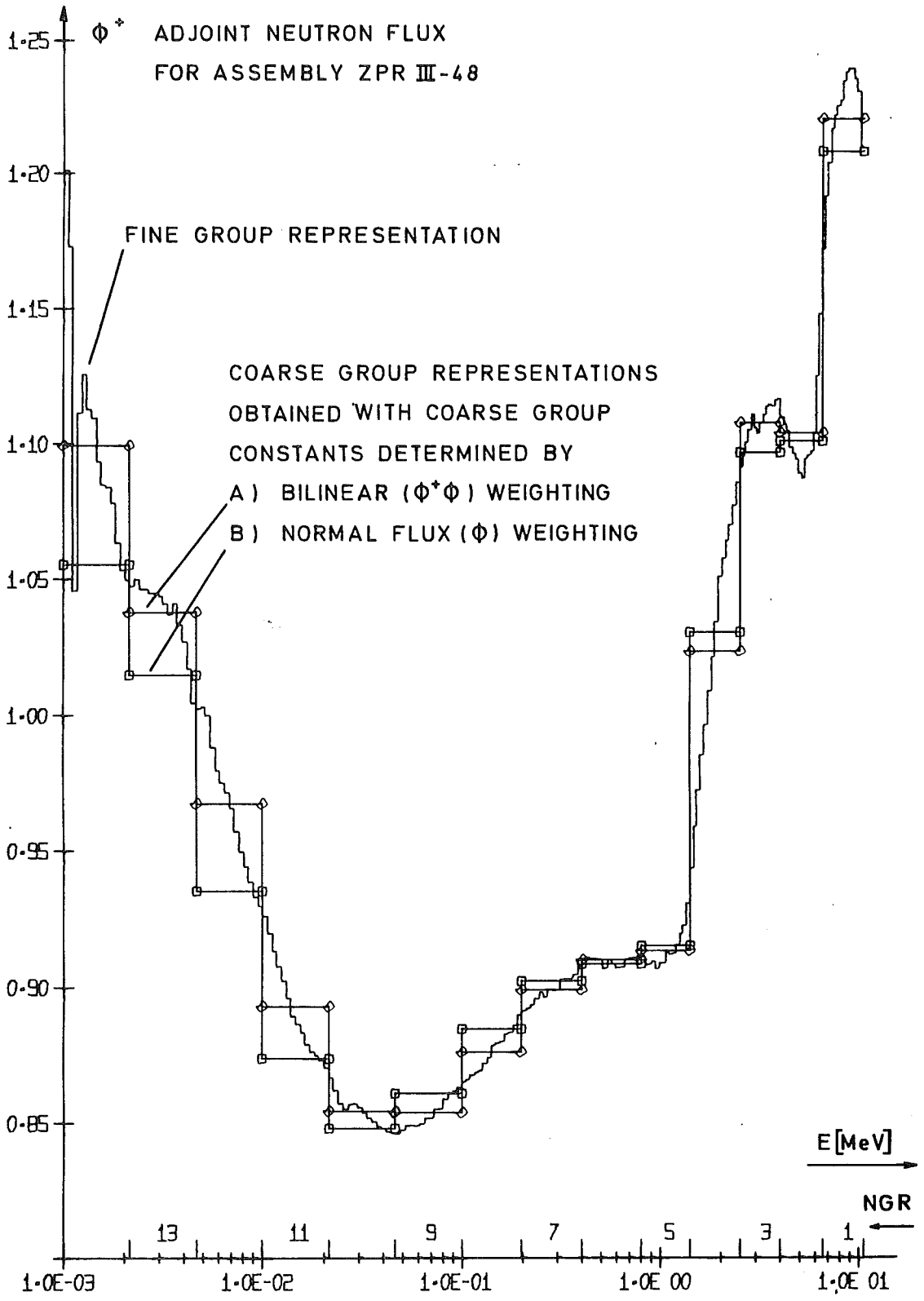

Fig. 2: Energy dependence of adjoint neutron fluxes

