Application of Real, Adjoint and Bilinear Weighting for Collapsing Group Constants Used in Space Dependent Neutron Diffusion Problems

E. Kiefhaber
Institut für Neutronenphysik und Reaktortechnik
Projekt Schneller Brüter

Kernforschungszentrum Karlsruhe

KERNFORSCHUNGSZENTRUM KARLSRUHE

Institut für Neutronenphysik und Reaktortechnik

Projekt Schneller Brüter

KfK 3430

Application of Real, Adjoint and Bilinear
Weighting for Collapsing Group Constants Used
in Space Dependent Neutron Diffusion Problems

Edgar Kiefhaber

Abstract

Conventional collapsing for group cross sections used in multigroup
nuclear reactor calculations is usually performed using normal (real;
direct) flux weighting. The application of more advanced collapsing proce-
dures using in an appropriate manner real, adjoint and bilinear weighting
was in the past restricted in general to fundamental mode problems.
Although the principles have been published for more than ten years, there
seems to exist little recent experience on the merits and possible diffi-
culties of these improved procedures for multidimensional diffusion
problems for practical purposes, e.g. in the nuclear design and analysis
of large Liquid Metal Fast Breeder Reactors (LMFBRs). The present work
indicates the nature of the problems which could possibly be encountered
in applying these procedures by tracing them back to the known close
correspondence between group collapsing and synthesis methods. It tries to
explain certain somewhat unusual features of the collapsed group constants
obtained by adjoint and bilinear weighting and describes the experience
gained in representative 1-dim. and 2-dim. test cases. It could be shown
for criticality and perturbation calculations that in general it is
advantageous to apply these improved collapsing methods if the necessary
precautions are taken. The possible disadvantages seem to be only minor
and the associated complications are considered to be tolerable. Compared
to the conventional collapsing procedures these improved procedures are
especially useful for multidimensional problems because their application
is well suited for that purpose. In the present study it could be proven
that they are favorable with respect to computer time and storage needed
due to the fact that the necessary number of coarse groups can be kept
fairly small without deteriorating too much the accuracy and reliability
of the coarse group results compared to reference results of corresponding
fine group calculations with uncollapsed group constants.

Anwendung von realer, adjungierter und bilinearer Wichtung zur Kondensation
von Gruppenkonstanten für ortsabhängige Neutronendiffusionsprobleme

Zusammenfassung

Bei der üblichen Kondensation von Multigruppen-Wirkungsquerschnitten für
nukleare Reaktorrechnungen wird in den meisten Fällen die normale (reale,
direkte) Flußwichtung benutzt. Die Anwendung verbesserter Methoden, bei
denen z. B. in angemessener Weise reale, adjungierte und bilineare Wich-
tung verwendet wird, war in der Vergangenheit häufig auf nulldimensionale
(ortsunabhängige) Probleme beschränkt. Ortsabhängige Probleme wurden
anscheinend in den letzten Jahren kaum mit solchen Methoden behandelt,
obwohl die Grundlagen, Vorteile und möglichen Schwierigkeiten seit langer
Zeit bekannt und veröffentlicht sind. Die vorliegende Arbeit versucht, auf
der Basis der bekannten Beziehungen zwischen der Gruppen-Kondensation und
den Synthesemethoden, die Besonderheiten dieser Methoden, sowie insbeson-
dere einige ungewohnte Eigenschaften der adjungiert und bilinear gewichte-
ten Querschnitte zu erläutern. Anhand repräsentativer 1- und 2-dimensiona-
ler Testfälle für Schnelle Natriumgekühlte Reaktoren wird gezeigt, daß es
bei entsprechend sorgfältigem Vorgehen sehr vorteilhaft ist, diese fort-
schrittlichen Wichtungsmethoden für Kritikalitäts- und Störungsrechnungen
anzuwenden. Im Vergleich zu konventionellen Wichtungsmethoden sind sie
gerade bei mehrdimensionalen Problemen besonders nützlich, da sie eine
deutliche Verringerung der Gruppenzahl zulassen und dementsprechend Ein-
sparungen an Rechenzeit und Speicherbedarf bewirken, ohne die Genauigkeit
und Zuverlässigkeit in merklichem Ausmaß nachteilig zu beeinflussen.

Table of Contents

I) <u>Introduction</u>

Group collapsing is a well established procedure in nuclear reactor calcu-
lations. Its mathematical foundation and derivation has been presented by
several authors (see e.g. /1/ - /4/) on the basis of synthesis methods.
Usually the weighting functions - which can be considered as some kind of
trial functions in the synthesis approach - are taken from solutions of
simplified problems which are (or are expected to be) similar to the geome-
trically more complex problem actually to be solved. In most cases normal
collapsing is applied, i.e. the many group weighting functions which are
taken to collapse fine group or many group cross sections to fewer, so-
called coarse group cross sections represent real (also called direct or
normal or forward) fluxes. The usefulness and quality of coarse group
cross sections determined in this way depend heavily on the quality of the
weighting functions, i.e. whether or not they are sufficiently good
approximations to the desired solution of the problem to be treated.

Besides this frequently used normal collapsing or conventional condensa-
tion procedure, basically corresponding to real flux collapsing, there
exist other collapsing possibilities which are characterized by the nature
of the corresponding weighting functions, namely adjoint flux collapsing
and bilinear collapsing, which uses both real and adjoint fluxes. These
less usual collapsing procedures have special advantages and require
special attention because some of their features and those of the desired
coarse group cross sections are rather strange and not in accordance with
the relations usually encountered in real flux group collapsing and valid
for group cross sections derived on the basis of usual real flux
collapsing.

In the past, the application of these unconventional procedures was mainly
restricted to fundamental mode problems, where the space dependence has
not to be taken into account explicitly. Thus, the experience with these
procedures for space dependent problems is somewhat restricted, although
they offer - at least in principle - certain favorable aspects with
respect to increased accuracy and reliability of nuclear calculations and
with respect to a reduction of the necessary computing time spent for such
calculations.

One additional aspect should be mentioned, namely that the application of refined calculational procedures is sometimes rendered more difficult by the lack of appropriate computer programs. Thus, for practical purposes the availability of calculational tools plays an important role. In the present study e.g. we suffered from the unavailability of diffusion- and perturbation-codes which could take into account special group-cross-sections or diffusion constants at region interfaces. The impact of this drawback becomes more evident in the discussion of the concept of staggered interfaces in Chapter II.

The present work aims at broadening the rather scarce knowledge in this field and at encouraging those who might adopt these still less conventional procedures to nuclear reactor calculations. The examples given here refer to calculations of nuclear characteristics of LMFBRs (in diffusion approximation for time-independent problems without explicitly taking into account the contribution of delayed neutrons), but the intrinsic features of the procedure suggest that its application may as well be useful or even more promising e.g. for intermediate and epithermal reactors with very pronounced variations in the energy dependence of the adjoint neutron flux in the energy range below about 1 keV, a region which is usually not very important for most characteristic quantities relevant to LMFBRs.

II) Remarks Concerning the Theoretical Foundation of Group Collapsing

Group collapsing as a special kind of flux synthesis methods is based on the assumption that the synthesized fine group solution for the group- and space-dependent neutron distribution in a reactor can be approximated with sufficient accuracy as a product of the following form:

$$f_{synth.}(i,r) = F_I(r) \cdot f_i$$

where i and I mean fine and coarse group indices, respectively, and f and F characterize the fine and coarse group neutron flux distribution, respectively. Usually f_i is chosen to be typical for special compositions or regions of a reactor composed of various material mixtures (compositions). Thus, f_i usually exhibits a step-function behavior if the space coordinate r crosses an internal material interface of the reactor configuration (this fact not being indicated explicitly in the above equation). If, in addition to normal real fluxes, adjoint fluxes or real and adjoint gradients are also used as weighting functions, one has to be aware that these functions are usually discontinuous at material interfaces too (internal boundaries).

Most derivations of synthesis methods applied in reactor physics are based on the variational principle, which is closely related to the well-known Hamiltonian principle of classical mechanics, as mentioned e.g. by Kaplan /2/. In accordance with this relationship there is also a close correspondence between the canonical integral and the functional established by Selengut and Wachspress (see list of references in /1/) for the multigroup neutron diffusion theory (see /5/ and the references given there). In their basic formulation of those neutron flux synthesis methods which permit the use of discontinuous trial functions, Wachspress and Becker /1/ illustrate some of the peculiarities and possible difficulties which may be encountered when using this approach. For the P1-approximation to the neutron transport equation a similar variational principle has been established by Henry /3/. This publication gives numerous comments concerning the application of discontinuous trial functions especially for bilinear weighting which seem to be very useful for the appropriate understanding of some problems encountered in group collapsing and upon using collapsed group constants obtained with bilinear weighting for the subsequent solu-

tion of space dependent neutron diffusion problems. The concept of the so-called "staggered interfaces", mentioned in /3/ p. 506, has been used later on also e.g. by Stacey (see /4/ and the references mentioned there on p. 455).

The problem of defining appropriate diffusion constants at material interfaces becomes even more complicated if two- or three-dimensional problems have to be solved instead of one-dimensional problems. As pointed out by Neta and Victory, Jr. in /5a/ - a publication which came to the author's knowledge only after having finished the present study - special complications can arise at so-called singular points, i.e. at those points where two interface curves or surfaces cross, where an interface curve or surface meets the external boundary, or where an interface or boundary has a discontinuous tangent (a corner).

The fact that group collapsing is basically related to synthesis-methods with discontinuous trial functions can probably most easily be demonstrated by using the functional J originally given by Stacey /4/. The relation given below is derived from the original eqn. (3) in /4/ by introducing the approximations and simplifications which are suitable for the present purpose. The notation uses the well-known abbreviations which are usual in reactor physics and for simplicity of the presentation does not distinguish between row- and column-vectors or between scalars, vectors, and matrices.

(II.1) $J = J_1 + J_2 + J_3 + J_4 + J_5$

(II.1.a) $J_1 = \int\limits_{\text{reactor}} dr \left\{ \phi^+ \left[\Sigma - k_{eff}^{-1} {}^*\chi^* \nu\Sigma_f \right] \phi + \psi^+ D \psi \right\}$

(II.1.b) $J_2 = \int\limits_{S_{in}:\text{ int. surfaces}} ds \cdot n \left((\phi_r^+ - \phi_\ell^+)\{(1 - \gamma)D_r \cdot \psi_r + \gamma D_\ell \cdot \psi_\ell\} \right.$

$\left. + \{\Omega\, \psi_r^+ D_r + (1 - \Omega)\psi_\ell^+ D_\ell\}(\phi_r - \phi_\ell) \right)$

(II.1.c) $J_5 = \int\limits_{S_o:\text{ ext. surfaces}} ds \cdot \{n\, \psi_{S_o}^+ \cdot D(\phi_{S_o} - L \cdot D\psi_{S_o} \cdot n) - \phi_{S_o}^+ \cdot D\psi_{S_o} \cdot n\}$

The terms J_3 and J_4 do not appear here, due to the simplifications men-
tioned above (e.g. time-independent problem, disregarding delayed neutrons).
Σ contains the scattering- and removal-contributions. ψ and ψ^+ mean the
gradients of the real and adjoint flux ϕ and ϕ^+. The indices ℓ and r
characterize the left- and right-hand boundaries of an internal interface
with respect to the unit normal vector n (for reasons of a simple pre-
sentation we have not specified row and column vectors explicitly and have
also omitted the specification of matrices; but those familiar with reactor
physics will easily be able to distinguish these quantities from scalars
even if this is not evident from the chosen notation). S_{in} and S_o are
internal or external surface boundaries, respectively. γ and Ω are arbi-
trary constants which are related to the continuity conditions at internal
interfaces and L defines the relation between flux and current on the
external boundary.

With respect to the application of coarse group constants in conventional
codes established to solve the diffusion equation some helpful remarks can
e.g. be found in the work of Lambropoulos and Luco /6/. Concerning the
progress achieved within the last 10 - 15 years it is somewhat disappoint-
ing to read the following corresponding statement on page 507 of Henry's
paper /3/ published in 1967:

> "Thus, the finite difference computer programs currently used for
> solving few-group equations are not directly applicable and, from the
> viewpoint of a consistent variational approach, it seems improper to
> evaluate the use of flux-adjoint weighted few-group cross sections
> without first extending these programs so that the boundary conditions
> ..... can be accounted for."