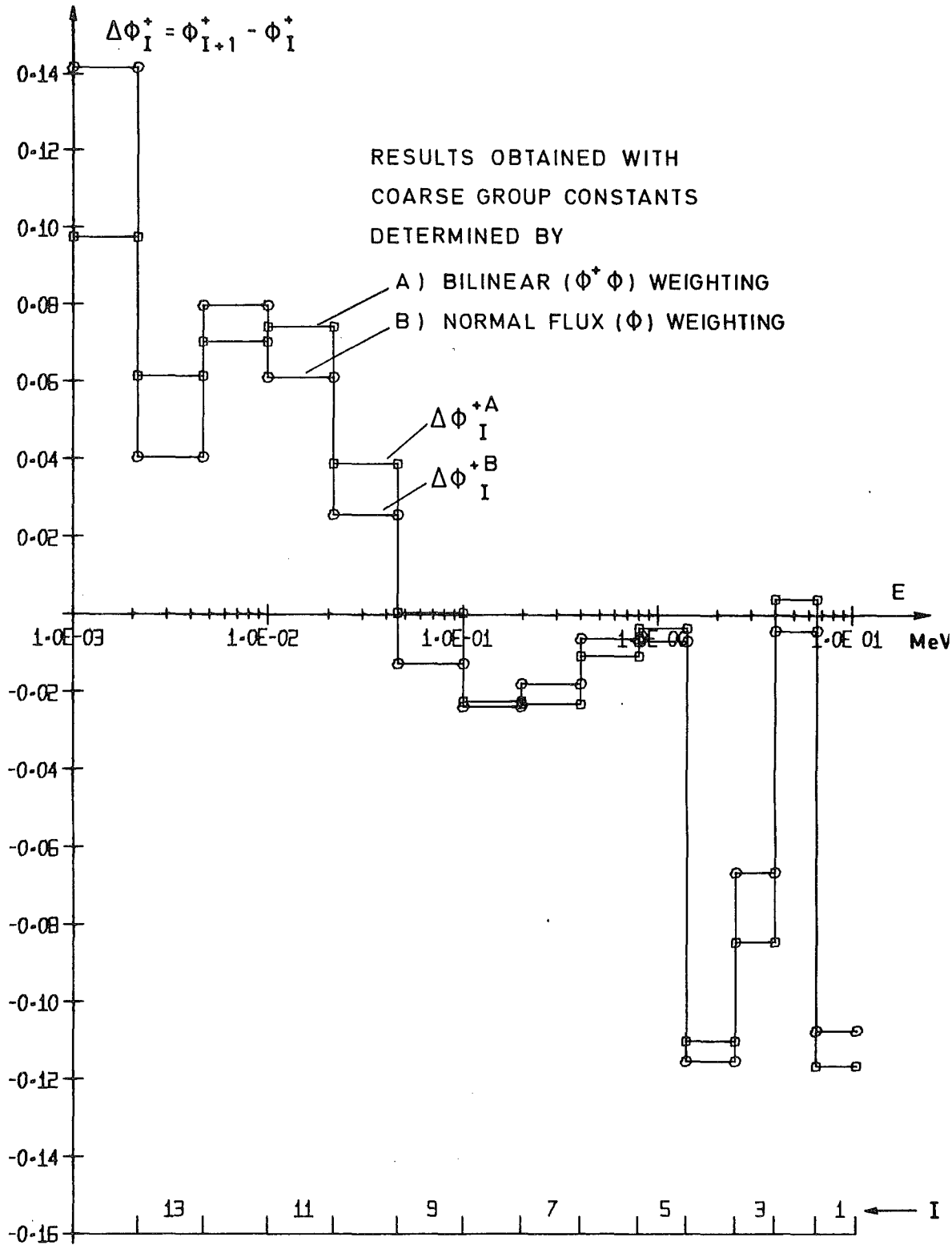

Fig. 3: Differences of adjoint fluxes

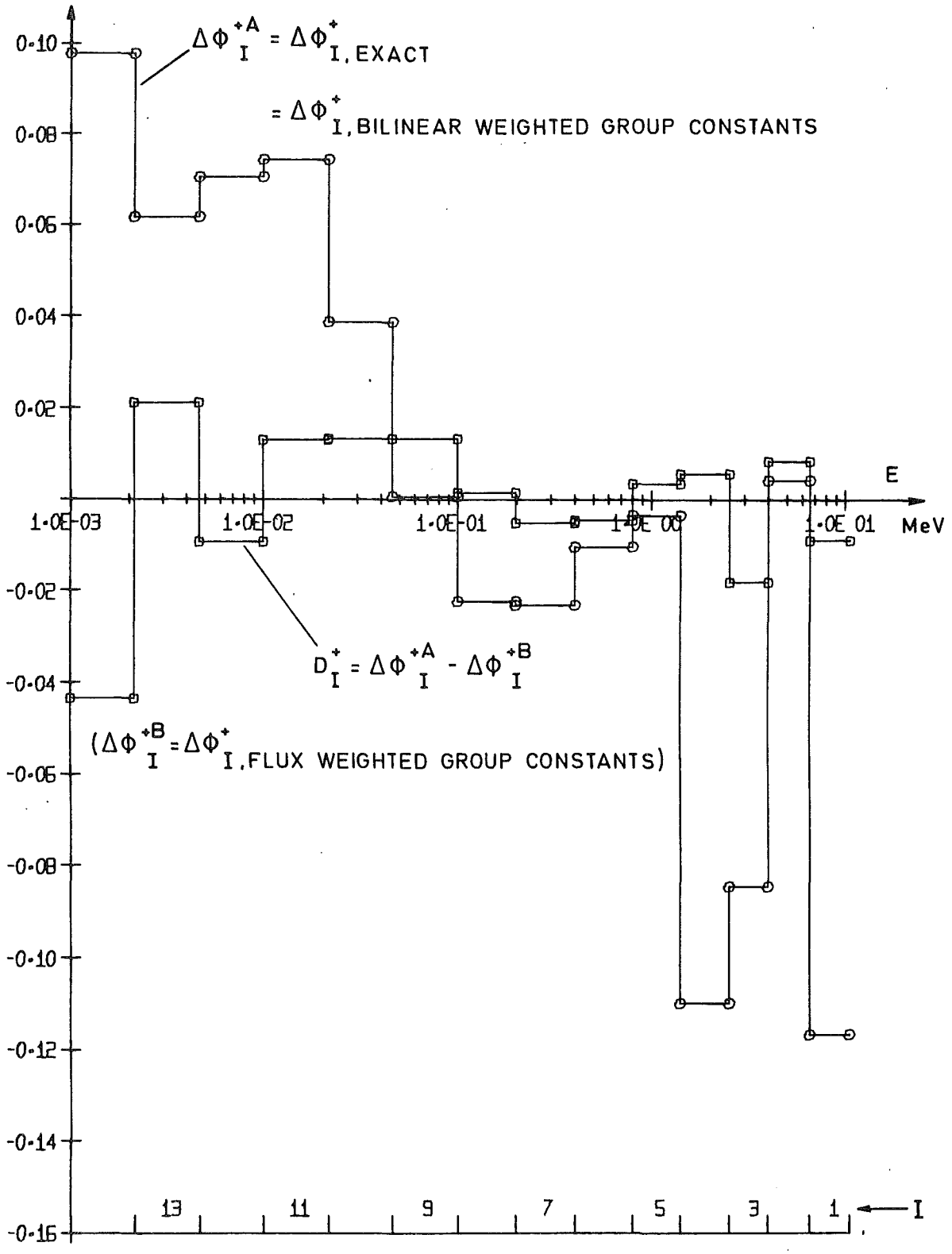