In the present author's opinion, even today most programs have not been
extended to include the capability of appropriately using flux-adjoint
weighted few-group constants. A further interesting detail has been men-
tioned by Henry (/3/, p. 498, p. 508) too, namely the use of direction-
dependent diffusion constants and corresponding weighting functions which
may - at least in principle - have different energy distributions for
different space directions, thus finally leading to the dyadic nature of
the diagonal elements of the diffusion matrix. As explained in /3/, the

diffusion matrix becomes even more complicated if the Pl-approximation is used instead of the usual diffusion approximation. Finally it should be mentioned, that the difficulties arising upon using bilinearly weighted group constants in diffusion programs could be considerably mitigated by using modified continuity conditions for the fluxes and currents at internal interfaces as has e.g. been shown by Terney and Srivenkatesan /7/. However, this modification, which also requires in most cases an extension of existing codes, brings about another ambiguity, namely the problem of overdetermination or arbitrariness concerning these continuity conditions at internal interfaces (for further details see also the comments by Buslik and the accompanying reply by Stacey published as Letters to the Editor in Nucl. Sci. Eng. pp. 112 - 115, 1972).

One potential remedy to overcome the problem of arbitrariness has probably up to now not been taken into consideration seriously. At least to the author's knowledge it has not been studied whether the initial ad hoc guess for the fluxes and gradients at material interfaces which is e.g. necessary to determine the R- and S-matrices used in the formulation of coarse group continuity conditions in /7/ could be improved, maybe iteratively during a coarse group diffusion calculation. Starting from a plausible recipe (e.g. 0.5, 0.5) for the combining factors for the fine group fluxes taken from the two neighboring regions of a plane interface, one could imagine that a reasonable improvement could be accomplished by modifying these two values for all fine groups comprised within a certain coarse group by using and analyzing the corresponding coarse group fluxes obtained during the corresponding coarse group diffusion calculations. Of course this could e.g. mean that the constants defining the continuity conditions would have to be changed e.g. for each source iteration of the diffusion programs. This would necessarily mean slight extensions of existing programs. On the other hand, one could expect that the values for the combining factors would remain nearly unchanged after the first few source iterations.

With respect to the influence of internal boundaries it may also be interesting to point out the anomaly observed by Rahnema and Pomraning /8/ which may arise if classic first order perturbation theory is applied to determine the reactivity effect associated with the displacement of

such a material interface. The reason for this deficiency of the standard first order perturbation expression comes from the fact that although there are only small differences for the real and adjoint fluxes between unperturbed and perturbed state, the corresponding differences for the real and adjoint gradients cannot be considered as to be sufficiently small in the sense of a first order perturbation, since the gradient is an unbounded operator. On the other hand, as mentioned in /8/, a shift of a material interface means that within a certain region the change of the material composition is usually not really small as it should be for the applicability of first order perturbation theory. A similar incorrectness could probably appear if the exact perturbation theory formalism is used not only to calculate the appropriate integral reactivity value caused by the considered perturbation but also - in a somewhat inappropriate but convenient way - to determine the corresponding so-called material worth traverse, i.e. local reactivity values.

The possible difficulty is connected with the procedure to obtain the suitable gradients at positions near the interfaces of the perturbed region, having in mind that these interfaces are frequently not present in the unperturbed configuration but are sometimes produced as external boundaries of the considered perturbation. If the gradients are directly supplied as part of the solutions to the unperturbed and the perturbed problem or if the external boundaries of the perturbed region are already present as possibly artificial interfaces in the unperturbed configuration, usually no problems should occur for deriving the desired integral or local reactivity values. However, if they are derived a posteriori from the solution obtained for the space dependent neutron flux, one has to take into account that the gradients may show a step-function behavior at these boundaries. Therefore, care has to be taken that the derivation of the gradients is no longer based on the assumption that the flux and its first derivative are continuous across those boundaries (an assumption which may be fulfilled for the unperturbed configuration if there the material properties do not vary across the interfaces possibly brought about additionally by the perturbation).

With respect to external boundaries it seems worthwhile mentioning that in some exceptional cases it may be important to accurately take into account

the influence of this boundary, e.g. on the eigenvalue, as indicated by the existence of the J5-term in (II.1.c). The appropriate treatment of this term could lead to deviations from the well known boundary constants applied to the boundary condition which is usually called logarithmic or diffusion boundary condition. However, this is mostly more or less an academic problem because the influence of such deviations is in most practical applications rather small due to the fact that the real and adjoint fluxes are usually fairly small at external boundaries of the nuclear system under study. (Of course, this statement concerning the usually negligible influence of the external boundary condition does not apply to such kinds of problems as e.g. shielding calculations or the determination of detector efficiencies in off-core positions, but on the other hand this kind of problems can in general not be treated by the application of diffusion theory, but has to be solved using e.g. transport theory where the problem of the logarithmic boundary condition does not exist). As could be expected, the boundary constants remain unchanged upon group collapsing for the conditions of vanishing flux or vanishing current (reflective boundary conditions) at the external boundary.

III) Unusual Features of Adjoint and Bilinear Weighted Coarse Group
     Constants

The appropriate basis for the collapsing procedure used for the present
study is given in Eqn. (II.1) taken from the publication of Stacey /4/. It
is most suitable for our purposes because it uses the gradients of the
real and adjoint neutron fluxes. These quantities can usually be provided
more easily than the similar quantities namely the real and adjoint
currents which are related to the former by Fick's law. Further useful
information concerning the topic discussed here has been published in the
comprehensive work of Wade and Bucher /9/ (see also the references given
there) and in the contributions of Kato et al. /10/ and of Freeman /11/.
These studies also give useful hints for the practical application of
group collapsing procedures which will not be repeated here.

For readers not too familiar with the relations used for group collapsing
it may be useful to present some formulae which are essential for the
understanding of peculiar features of adjoint and bilinear weighting; the
following formulae are given for bilinear weighting, the relations for
real and adjoint weighting can then be easily derived by introducing the
additional approximative assumptions that the adjoint flux is constant or
that the real flux as a function of lethargy is constant (i.e. that $f(i) = u(i)$) for real or adjoint weighting, respectively.

(III.1) $\text{SIGMA}(I) = \sum_i (a(i)*sigma(i)*f(i))/(A(I)*F(I))$ (usual group cross sections)

(III.2) $\text{NUSF}(I) = \sum_i (nusf(i)*f(i))/F(I)$ (neutron production cross section)

(III.3) $\text{CHI}(I) = \sum_i (a(i)*chi(i))/A(I)$ (fission neutron spectrum)

(III.4) $\text{DIFKO}(I) = \sum_i (b(i)*difko(i)*g(i))/(B(I)*G(I))$ (diffusion constant)

(III.5) $\text{SMTOT}(I \to J) = \sum_i \sum_j (a(j)*smtot(i \to j)*f(i))/(A(J)*F(I))$ (scattering matrix)

where

(III.6) $U(I)$ = Sum $u(i)$ (coarse and fine group lethargy widths)
              i

(III.7) $F(I)$ = Sum $f(i)$ (coarse and fine group real fluxes)
              i

(III.8) $G(I)$ = Sum $g(i)$ (coarse and fine group real gradients)
              i

(III.9) $A(I)$ = Sum $(a(i)*u(i))/U(I)$ (coarse and fine group adjoint
              i fluxes)

(III.10) $B(I)$ = Sum $(b(i)*u(i))/U(I)$ (coarse and fine group adjoint
              i gradients)

and small and capital letters are used to characterize fine and coarse
group data, respectively. The summations are extended over all fine groups
i or j corresponding to the considered coarse group I or J.

It may not be evident at first glance that (III.1) is in general not
equivalent to the well known averaging procedure. This would require the
following relation (III.11) which becomes identical to (III.1) only in the
case that the adjoint flux $a(i)$ is constant, i.e. in the case of real flux
weighting.

(III.11) $SIGMA(I)$ = $Sum(a(i)*sigma(i)*f(i))/Sum(a(i)*f(i))$
                        i i

(Usual averaging formalism; not used in bilinear weighting for group
collapsing!)

In the following only some unusual features will be mentioned which may
appear somewhat surprising or curious to users accustomed to normal flux
weighted coarse group constants. Four fairly trivial points should be
mentioned at the beginning:

(1)   If so called diffusion weighting functions i.e. flux gradients are
      going to be used, one should make sure that the derived coarse group
      diffusion constants are determined in a reliable way. This means that
      one should especially be careful if, within a certain coarse group, a
      change of sign occurs for the fine group energy distribution. In such
      cases the application of the corresponding coarse group diffusion con-
      stant might become doubtful. Sometimes the situation can be improved
      by slight changes of the energy group boundaries of the coarse groups
      but in other cases additional measures have to be taken e.g. replac-
      ing at least within this coarse group in question the fine group
      gradients by the fine group fluxes. In most cases the effect of this
      replacement seems to be tolerable because in the concerned coarse
      group the neutron leakage is usually small (in accordance with the
      change of sign of the fine group distribution) so that a somewhat
      inadequate diffusion constant will not appreciably change the spatial
      distribution of the neutrons determined in coarse group diffusion
      calculations.

(2)   As is evident from the formulae for adjoint and bilinear weighting,
      in these cases it is necessary to make use of the fine group lethargy
      widths which are not usually required for group collapsing with nor-
      mal (real) flux weighting.

(3)   As is also evident from the perturbation formalism, it is essential
      to collapse adequately the differences of group cross sections. Since
      usually the group cross sections for the perturbed and unperturbed
      compositions are collapsed individually, it is recommended (but not
      absolutely necessary from program requirements) to have the same set
      of weighting functions for both compositions; otherwise in the course
      of group collapsing the reactivity effect of a change in the material
      composition is mixed up with the additional (and mostly undesired)
      effect of using different weighting functions for the two composi-
      tions defining the material perturbation.

(4)   It is advisable to provide for a sufficient numerical accuracy (e.g.
      by using double precision datafields) of the collapsed group con-
      stants. Of course, this depends on the kind of problem to be treated

and mainly concerns the elements of the scattering matrix which are determined by means of double sums. Therefore, the above aspect is of extraordinary importance if a fine or ultra-fine group structure (having usually far more than several hundred energy groups) is collapsed to a rather coarse group structure (with about 10 - 30 energy groups).

The most important unusual features of adjoint and bilinear weighted group constants, which might become important for some balance algorithms in diffusion codes and which the user accustomed to conventional, flux weighted group constants should bear in mind, are probably the following ones:

(5)   The group sum of the fission spectra (for the prompt as well as for the delayed neutrons) does no longer add up to unity.

(6)   The usual balance relations for the group cross sections used in diffusion codes are no longer valid, i.e. even in the absence of (n,2n)- and (n,3n)-reactions the sum of the group transfer elements of the scattering matrix is in general different from the difference between the removal and the absorption group cross section. This fact also has to be taken into account for the interpretation of individual terms of perturbation calculations.

(7)   Due to the fact that the adjoint and bilinear weighting do not correspond to the usual formation of weighted averages (as does real flux weighting), the value of a collapsed group constant may under certain conditions lay outside the range of the values covered by the corresponding fine group constant. It is especially surprising that, assuming for a special nuclear reaction a constant value for all fine group cross sections within a specific coarse group, the corresponding coarse group constant is generally different from that constant value.

These problems have already been mentioned by Pitterle (see /12/ p. 44) and it might be useful to repeat some of his comments:

"However, when adjoint weighting is included, the average values of the total cross sections are no longer equal to the sum of the average values

for each of the parts comprising the total cross section. This results of course since the total cross sections enter the group equations as loss terms while the transfer cross sections enter as source terms and are thus subjected to different importance weighting factors. Thus with the adjoint weighted parameters one must accept relationships between the cross sections different from the fundamental energy dependent cross sections or from the flux weighted cross sections. The flux averaged definition of removal cross section maintains neutron conservation as the number of neutrons transferred to other groups is exactly the difference between total removal and total absorption for the group. However, this is no longer true for the bilinear averaged constants due to the differences in transfer and removal cross sections discussed above."

The following remark seems to be adequate with respect to the application of bilinear weighting: contrary to normal flux weighting bilinear weighting takes into account changes of the neutron importance suffered in scattering processes; this is especially important for those scattering processes which take place in the fine groups collapsed to one coarse group (within-group scattering). Therefore the change of sign in group-dependent reactivity contributions (especially for the so called degradation- or moderation-term) is less important for the choice of coarse group boundaries when using bilinear weighting than when using usual flux weighting. For this reason fundamental mode calculations (with group-independent buckling values) would reproduce the eigenvalue and the eigenvalue differences (i.e. material worths) when using bilinear weighting in the appropriate way even if group collapsing reduced the number of coarse groups down to only one. On the other hand, for space dependent problems the question of separability of the real and adjoint distribution into two components, one being energy dependent and the other space dependent, plays a dominating role in group collapsing and the question of choosing appropriate coarse group boundaries (see also the corresponding discussion in /12/). Two aspects which are related to each other have to be considered simultaneously: (a) the difference between the energy dependence of the flux and the gradient (for the same zone); i.e. the fact that the proportionality factor between the gradient and the flux is usually not constant for the fine groups taken together in one coarse group and (b) the difference in the energy dependence of each of these quantities

between neighboring zones (both aspects apply to the real as well as to the adjoint distributions). The first point is mainly important for the possible inclusion of diffusion weighting functions whereas the second one could result in the recommendation to subdivide an originally uniform zone into several artificial zones by introducing so-called transition zones to obtain improved results upon application of group collapsing. But with respect to introducing artificial zones one should be aware that first of all it is necessary to have available reasonable approximate weighting functions for all zones (regions) and secondly the advantage of having appropriately weighted the group constants in the neighborhood of material interfaces (transition regions) may at least be partially counterbalanced by the disadvantage of the necessity to include more internal boundaries where - in the sense of the synthesis approach - the fine group trial functions are discontinuous.

IV) Experience Gained during Test Applications

A) General Remarks

As a more or less trivial test of the weighting procedures the earlier /13/ fundamental mode problems were repeated to verify the appropriate performance of the program which was rewritten to deal with diffusion weighting functions and to include collapsing of group constants for the delayed neutrons.

Results for space dependent neutron diffusion problems using coarse group constants which have n o t been determined by the usual flux weighting are only seldom to be found in the published literature. The comprehensive study published by Wade and Bucher /9/ is essentially confined to the condensation of the energy group structure, i.e. to collapsing group constants for space independent problems. Nicholson and coworkers (see e.g. /14/, /15/) have studied the problem of spatial collapsing or spatially averaged group constants without touching the problem of simultaneous energy group collapsing. The early work of Pitterle /12/ was devoted to the problem of collapsing group constants for space dependent problems and perturbation calculations and applying for this purpose adjoint and bilinear weighting procedures in addition to the usual real (or normal) flux weighting. His work gives a clear presentation of the mathematical background and the neutron physics aspects relevant to explain and understand the important intrinsic features of the method which he probably described extensively for the first time. Nevertheless one should be aware that nearly twenty years have passed since that work was done. Meanwhile the calculational tools have been improved considerably, and in accordance the accuracy requirements have been increased drastically. Moreover, in earlier times the topics of interest in reactor physics were mainly in the field of thermal reactors whereas nowadays fast reactors and especially their safety behavior is of dominating importance. Criticality differences exceeding $1 \cdot 10^{-3}$ as found in the tables of Pitterle's work would be considered intolerable for present standard design tools. Pitterle /12/ has given only very few results from perturbation theory calculations which, however, seem to be sufficiently promising to justify the application of bilinear weighting for that purpose.

Therefore, it seems desirable to continue the kind of study originally launched by Pitterle in 1965 mainly for the following reasons:

(1) At present the accuracy requirements are appreciably higher than in 1965.

(2) At present advanced calculational tools are available, i.e. there exist improved possibilities to use better weighting functions for group collapsing than the rather crude approximations at hand in 1965.

(3) At present the reactor geometry is modelled in sufficient detail so that 3-dimensional diffusion calculations are no longer performed only for exceptional occasions. Thus, weighting functions can fairly easily be derived from 1- or 2-dimensional calculations.

(4) The influence of the coarse group constants used for the continuity conditions discussed before (i.e. the necessity to include a term of the general form of J_2, as given in (II.1.2) in the functional in order that its stationarity implies satisfaction of the flux and current continuity conditions) has been described in the literature e.g. by Henry /3/ and Stacey /4/ after Pitterle /12/ had completed his work. So this aspect might not have deserved the desirable attention in his study.

(5) As stated by Pitterle /12/, his calculations had to be considered as an initial investigation of the problem, indicating that bilinear averaged parameters yield appreciably better results for perturbation theory calculations than flux averaged parameters.

Compared to the work of Pitterle we are dealing here with fast reactors only, but it is expected that similar results could be obtained for other types of reactors as well, an assumption which is supported by the results presented already by Pitterle. For obvious reasons it seemed appropriate (a) to use fairly realistic reactor configurations in order to obtain results which are readily transferable to practical problems and are not only based on idealized simplified models, and (b) to consider several kinds of perturbations which frequently have to be treated in reactor design calculations and are important for the safety behavior of fast reactors.

B) Specific Results for a One-Dimensional LMFBR-Benchmark

a) Description of the Calculation Model

As 1-dimensional test case a spherical model /16/ of the well known assembly ZPR III-48 has been chosen, made up of one core and one blanket region. The basic calculations were performed using 26 energy groups of the widely used Russian ABBN structure /17/. The corresponding results were taken as reference data to which the coarse group results have to be compared. Several coarse group structures were tried using 13, 9 and 7 coarse groups. This presentation will deal mainly with the 7 group results because they can be considered as the most rigorous test of the method. Some 9 group results are also given in addition. The other data not mentioned here have helped to confirm the tendencies and conclusions drawn in the following.

The choice of the coarse group scheme was based on the space and energy dependence of the real and adjoint neutron fluxes and the corresponding gradients and the energy dependence of some perturbations studied like the sodium-void reactivity effect. Other additional aspects which may influence such a choice could e.g. be the fission rate or the absorption rate of special materials. For the present purpose the 7 coarse groups were distributed in the following way among the original 26 groups according to the indicated criteria:

New group	Original Groups	Most important reason
1	1 - 4	Fast fission effect
2	5 - 7	High leakage contribution
3	8 - 10	High reaction rates
4	11 - 12	Fairly large Doppler contribution
5	13	Sodium-resonance; non-separability
6	14 - 16	Fairly large Doppler contribution
7	17 - 26	Remaining low energy groups

The adequacy of the chosen coarse group structure may also be deduced from the curves presented in Figs. 1 - 4 and 11 - 14 (these Figs. were not available at the time when the 7 group structure was fixed). For the sake of completeness it should be added that the global shape of the energy dependence of the normalized real and adjoint gradients is similar to that of the corresponding normalized real and adjoint fluxes; the existing deviations between gradients and fluxes will be explicitly discussed later on. Having available in such a graphical form the space- and energy-dependence of the real and adjoint fluxes and gradients for representative weighting functions will in the future probably facilitate the appropriate choice of coarse group boundaries.

Of course, the choice of the group structure has to be adapted to the kind of problem to be solved; therefore, it may be different if one or several of the following quantities have to be determined: criticality, power distribuiton, reactivity effect of the displacement or removal or addition of certain materials (e.g. absorber, coolant, steel, fuel), reactivity effect of a change of the fuel temperature (Doppler effect). Furthermore, the optimum choice is certainly dependent on the type of reactor studied (e.g. whether the neutron spectrum is fast, epithermal or thermal).

For the test case studied here, the weighting functions have been taken from 26-group one-dimensional diffusion calculations for the same con-figuration. The convergence criteria were chosen intentionally rather poor in order to obtain only approximate solutions which will - at least slightly - deviate from the exact solutions. For the same reason we used, as usual in practical applications, zone-averaged quantities as weighting functions although an absolutely exact treatment would require to use space-dependent weighting functions which would exhibit different energy dependencies for each point. However, such a strict procedure is - if at all - only possible for idealized problems and is inadequate for realistic purposes. For the sake of completeness it should also be mentioned that in a very few exceptional cases the diffusion weighting function was modified in certain coarse groups: in order to avoid possible difficulties the corresponding (real or adjoint) fine-group flux was used instead of the gradient, if for the latter a change of sign occurred for the fine group values comprised within one coarse group (see also point (1) in Chapt. III).

It might be useful to mention that the application of weighting functions obtained from fundamental mode calculations could sometimes be a too crude approximation especially for the spectra in the blanket and reflector regions. As already indicated by Pitterle (see /12/ p. 97 and p. 106) this problem is usually more severe for the adjoint than for the real flux.

b) Results for Criticality Values

Apart from fortuitous exceptions, the results obtained for the one-dimensional test case could be summarized as follows:

(1) The k_{eff}-deviations increase as the total number of coarse groups decreases.

(2) The k_{eff}-deviations obtained with real flux weighting are considerably smaller than those obtained with adjoint flux weighting. In many cases a crude approximation for the real flux turns out to be more suitable than a fairly good approximation for the adjoint flux.

(3) The k_{eff}-deviations decrease as the number of artificial zones increases; this turns out to be less important for the real flux than for the adjoint flux weighting.

(4) The improvement observed when using diffusion weighting functions is usually more pronounced for adjoint than for real flux weighting.

(5) The use of bilinearly weighted coarse group constants, taking real and ajoint weighting functions for the individual zones of the reactor, leads to unacceptable k_{eff}-deviations.

(6) Contrary to the results obtained by Pitterle /12/, we found that even the k_{eff}-differences, i.e. the change in reactivity for a certain perturbation, was less accurate when bilinearly weighted coarse group constants were used instead of normal flux weighted ones.

(7) The results obtained with bilinear weighted group constants could be considerably improved if either a uniform real or a uniform adjoint flux are used as weighting functions (such uniform functions could be derived e.g. by integrating over all zones of the whole reactor). In the former case the results are superior to those obtained with pure adjoint flux weighting (equivalent to using a real flux which is constant in lethargy) and in the latter case usually slightly better than with pure real flux weighting (equivalent to using an adjoint flux which is assumed constant in lethargy).

A few characteristic results should be sufficient to demonstrate the essential features mentioned before. The fine- and coarse- (7) group structure used have already been specified in the text before. The 9 coarse groups were collapsed from the basic 26 fine groups in the following manner:

Coarse group	1	2	3	4	5	6	7	8	9
Fine group	1-5	6	7	8	9-12	13	14	15-18	19-26

The perturbation considered here consisted in completely voiding the sodium of the core region. In the following Tables I and II f and a indicate the real and adjoint flux, respectively, g and b the corresponding gradients (see also formulae (III.7) - (III.10)), and the indices N and P characterize the normal and perturbed case. The bar above f or a means that the global quantity (uniform weighting function) derived for the whole reactor is used whereas otherwise the zone-dependent weighting functions are applied. The inclusion of functions in brackets means that these functions are used for bilinear weighting.

Table I

Typical results obtained for the spherical model of
ZPR III-48 upon group collapsing to 7 coarse groups

Reactor configuration	Weighting function(s)	Ratio of coarse-group to fine-group results for k_{eff} Total number of zones in the reactor		
		2*)	4**)	5***)
Normal	f_N	1.0029	1.0028	1.0028
Perturbed	a_P	0.9930	0.9959	0.9962
Normal	f_N, g_N	1.0008	1.0003	1.0003
Perturbed	a_P, b_P	1.0048	0.9985	0.9988

*) Basic model: core-radius: 45.245 cm, blanket thickness: 30 cm

**) 2 artificial interfaces; one in the core at R = 30. cm
and one in the blanket at R = 55. cm

***) 3 artificial interfaces; two in the core at R = 30. cm and R = 40. cm,
and one in the blanket at R = 50. cm

Please note: At the time when deciding on the zone-subdivisions the drawings of Figs. 1 and 2
were not yet available.

Table II

Typical results obtained for the spherical two-zone model of ZPR III-48
upon group collapsing to 9 coarse groups

Reactor Configuration	Weighting function(s)	Ratio of coarse-group to fine-group results for k_{eff}
Normal	f_N	0.9985
Perturbed	f_N	0.9985
Perturbed	a_P	0.9904
Normal	(a_P, f_N)	1.0063
Perturbed	(a_P, f_N)	1.0082
Normal	$(\overline{a_P}, f_N)$	1.0006
Perturbed	$(\overline{a_P}, f_N)$	1.0012
Normal	$(a_P, \overline{f_N})$	1.0049
Perturbed	$(a_P, \overline{f_N})$	1.0068

The reason for the result mentioned in (2) above is the following,
explaining also the facts mentioned in (3) and (4): The approximation of
separability mentioned before, which is equivalent to the assumption of
the adequacy of the buckling concept for all fine groups making up a
certain coarse group is usually less well justified or satisfied for the
adjoint than for the real flux. The values for the adjoint flux are
roughly fairly equal in magnitude whereas for the real flux we observe in
typical fast reactor applications that the group values usually differ by
several orders of magnitude (see e.g. Figs. 3 and 4). Even within one
coarse group we find for the real flux that frequently only a few fine-
groups are of dominating influence, the other ones contribute only minor
portions to the total coarse group real flux; for the adjoint case, how-
ever, all fine groups within one coarse group are of nearly equal impor-
tance. Therefore they have roughly the same influence on the adjoint-flux-
weighted collapsed group constants whereas the real-flux-weighted col-
lapsed group constants are in many cases mainly determined by the few fine

groups which form the major portion of the total flux in the corresponding coarse group. In that case it is usually sufficient that the assumption of separability is valid for these few groups only.