Fig. 4 : Comparison of adjoint flux differences

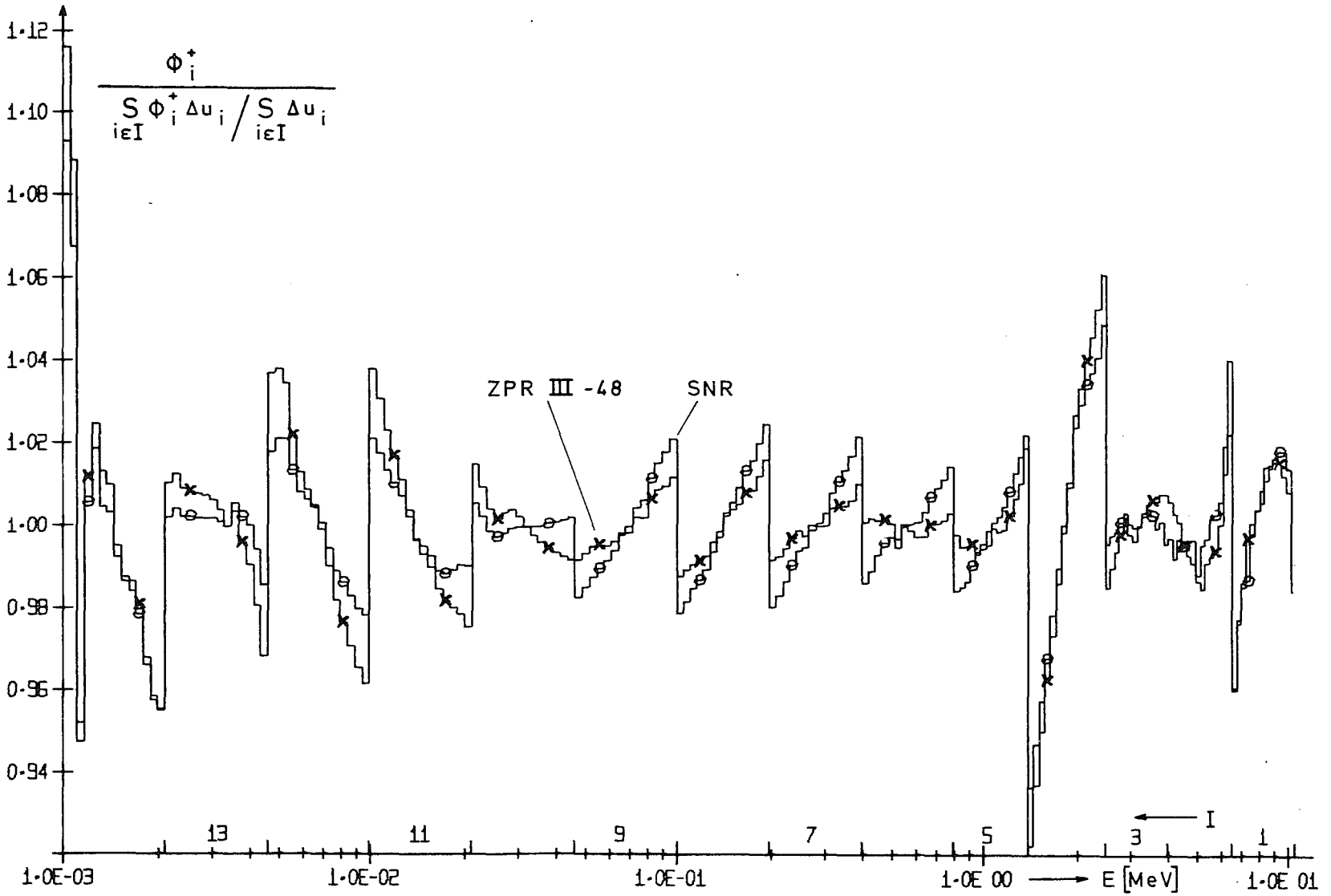