Figs. 5 and 6 show that in the energy range 20 keV - 800 keV which is of dominating influence for the important reaction rates and accordingly also for the neutron balance, the ratio of the adjoint flux in zone 2 to that in zone 1 shows a pronounced energy-dependence whereas the equivalent ratio for the real flux shows a nearly constant value. The global shape of the corresponding curves for the ratio of the normalized real and adjoint gradients in the two zones is roughly similar to that for the real and adjoint fluxes shown in Figs. 5 and 6.

The above argument that for the real flux a few fine groups are of dominating influence whereas for the adjoint flux this influence is nearly equally shared between all fine groups within one coarse group applies to the group dependent ratio of gradients to fluxes too, which is responsible for the result (4) mentioned before.

As can be seen from Figs. 7 - 10, that ratio varies appreciably as a function of energy although the overall form of the group dependence of the normalized real and adjoint gradients looks roughly like that of the corresponding real and adjoint fluxes. This variation is usually more pronounced for the outer zone (zone 2 ≡ blanket) than for the inner zone (zone 1 ≡ core) as can be seen by comparing Fig. 7 with Fig. 8 and Fig. 9 with Fig. 10, respectively. As already mentioned before, this variation is smaller for the real than for the adjoint quantities if one considers only the mainly important energy range from ∿ 20 to 800 keV. A comparison of Fig. 5 and Figs. 7 and 8 with Fig. 6 and Figs. 9 and 10, respectively illustrates that in the important energy range the assumption of separability of space and energy dependence is better fulfilled and the omission of extra diffusion weighting functions is better justified for the real than for the adjoint weighting.

The reason for the unsatisfactory behavior of bilinearly collapsed group constants stated in (5) above is related to the problem of staggered interfaces mentioned in Chapter II. The discussion presented there applies also to the facts stated in (6) and especially in (7) above.

Before going on to the discussion of perturbation theory results, the following remark seems to be adequate to illustrate the influences of two of the three quantities entering the determination of coarse-group reactivity values, namely of the coarse-group real and adjoint fluxes which are necessary in addition to the coarse-group cross-section differences. As could be expected, the coarse-group real flux is in fairly good agreement with the appropriate average fine-group real flux if real weighting functions were used to derive the coarse-group cross sections (see Fig. 11). In an analogous manner, the coarse-group adjoint flux is close to the appropriate average fine-group adjoint flux if adjoint weighting functions were used to derive the coarse-group constants (see Fig. 14); for fundamental mode problems exact agreement will be obtained in these cases as can be easily proven mathematically. Figs. 12 and 13 show that in both cases the respective complementary coarse-group quantity shows considerable deviations from the corresponding average of the fine group quantity, in Fig. 12 e.g. in the ranges 0.2 to 2 keV, 20 - 200 keV and above 1.4 MeV and in Fig. 13 especially in the range 20 - 200 keV. In order to avoid possible misinterpretations, it should be mentioned that the group dependence is only shown in a restricted energy range. Therefore, the apparent deviation in the last coarse-group of Fig. 14 does not really exist but is simply caused by the fact that this coarse-group includes more fine groups than shown in the figure and the coarse-group value is representative of the average of <u>all</u> fine groups comprising this coarse group. From the above discussion it is evident which coarse-group real and adjoint fluxes have to be applied to derive well-founded reasonably accurate coarse-group reactivity values within the framework of perturbation theory by application of the consistent collapsing formalism and that then, quite naturally, bilinear weighting is required for collapsing the group cross section differences.

c) Results of Perturbation Theory Calculations

As has been shown in previous studies /9/, /12/, /13/, bilinear weighting is especially suited for the calculation of reactivity changes caused by changes in group cross sections which are induced by variations in the material compositions of certain reactor zones. Therefore, we studied some

typical cases characteristic for design applications, namely the sodium-void effect and the Doppler effect. Besides these two well-known quantities we included also the reactivity effect (material worth) of hydrogen because this quantity is known to be extremely sensitive to the influence of group collapsing. It should, therefore, give valuable information on the adequacy and efficiency of the group collapsing methods applied here. Results will be presented here only for the 7 coarse group scheme although other coarse group schemes have been used too to confirm the tendencies and conclusions indicated in the following.

Since there are several possibilities and quite a lot of combinations of choosing weighting functions for group collapsing, performing diffusion calculations with coarse group constants and subsequent coarse group perturbation calculations, the notation used in the following to specify the individual cases in a unique way is somewhat complicated and lengthy.

We use EPT to characterize results from Exact Perturbation Theory calculations and FOP for those obtained with First Order Perturbation theory calculations. Small and capital letters mean fine and coarse group quantities, respectively. x and X are used for fine and coarse group cross sections and xd and XD corresponding cross section differences. Thus $F_N(X_N : a_P \cdot x_N \cdot f_N)$ means the coarse group real flux for the normal reactor configuration determined by a diffusion calculation where bilinearly weighted cross sections have been used obtained when using the fine group adjoint flux for the perturbed reactor configuration and the corresponding real flux for the normal (unperturbed) configuration; diffusion weighting functions were not applied in that example given above.

c1) Results for Exact Perturbation Theory

For exact perturbation theory we distinguished between the two basically different procedures:
(a) the usual one, EPTU, which, in our opinion, corresponds to a
     frequently used conventional way to apply coarse group constants for
     determining reactivity effects (admittedly this choice is somewhat
     arbitrary and may reflect personal preferential custom),

(b) an improved way, EPTI, which is offered by the availability of options
for real, adjoint and bilinear weighting.

The following scheme specifies how the coarse-group quantities are
determined:

Procedure	Determination of cross sections and cross sections differences		
	X_P for A_P	XD	X_N for F_N
EPTU	$x_P \cdot f_N$	$xd \cdot f_N$	$x_N \cdot f_N$
EPTI	$a_P \cdot x_P$	$a_P \cdot xd \cdot f_N$	$x_N \cdot f_N$

The following Table III presents a comparison of the ratio of coarse to
fine group integral sodium-void reactivities determined for the 5-zone
model of ZPR III-48. Similar results have been obtained for the 4- and
2-zone models too.

Table III : Ratios of coarse to fine group integral sodium-void
             reactivities for the ZPR III-48 core

	Procedure			
	EPTU		EPTI	
Diffusion weighting functions used	no	yes	no	yes
Number of the core zone				
1	1.2822	1.4908	1.0498	0.9605
2	1.0141	1.0474	0.9746	0.9699
3	0.9889	1.0079	0.9539	0.9531
Total	1.0179	1.0547	0.9695	0.9618

Before going on to discuss the data given in Table III it should be men-
tioned that intentionally we have chosen an example which is not a typical
model case. However, it exemplifies that only a thorough analysis and care-
ful interpretation of the results allows to draw the appropriate conclu-
sions based on common understanding of neutron physics as well as on the
sophisticated insight into the details of numerical evaluations. The
general trends observed can be stated as follows (although not always
evident from the above Table III as will discussed below):

(8) The usually applied procedure EPTU is in general inferior to the more
     refined procedure EPTI. Its efficiency is underlined by the fact that
     the deviations in Table III even for the most crucial values for core
     zone 1 are below about 5% whereas for EPTU they amount to roughly
     50%.

(9) Using diffusion weighting functions in addition to the usual flux
     weighting functions brings about a reduction in the deviations be-
     tween corresponding energy-dependent individual contributions in the
     fine and coarse group results (usually by about a factor of 2 - 3).

The data presented in Table III seem not to confirm the two above state-
ments, but sometimes seem to indicate the opposite behavior. The explana-
tion for this apparent contradiction comes from the extensive cancellation
of positive and negative terms. Such kind of partial mutual compensation
occurs already for the reactivity effect of the inner core zone without
using diffusion weighting functions. The following detailed list of the
individual contributions (given for fine group results obtained for the
5-zone model) shows that the net degradation term is less than 3 % of the
positive scattering (or degradation) term, respectively; furthermore, for
this core zone the (positive) sum of the net degradation term and the
capture term are nearly compensated by the (negative) diffusion term, so
that finally the net reactivity amounts only to 1.5 % of the positive
degradation term. This fact clearly indicates that even the fine group
result for this particular net reactivity is fairly sensitive to numerical
accuracy so that the same quantity will be subject to even worser
uncertainty conditions if it is determined in a coarse group structure
established by group collapsing.

Table IIIa:

Individual contributions to the sodium-void reactivity of core zone No. 1; in brackets is indicated the ratio to the corresponding fine group result

	Fine group results	Coarse group results	
		without using diff. weight funct.	using diff. weight. funct.
Capture :	21.70/-4	21.77/-4 (1.0032)	21.73/-4 (1.0012)
Fission :	1.48/-4	1.49/-4 (1.0035)	1.48/-4 (1.0013)
Diffusion :	-38.33/-4	-37.89/-4 (0.9886)	-37.94/-4 (0.9899)
Source : (Production)	-4.41/-4	-4.43/-4 (1.0043)	-4.42/-4 (1.0020)
Pos. Degrad. :	443.63/-4	388.15/-4	387.80/-4
Neg. Degrad. :	-430.86/-4	-376.22/-4	-375.17/-4
Degrad. Sum :	12.77/-4	11.93/-4 (0.9348)	12.63/-4 (0.9893)
$\Delta(-1/k)$	-6.79/-4	-7.13/-4 (1.0498)	-6.52/-4 (0.9605)

Although the agreement for each individual term is improved when the usual weighting functions are supplemented by diffusion weighting functions, the absolute value of the deviation for the net reactivity remains nearly unchanged and would, therefore, not indicate any significant advantage of the inclusion of diffusion weighting functions.

This is due to the fact that the deviations of the diffusion and net degradation term are to a large extent fortuitously cancelling each other if no diffusion weighting functions are applied and that this partial cancellation does no longer occur if diffusion weighting functions are used. The fact that the deviation for the diffusion term is not significantly reduced may possibly be related to the problem of staggered interfaces and the correlated difficulty that usual perturbation codes have no

option to include an extra term to account for the effect of discontinui-
ties in the collapsed group constants brought about by weighting functions
which are different in neighboring regions of an interface. The fact that
the deviation for the degradation term is reduced comes about in a rather
indirect way: the use of diffusion weighting functions leads to slightly
changed coarse group diffusion constants which in turn cause minor varia-
tions in the space- and group-dependence of the coarse-group real and
adjoint neutron fluxes determined by corresponding diffusion calculations.

A detailed investigation of the numerical results presented in the
following indicates that the inclusion of diffusion weighting functions
leads to a reduction of the deviations to the corresponding correct
individual coarse group degradation contributions thus that the already
small maximum absolute difference of about 0.5 % could be further reduced
to about 0.25 % if the more refined collapsing procedure is applied. It is
somewhat surprising, that even these relative small improvements in the
groupwise net degradation terms caused by the additional use of diffusion
weighting functions results in this case in a significant improvement of
the total degradation term. However, it is not completely clear if this
effect and especially its magnitude is of a general nature or just fortui-
tously comes from accidental compensation effects arising in the special
case studied here.

Table IIIb:
Group dependent values for the net degradation term (in brackets is
indicated the ratio to the correct values given in column 2)

Coarse group	Derived from fine group results	Obtained without using diffusion weighting function	Obtained upon using diffusion weighting function
1	1.721791/-2	1.715345/-2 (0.996256)	1.721419/-2 (0.999784)
2	1.157352/-2	1.163528/-2 (1.005336)	1.156161/-2 (0.998971)
3	-1.321265/-2	-1.322718/-2 (0.998894)	-1.318877/-2 (0.998193)
4	-1.748375/-2	-1.757822/-3 (1.005403)	-1.743871/-2 (0.997424)
5	1.000195/-2	1.002670/-2 (1.002475)	1.000384/-2 (1.000189)
6	-2.238053/-2	-2.246130/-2 (1.003609)	-2.240869/-2 (1.001259)
7	-1.751690/-4	-1.757328/-4 (1.003219)	-1.753381/-4 (1.000965)
Sum	1.276650/-3	1.193404/-3 (0.934793)	1.262967/-3 (0.989282)

c2) Results for First Order Perturbation Theory

For first order perturbation (FOP) theory calculations we proceeded in the
analogous way as for the exact perturbation theory case, i.e. we dis-
tinguished between two different procedures which could be characterized
as follows, using the abbreviations defined above:

Procedure	Determination of cross sections and cross section differences		
	X_N for A_N	XD	X_N for F_N
FOPU	$x_N \cdot f_N$	$xd \cdot f_N$	$x_N \cdot f_N$
FOPI	$a_N \cdot x_N$	$a_N \cdot xd \cdot f_N$	$x_N \cdot f_N$

The corresponding results for the prompt neutron lifetime, the central
sodium-void reactivity effect, the central Doppler reactivity effect, and
the central hydrogen reactivity effect (material worth) are shown in Table
IV below.

Table IV :   Ratio of coarse-group (7) to fine-group (26) first order
             perturbation theory results for the ZPR III-48 Core

Quantity	Calcul. Proc.	FOPU		FOPI	
	Use of Diff. Weight. Funct.	no	yes	no	yes
Prompt neutron lifetime		0.9937	0.9953	1.0040	1.0025
Central sodium void react.		0.9841	0.9600	0.9703	0.9851
Central Doppler react.		0.9085	0.9095	0.9808	0.9798
Central hydrogen material worth		0.4855	0.5096	0.9085	0.8992

The discussion of the results presented in Table IV goes along the same lines as that for the results of Table III. Therefore the arguments, especially those for the sodium-void reactivity will not be repeated. Detailed examinations concerning the influence of using diffusion weighting functions lead to the conclusion that their application does not produce significant improvements in FOP results; nevertheless their application is suggested if it is possible without complications because they are advantageous with respect to the criticality parameter as already mentioned above.

As could be expected from the nature of the problem and the intrinsic features of the adopted improved collapsing method, the coarse group results could be drastically ameliorated, if one applies the new method in an adequate way, i.e. using real, adjoint and bilinear weighting for suitable purposes. The Doppler reactivity effect and the hydrogen material worth are convincing examples underlining the prospects of the improved collapsing method and the associated calculational technique which has to be followed. Figs. 15 - 18 show that with this improved method the coarse-group quantities are in close correspondence with the related fine-group quantities whereas for the usual method such a good agreement for the group-dependence can only be established for the real neutron flux, but then the adjoint flux and the perturbation results are inevitably in less favorable agreement. In other words, the additional application of adjoint and bilinear weighting allows to properly determine the coarse group energy dependence of the adjoint flux and the appropriately weighted cross section differences, so that one is able to derive reasonable coarse-group values for reactivity effects, especially of those which are sensitive to details of and slight spectral shifts in the energy distribution of the adjoint flux.

The shaded area in Fig. 15 and Fig. 16 in the energy range around 1 keV should indicate that the total reactivity contribution of the concerned coarse-group is in reasonable agreement with the average contribution of the corresponding fine groups if the improved collapsing method is applied and that remarkable differences may occur when the usual collapsing method is used. The same conclusion applies for the most important individual contribution, namely the capture term in the same energy range as can also be

deduced from Figs. 15 and 16. In Figs. 17 and 18 is shown the most impor-
tant contribution to the hydrogen material worth, namely the so-called
moderation term, which is related to the change of the neutron importance
due to scattering processes. In that case the improved collapsing forma-
lism leads to significantly better agreement between coarse- and fine-
group reactivity values in almost the whole energy range. By comparing
Fig. 17 and Fig. 18, the advantage of the new, consistent collapsing
method becomes immediately evident for all coarse groups below 1.4 MeV.

It seems to be worthwhile to mention that the deviations in the group-wise
reactivity-contributions are usually fairly small between the usual and
the consistent methods; most times they are remaining below 5 % and are
exceeding 10 % only in a very few cases. For fissile and absorber mate-
rials the amount of the deviation for the total reactivity is in general
tolerable because it is acceptably low (i.e. well below 5 %). For pre-
dominantly scattering materials (with nearly equal positive and negative
degradation terms) or for those cases where effects of opposite signs to a
large extent cancel each other (e.g. leakage and moderation effect), the
observed discrepancies, which do not seem to be prohibitively large at
first sight, may eventually be responsible for quite significant devia-
tions in the total reactivity value predicted by usual and consistent
coarse-group perturbation calculations. In such cases the improvement
brought about by using the consistent method is obvious and, due to this
advantage, its application is therefore highly recommended.

It is natural, that an optimum choice of the coarse group structure
depends on the kind of the intended application i.e. k_{eff}-calculation,
type of reactivity effect etc. According to the experience gained in this
study, the 7-group structure used here can obviously be recommended for a
broad class of possible applications in the field of nuclear studies for
LMFBRs: the number of coarse groups remains sufficiently small and most of
the characteristic nuclear reactor parameters can be determined such that
the associated uncertainties do not exceed amounts which are considered to
be tolerable for practical purposes.

C) Results for a Two-Dimensional Reactor Model

a) Description of the Calculation Model

Having obtained satisfactory results for the application of the improved
collapsing methods for one-dimensional diffusion and perturbation
calculations we tried to verify the adequacy of the new procedures for
more realistic two-dimensional problems too. We used a cylindrical model
of a conventional design of a 1300 MW_e-LMFBR, with two core zones of
different enrichment. It is internally labelled HOM1 to distinguish it
from a corresponding design for an unconventional, so-called heterogeneous
core design and has been described e.g. in /18/. The details of the design
will not be specified here but it should be mentioned that we studied an
end-of-burnup-cycle condition where the control rods are withdrawn nearly
up to the upper core blanket interface. The normal reactor configuration
was modified to obtain a representative perturbed configuration by
removing most of the sodium out of the upper blanket and the (axially)
neighboring 2/3 of the core region; for the perturbation calculations,
i.e. to obtain the group cross section differences, this removal was
supposed to take place in all regions of the reactor. Two coarse group
condensation structures were used: a 12-group scheme which was the
standard one for determining reactivity coefficients for subsequent safety
studies and the 7-group scheme proved to be useful in the preceding
one-dimensional test cases.

The 12-group scheme is related to the 26-group scheme in the following
way:

Coarse group	1	2	3	4	5	6	7	8	9	10	11	12
Fine group(s)	1-2	3-4	5-6	7	8-9	10-11	12	13	14	15	16	17-26

In order to have appropriate but still somewhat approximate weighting
functions we performed 2-dimensional 26-group diffusion calculations with
less stringent convergence criteria (e.g. $1 \cdot 10^{-2}$ for the eigenvalue) than
usually used for production runs. Only flux weighting functions were used
for group collapsing because no gradients were easily available.

Generally the experience gained during the study for the one-dimensional geometry cases confirmed especially that adjoint flux collapsing is less advantageous than real flux collapsing as far as the coarse group eigenvalue is concerned. Three kinds of perturbation calculations, described below, have been done using the methods which can be characterized as follows using the nomenclature explained before:

Calculational Method	Procedure to derive coarse group constants			
	X_P for A_P	$XD = X_P - X_N$ with		X_N for F_N
		X_P from	X_N from	
M1	$x_P \cdot f_N$	$x_P \cdot f_N$	$x_N \cdot f_N$	$x_N \cdot f_N$
M2	$x_P \cdot f_P$	$x_P \cdot f_P$	$x_N \cdot f_N$	$x_N \cdot f_N$
M3	$a_P \cdot x_P$	$a_P \cdot x_P \cdot f_N$	$a_P \cdot x_N \cdot f_N$	$x_N \cdot f_N$

M1 is a frequently used method which avoids adjoint and bilinear weighting and uses only real fluxes for the unperturbed configuration. M2 also avoids these additional weighting complications but uses real fluxes for the unperturbed and the perturbed configurations and, thus, yields coarse group reactivity values which should be exact for the specific perturbation considered (in fact this is not strictly valid because region-averaged instead of space-dependent weighting functions are used). M3 corresponds to the improved collapsing method offered by the availability of adjoint and bilinear weighting.

b) Results for Sodium-Void Reactivities

As representative results, the following table shows the results of integral perturbation calculations for two perturbations: P1 the transition from the normal to the partially voided reactor, P2 corresponding to the removal of most of the sodium from all regions of the reactor.

Table V: Typical Results for the Effect of Group Collapsing Applied
to a 2-dim. LMFBR-Model

Calculational Method	Number of coarse groups	Ratio of coarse-group to fine-group sodium-void reactivities for perturbation	
		Partial Voiding; P1	Global Voiding; P2
M1	12	0.9593	0.9474
M1	7	1.0422	1.0661
M2	7	1.0144	1.0328
M3	7	1.0033	1.0094

The values presented in Table V clearly demonstrate the superiority of the
improved collapsing method to those commonly used and show that even with
a reduced number of coarse groups it is able to produce results which are
superior to those obtained with more coarse groups if the usual collapsing
method M1 is applied.

Having already confirmed the superiority of the improved collapsing method
M3 compared to the conventional one, M1, on the basis of integral perturba-
tion results we were also able to show its merits on the basis of local
quantities, namely for the Na-void reactivity effect of each node of the
2-dim. RZ-model. Generally the following typical deviations between the
coarse group results and the corresponding fine group results were
observed in the fuel regions of core nodes with positive sodium-void
contributions:

M1 (12 groups) :   -2 % to -5 %
M1 (7 groups) :   0 % to +4 %
M2 (7 groups) :   -2 % to +2 %
M3 (7 groups) :   -1 % to +1 %

Bearing in mind the fairly good quality of the weighting functions used in these test cases, the deviation of ± 1 % for M3 is quite acceptable whereas differences of up to 5 % seem somewhat high indicating the need to apply improved calculational methods.

Similar advantages were also obtained for the blanket nodes. A detailed comparison for these nodes shows that method M3 with 7 groups leads to similar deviations as method M1 with 12 groups. Thus, the application of the improved collapsing method could really be considered as a successful demonstration of the potential improvements attainable when using this new tool. For the sake of completeness it should be mentioned that in the immediate neighborhood of the zeros of the local Na-void reactivity effect neither collapsing method is able to produce satisfactory results in all cases. But this behavior is obviously due to the effects of large mutual cancellations of positive and negative contributions already mentioned before.

V) Conclusions

Before discussing the merits of the improved collapsing method and the
special inherent features one should bear in mind when applying it for the
numerical solution of space dependent coarse group neutron diffusion
problems it may be worthwhile to mention a general problem common to
almost all collapsing procedures: it is practically always necessary to
use approximate weighting functions which are in almost all cases given
only for certain material regions (or spatial domains); therefore, the
coarse group cross sections are usually constant within corresponding
specified regions, a feature which is favorable to facilitate the
numerical solution to the coarse group diffusion equation but which
represents an approximation to the rigorous treatment requiring the
derivation and use of space dependent coarse group constants even within a
region containing a completely homogeneous material. In realistic
applications such a complicated treatment is nearly impossible because
appropriate space dependent weighting functions are most times not
available and even then would usually be only an approximation to the
correct multidimensional fine-group solution which - in principle - would
be necessary for that purpose.

According to the experience gained from the present study, the following
procedure for the application of group collapsing seems to be reasonable:

A) If only criticality, power distribution, breeding ratio, absorber rod
    reactivities or similar quantities are to be determined, usual (real
    or normal) collapsing might be sufficient (if possible with inclusion
    of so-called diffusion weighting functions); the necessary weighting
    functions could e.g. be obtained from a multi-dimensional fine group
    diffusion calculation with very moderate accuracy requirements of
    about 1 - 5 % in k_{eff}.

B) In those few cases where e.g. reliable detector efficiencies are to be
    determined by using the importance function obtained as solution of
    the adjoint multigroup problem, the application of adjoint weighting
    seems to be appropriate, where the adjoint weighting functions (to-
    gether with the corresponding adjoint diffusion weighting functions)

could be obtained in an analogous manner as indicated above for the real weighting functions.

C) If reactivity values as e.g. the sodium-void effect, the Doppler effect or the material worth of special isotopes or elements are to be determined, a more refined procedure seems to be adequate: three types of collapsed (coarse) group constants should be established using real, adjoint and bilinear weighting, respectively. Bearing in mind the extreme sensitivity of these reactivity values to details of the energy distribution of the real and adjoint fluxes, it seems favorable to derive the weighting functions from rather accurate multi-dimensional fine group calculations where the k_{eff} uncertainty margin should probably be at least below 1 %.

The above suggestions A) - C) are plausible from general knowledge of reactor physics. Further applications for realistic problems will hopefully show that they usually lead to reasonable, acceptably accurate and reliable results. However, in some special cases it may turn out that special classes of problems require an even more refined treatment or at least higher accuracies in the preparation of weighting functions.

In the present study the improved collapsing method has mainly been applied to 1-dim. and 2-dim. test cases supposed to cover a sufficiently broad class of typical problems encountered in nuclear calculations for fast reactors. It could be shown in this presentation that the suggested method has the following advantages compared to the usual collapsing method using flux weighting only:

(1) Using the same number of coarse groups it leads to more accurate and reliable results.

(2) If the same requirements concerning the tolerable deviations between corresponding coarse and fine group results should be satisfied, the new method allows to use an appreciably smaller number of coarse groups with the additional advantage of a significant reduction of the storage and computer time needed mainly for multidimensional diffusion calculations.

The following precautions should be taken for the appropriate and promising application of the new collapsing method for space dependent problems especially when standard diffusion and perturbation codes are used to determine reactivity values:

(3) Three sets of coarse group constants have to be produced using real, adjoint and bilinear weighting, respectively.

(4) The choice of the necessary weighting functions for group collapsing has to be done in a consistent manner and should take into account the subsequent use of these coarse group sets; this is especially important for the bilinearly weighted group constants of unperturbed and perturbed compositions used in perturbation calculations and also for the so called normalization integral entering as the denominator into the perturbation expressions.