Fig. 5: Fine group adjoints, normalized to unity in each coarse group I

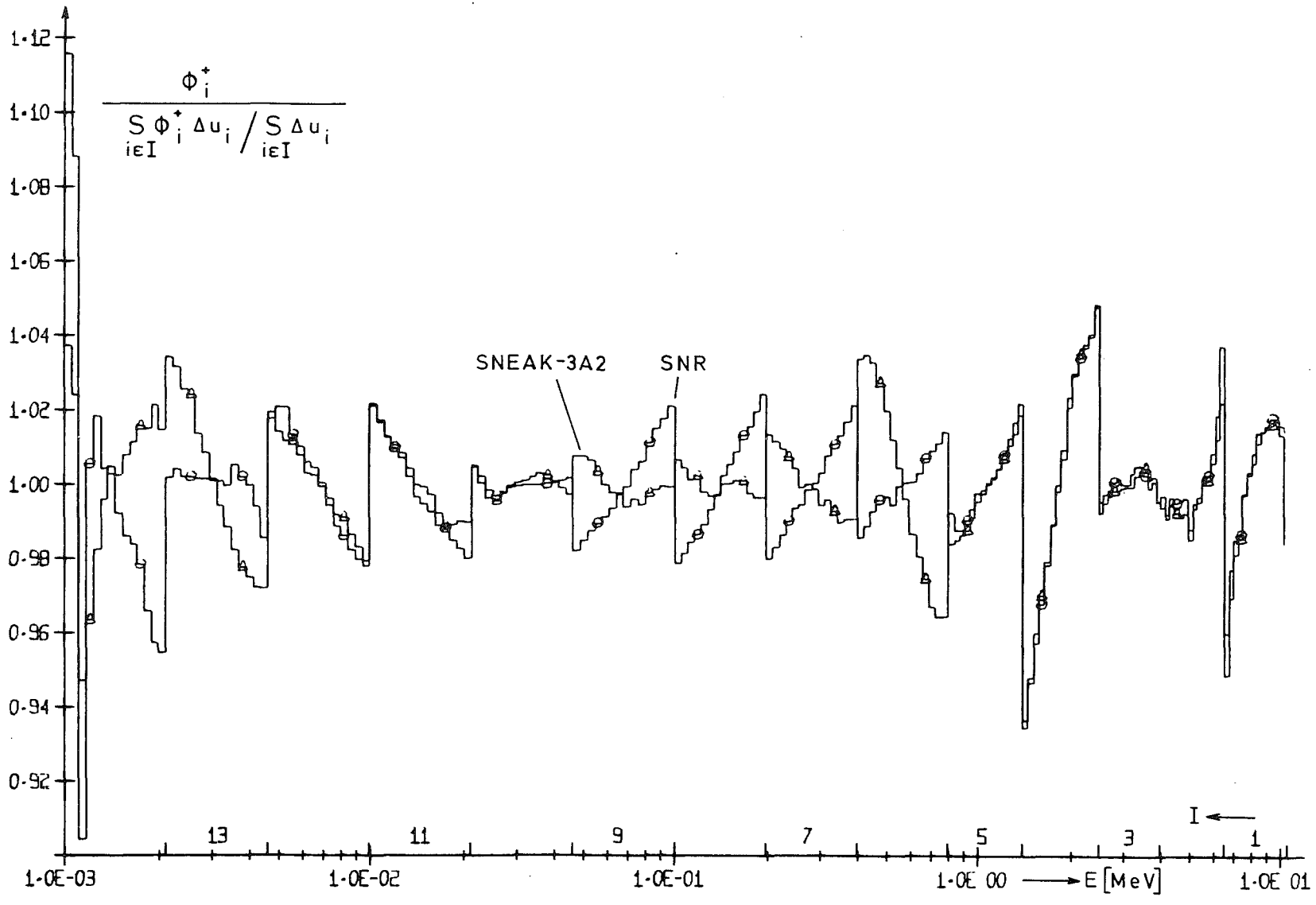

Fig. 6: Fine group adjoints, normalized to unity in each coarse group I

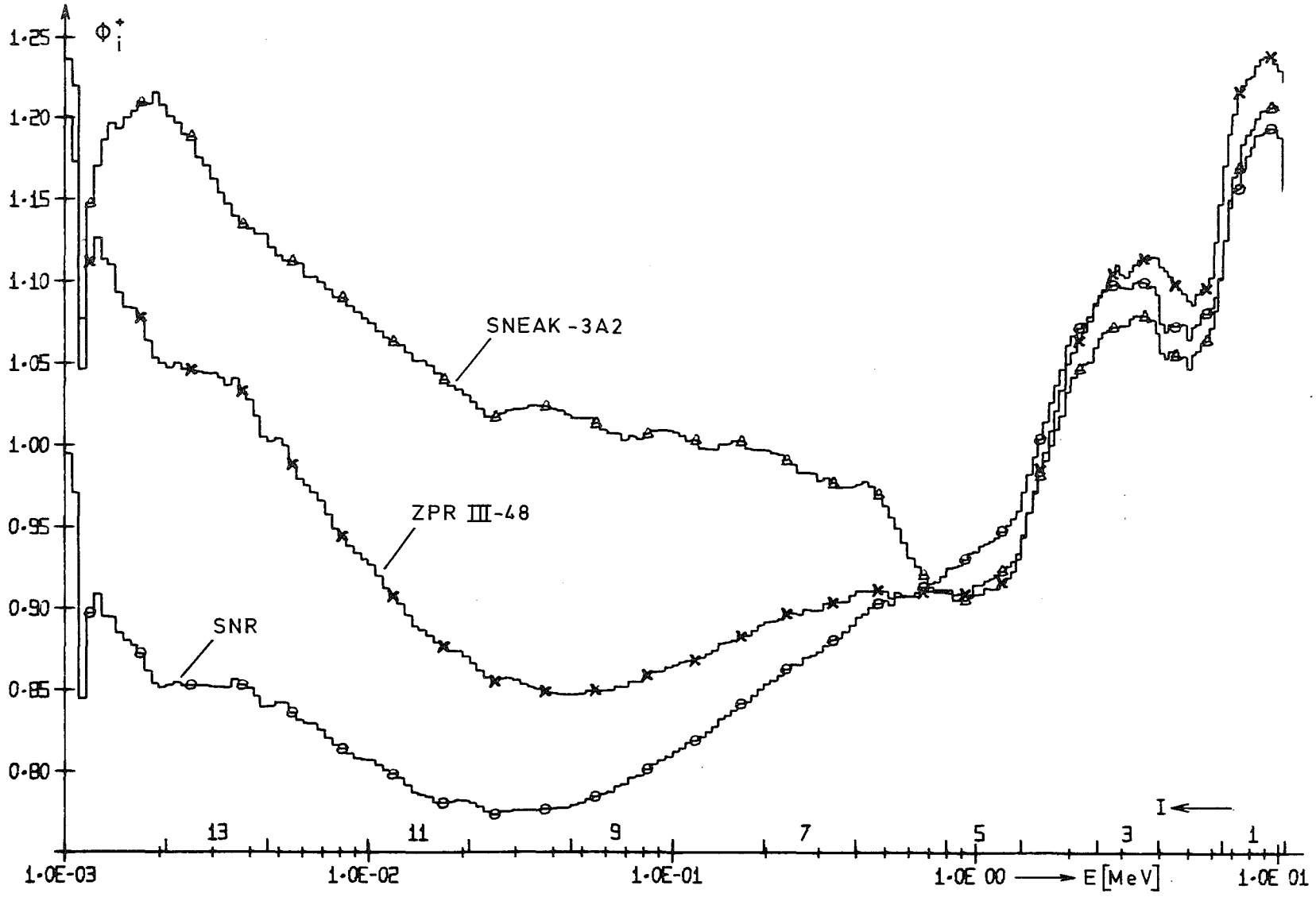

Fig. 7: Fine group representation of adjoint fluxes for SNR, ZPR III-48, SNEAK-3A2