(5) In general, normal flux weighting leads to smaller differences between coarse and fine group eigenvalues than adjoint flux weighting. Therefore, the latter should be used preferably to generate coarse group constants which are subsequently used for determining coarse group adjoints.

(6) Special care has to be taken if bilinearly weighted coarse group constants are applied for eigenvalue calculations. Difficulties are encountered - at least with usual diffusion codes - upon fulfilment of the continuity conditions at internal interfaces. The nature of the problem has been described previously in the literature (see e.g. /1/, /4/), and a remedy has been proposed (which is at least possible in principle but somewhat tedious and complicated in practice), namely the use of artificial, so called "staggered" interfaces.

(7) If so called diffusion weighting functions are applied to collapse diffusion constants, additional difficulties may arise which are related to the one above and refer to the appropriate definition of coarse group diffusion constants to be used in equating the real or adjoint neutron currents of both sides of an internal material interface. The proper treatment of such discontinuities in coarse group

diffusion calculations may necessitate modifications in existing usual
diffusion codes.

(8) When applying the improved collapsing method for space dependent
problems one should always be aware that usually it cannot be avoided
that the coarse group adjoint equation based on coarse group constants
obtained by adjoint weighting is in general not equivalent or directly
related to the adjoint of the real (or direct) equation based on
coarse group constants obtained by real weighting. Although this
feature, i.e. the non-commutativeness of the two operations, namely
group collapsing and transition from the direct to the adjoint equa-
tion, seems to be undesirable from a more mathematical point of view,
it has been shown in typical practical applications that this princi-
pal drawback is no real basic disadvantage and should not be a severe
obstacle against using this method.

Acknowledgements

VI) <u>References</u>

/1/ E. L. Wachspress and M. Becker: Variational Synthesis with
     Discontinuous Trial Functions. Int. Conf. on the Application of
     Computing Methods to Reactor Problems, Argonne National Laboratory,
     ANL-7050, 191, 1965.

/2/ S. Kaplan: An Analogy Between the Variational Principles of Reactor
     Theory and those of Classical Mechanics. Nucl. Sci. Eng. 23, 234,
     1965.

/3/ A. F. Henry: Few-Group Approximations Based on a Variational
     Principle. Nucl. Sci. Eng. 27, 493, 1967.

/4/ W. M. Stacey, Jr.: Variational Flux Synthesis Methods for Multigroup
     Neutron Diffusion Theory. Nucl. Sci. Eng. 47, 449, 1972.

/5/ G. I. Bell, S. Glasstone: Nuclear Reactor Theory. Van Nostrand
     Reinhold Company.

/5a/ B. Neta and H. D. Victory, Jr.: On the development of a convergence
     theory of synthesis methods for solving diffusion equations. Progress
     in Nuclear Energy, Vol. 8, pp. 283-293, 1981.

/6/ P. Lambropoulos and V. Luco: Functionals for Discontinuous Trial
     Function Flux Synthesis. Journal of Nuclear Energy, 24, 551, 1970.

/7/ W. B. Terney and R. Srivenkatesan: Few Group Methods for Fast-Reactor
     Transients. Nucl. Sci. Eng. 53, 337, 1974.

/8/ F. Rahnema and G. C. Pomraning: An Anomaly in the Use of Perturbation
     Theory. Nucl. Sci. Eng. 78, 393, 1981.

/9/ D. C. Wade and R. G. Bucher: Conservation of the Adjoint Neutron
     Spectrum by Use of Bilinear-Weighted Cross Sections and Its Effect on
     Fast Reactor Calculations. Nucl. Sci. Eng. 64, 517, 1977.

/10/ Y. Kato, T. Takeda and S. Takeda: A Coarse-Mesh Correction for Neutron Diffusion Calculations. Nucl. Sci. Eng. 61, 127, 1976.

/11/ L. B. Freeman: Space-Energy Few-Group Neutron Cross Sections for Large, Complex Core Calculations. Nucl. Sci. Eng. 78, 342, 1981.

/12/ T. A. Pitterle: Bilinear Averaging for Diffusion Theory Parameters. Dissertation, University of Wisconsin, University Microfilms Inc. (1965).

/13/ E. Kiefhaber: Fine Group Calculations for Reactivity Coefficients of Structural Materials in Fast Reactors. KfK 1759, Februar 1973.

/14/ M. Komata, R. B. Nicholson, and E. M. Page: A Bilinear Formulation for Spatial Cross-Section Averaging. Nucl. Sci. Eng. 50, 220, 1973.

/15/ R. G. Palmer, J. P. Plummer, and R. B. Nicholson: A Study of Several Methods for Analysis of Critical Assembly Heterogeneity. Nucl. Sci. Eng. 50, 229, 1973.

/16/ ENDF-202; Cross Section Evaluation Working Group Benchmark Specifications, BNL 19302, November 1974.

/17/ I. I. Bondarenko et al.: Group Constants for Nuclear Reactor Calculations. Consultant Bureau Enterprises, Inc., N.Y. (1964).

/18/ A. Mockel, R. de Wouters, S. Pilate, G. Buckel, E. Kiefhaber, A. Polch, D. Thiem, U. Wehmann: Design and nuclear analysis of large homogeneous and heterogeneous LMFBR cores using multi-dimensional diffusion codes. Fast Reactor Physics, Internat. Symp., Aix-en-Provence, France, September 24 - 28, 1979, IAEA-SM-244/30.
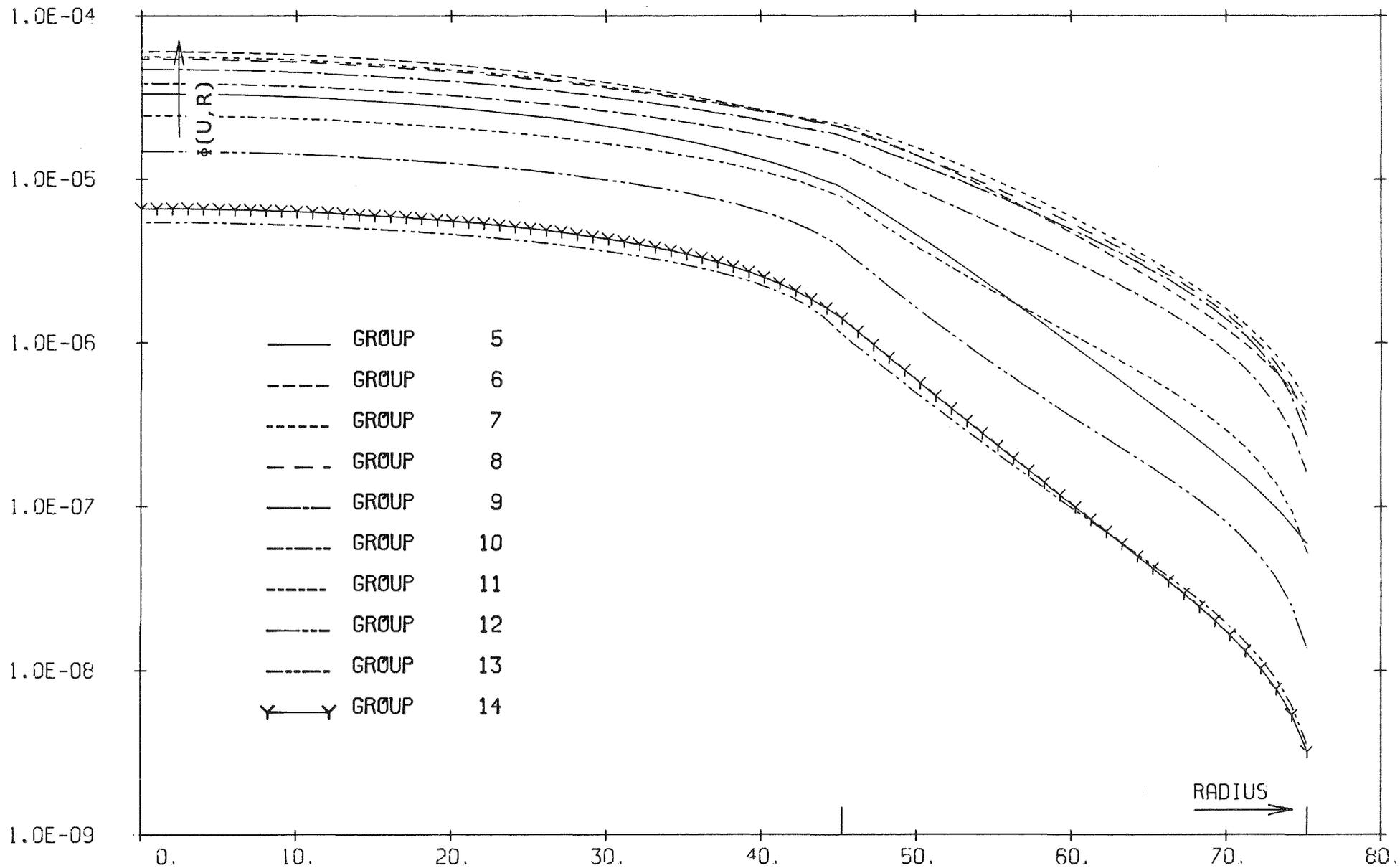
FIG. 1: ZPR III-48 SPHERICAL MODEL; REAL NEUTRON FLUX $\Phi(U,R)$

IN THE ENERGY GROUPS 5-14 AS A FUNCTION OF THE RADIUS R

- 45 -
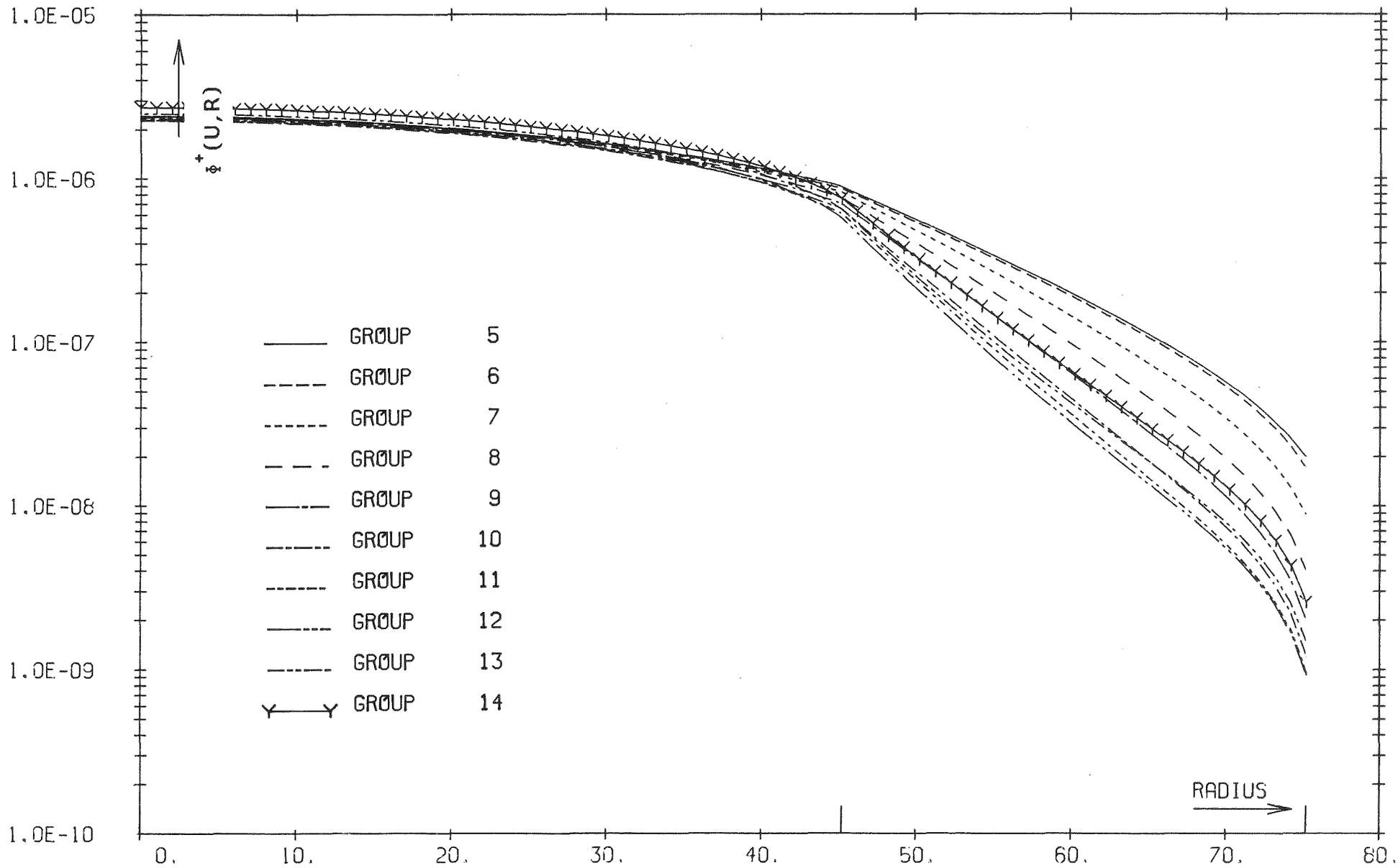
FIG. 2: ZPR III-48 SPHERICAL MODEL; ADJOINT NEUTRON FLUX $\Phi^+(U,R)$
IN THE ENERGY GROUPS 5-14 AS A FUNCTION OF THE RADIUS R
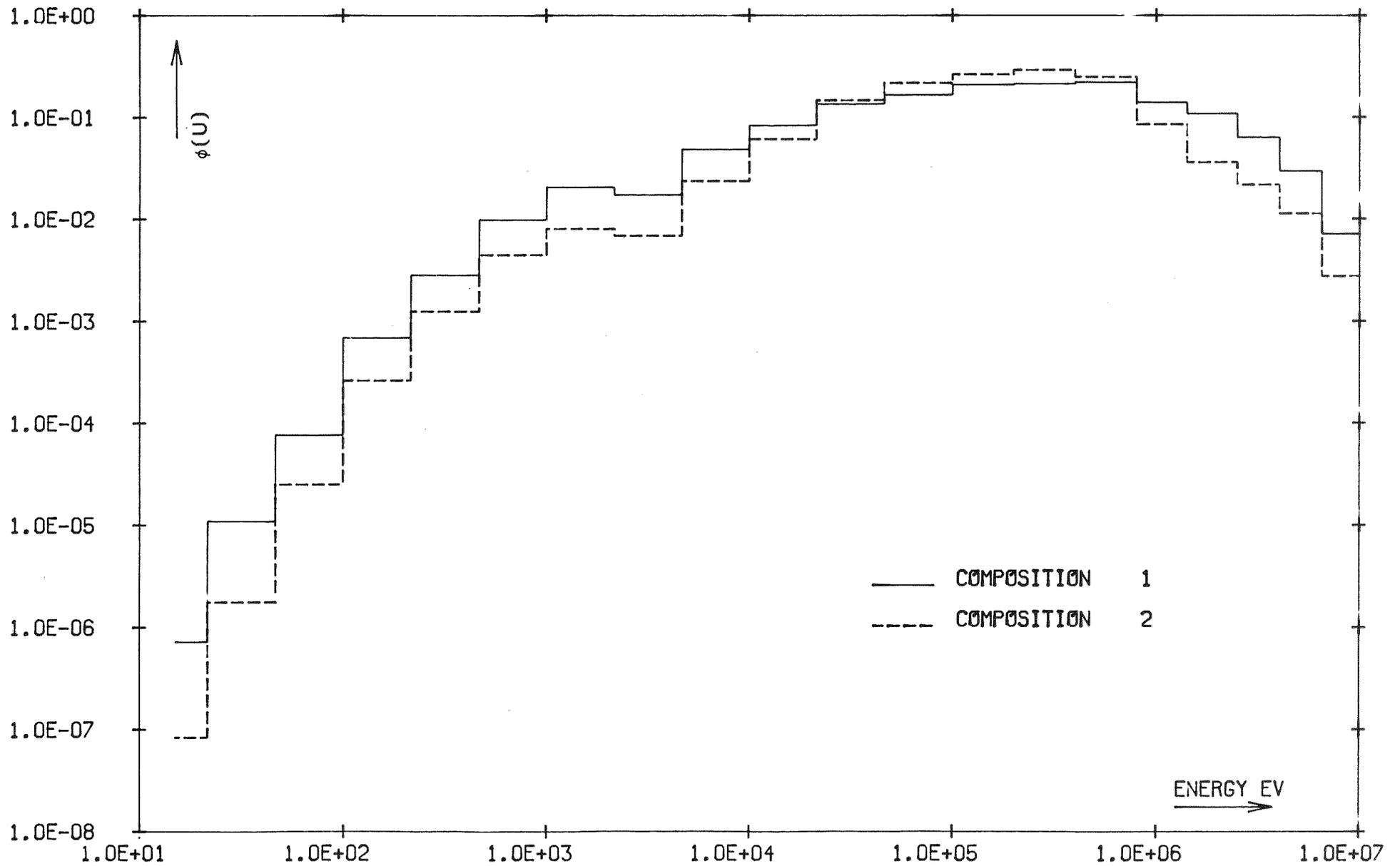
FIG. 3: ZPR III-48 SPHERICAL MODEL; NORMALIZED REAL INTEGRAL NEUTRON
FLUXES $\phi(U)$ FOR ZONE 1 AND ZONE 2 AS A FUNCTION OF LETHARGY U
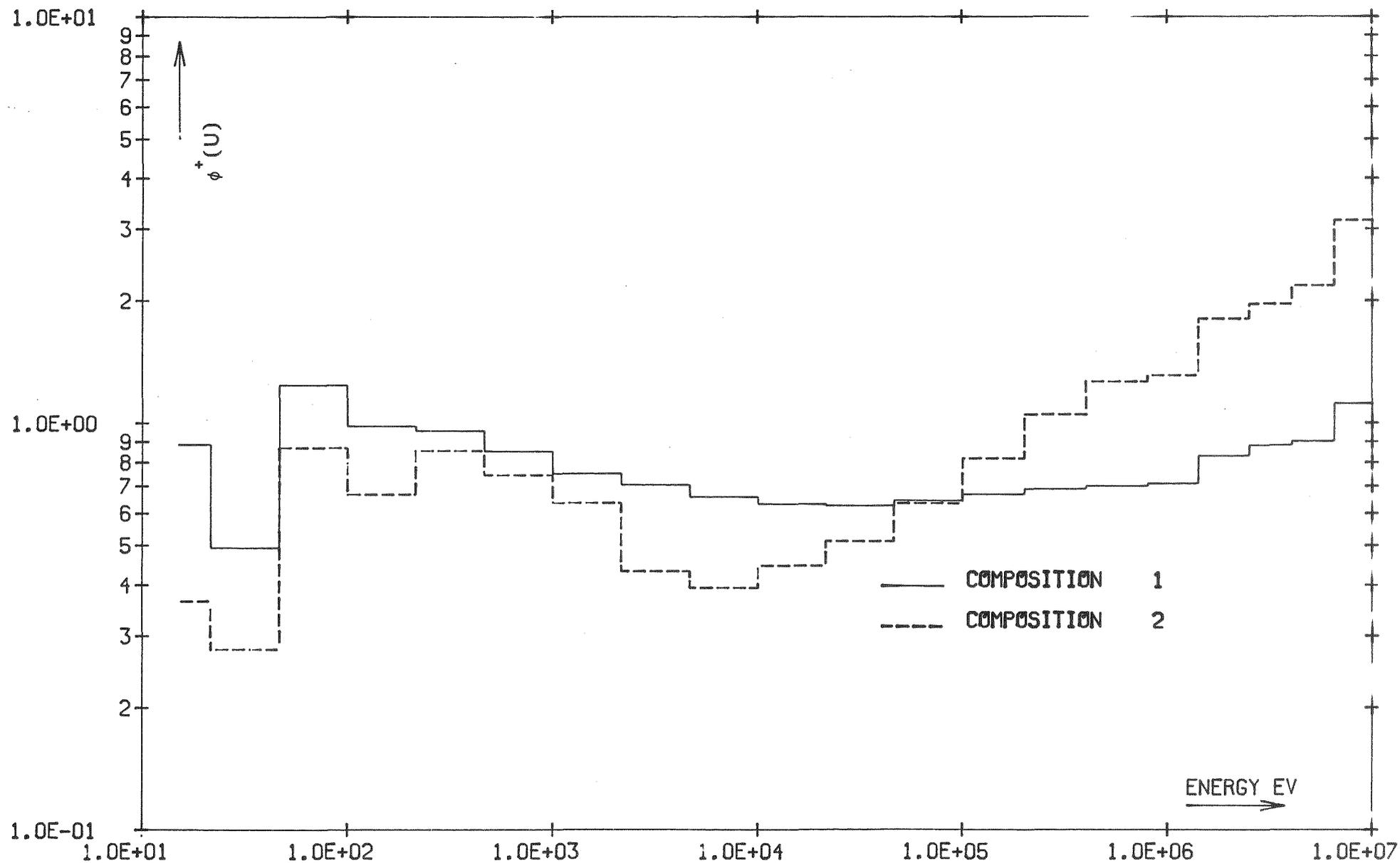
FIG. 4: ZPR III-48 SPHERICAL MODEL; NORMALIZED ADJOINT INTEGRAL NEUTRON
FLUXES $\phi^+(U)$ FOR ZONE 1 AND ZONE 2 AS A FUNCTION OF LETHARGY U
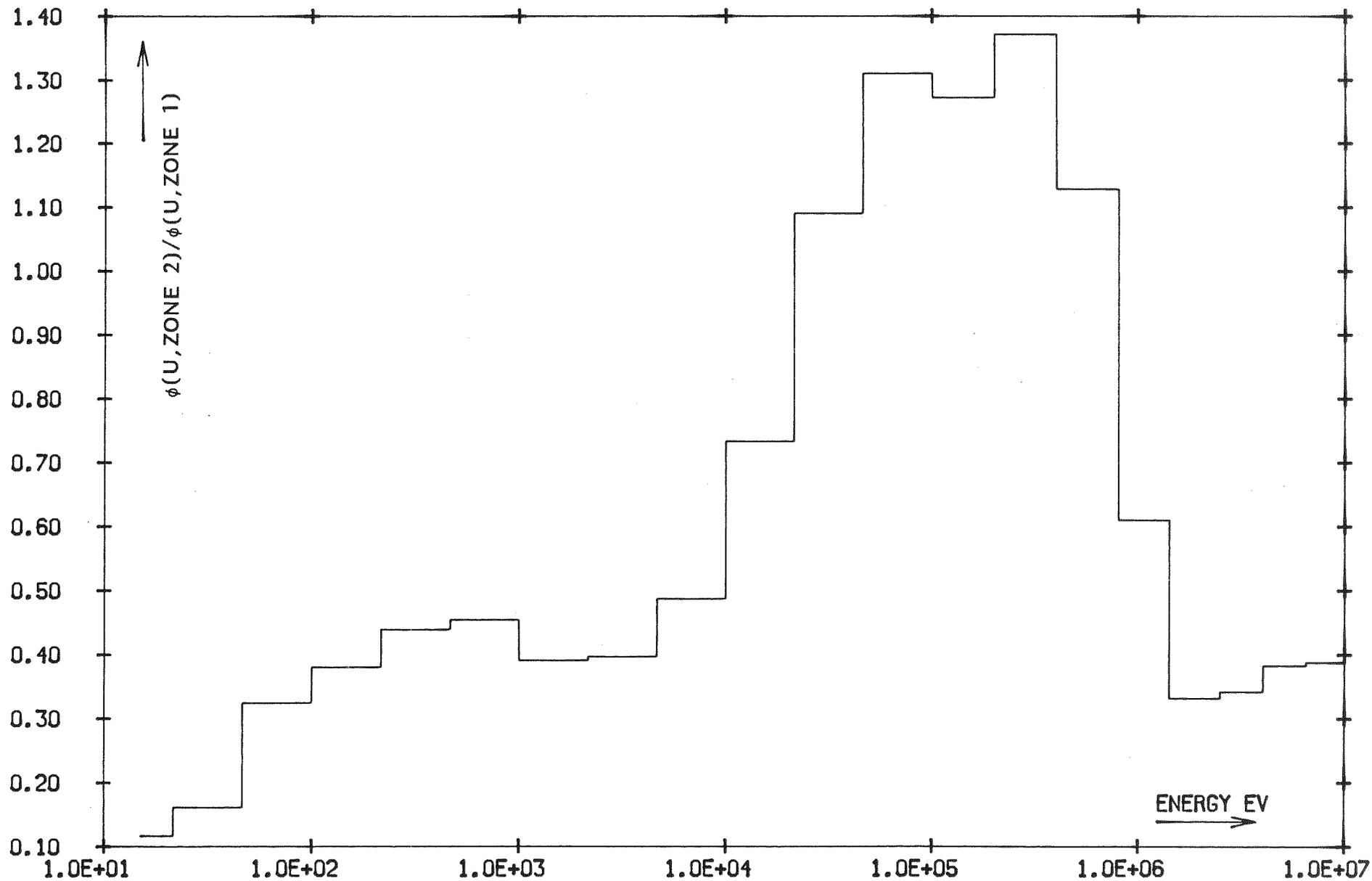
FIG. 5: ZPR III-48 SPHERICAL MODEL; RATIO OF NORM. REAL INTEGRAL NEUTRON
FLUXES φ(U) OF ZONE 1 AND ZONE 2 AS A FUNCTION OF LETHARGY U

FIG. 6: ZPR III-48 SPHERICAL MODEL; RATIO OF NORM. ADJOINT INTEGRAL NEUTRON FLUXES $\phi^+(U)$ OF ZONE 1 AND ZONE 2 AS A FUNCTION OF LETHARGY U
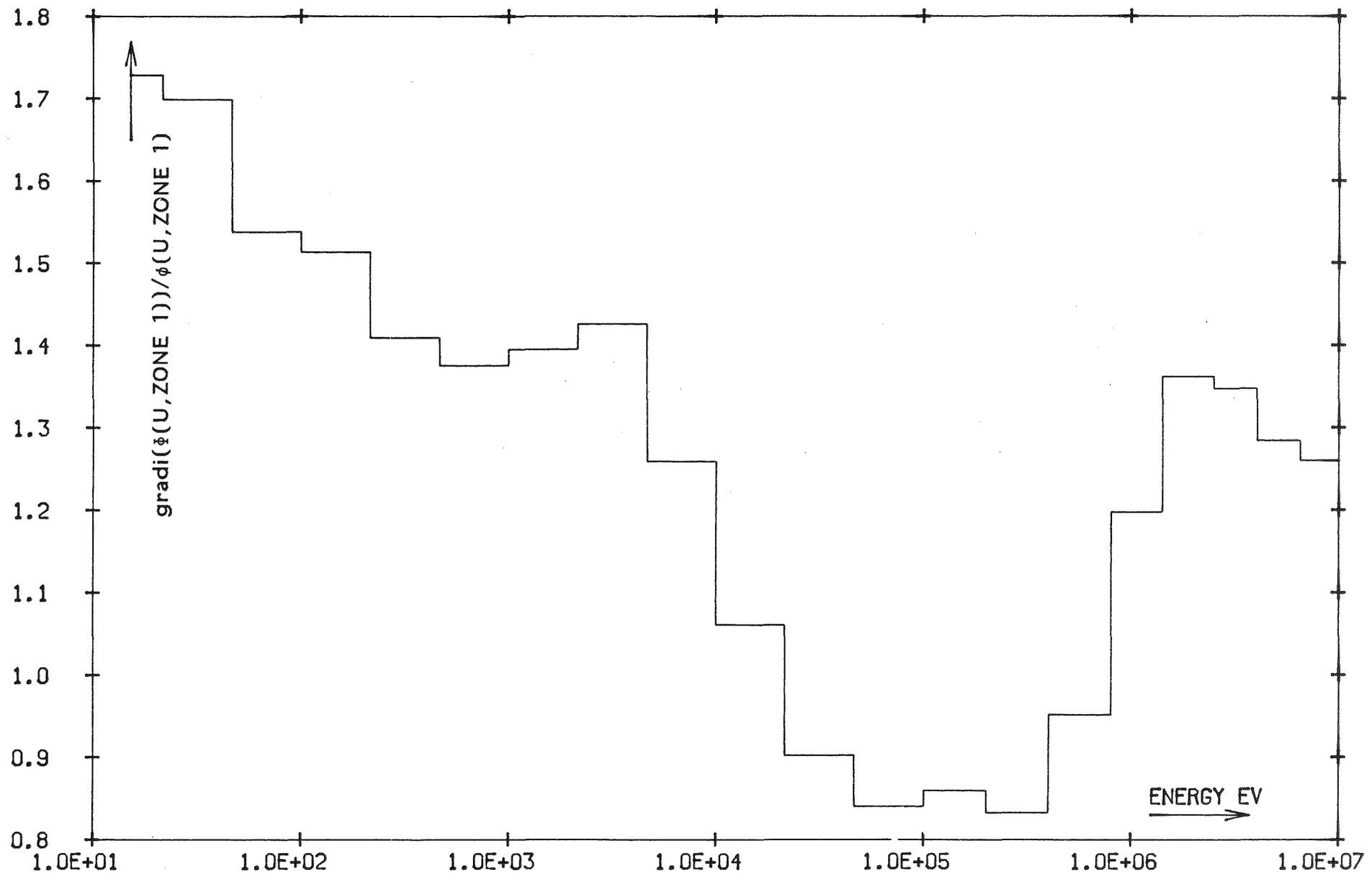
FIG. 7: ZPR III-48 SPHERICAL MODEL; RATIO OF NORMALIZED REAL GRADIENT-
INTEGRAL TO NORMALIZED REAL FLUX-INTEGRAL FOR ZONE 1
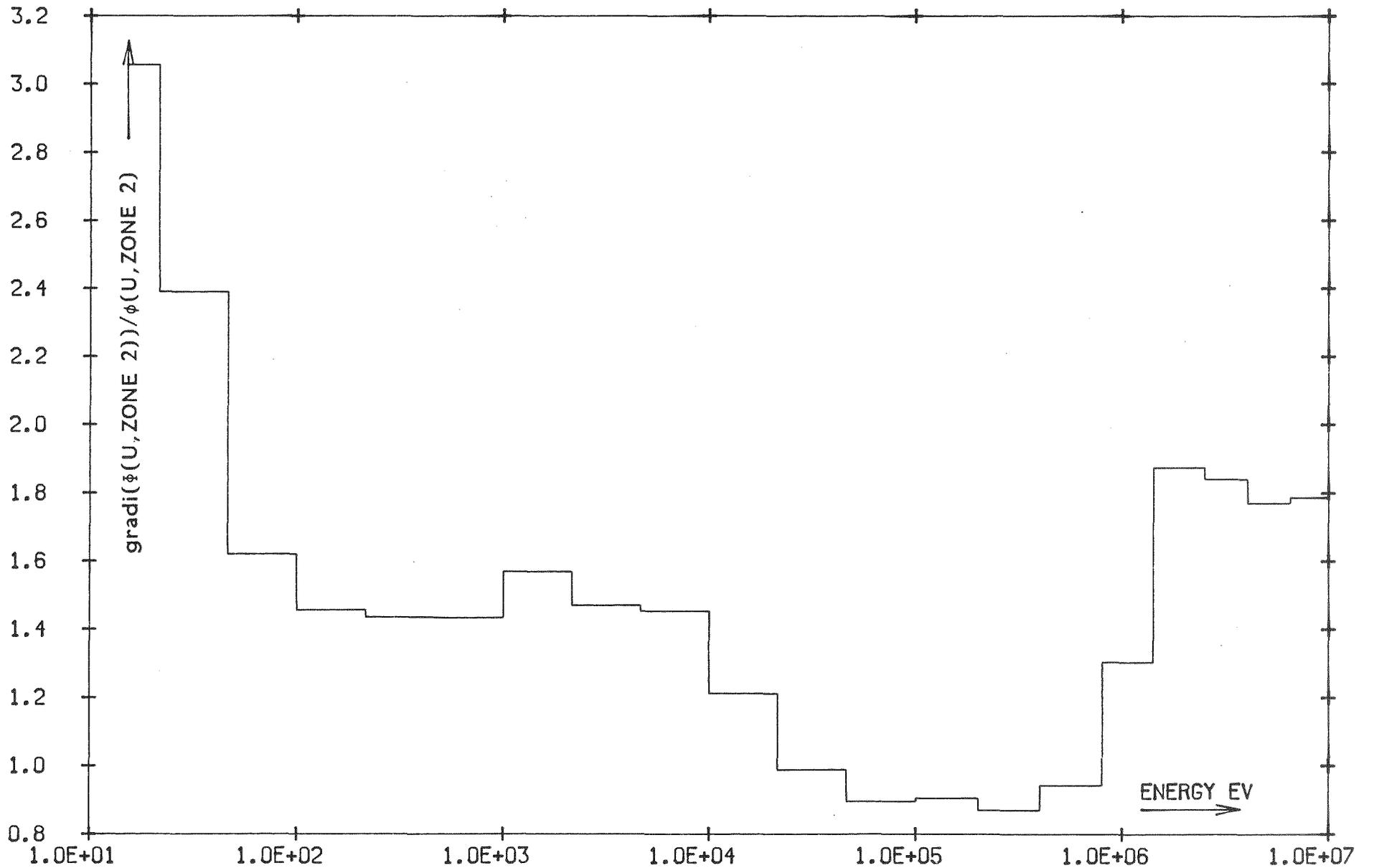
FIG. 8: ZPR III-48 SPHERICAL MODEL; RATIO OF NORMALIZED REAL GRADIENT-
INTEGRAL TO NORMALIZED REAL FLUX-INTEGRAL FOR ZONE 2
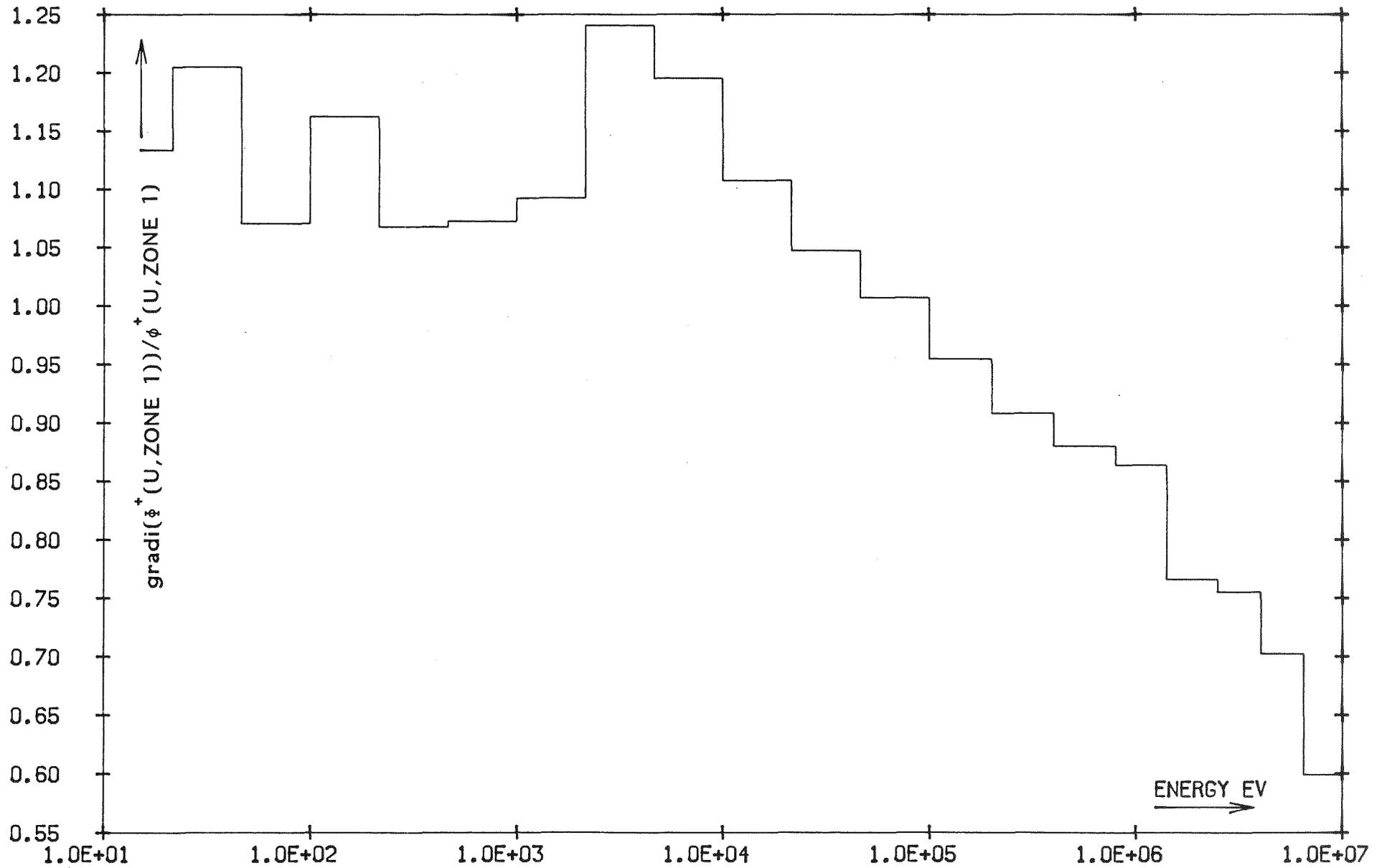
FIG. 9: ZPR III-48 SPHERICAL MODEL; RATIO OF NORMALIZED ADJOINT GRADIENT-
INTEGRAL TO NORMALIZED ADJOINT FLUX-INTEGRAL FOR ZONE 1
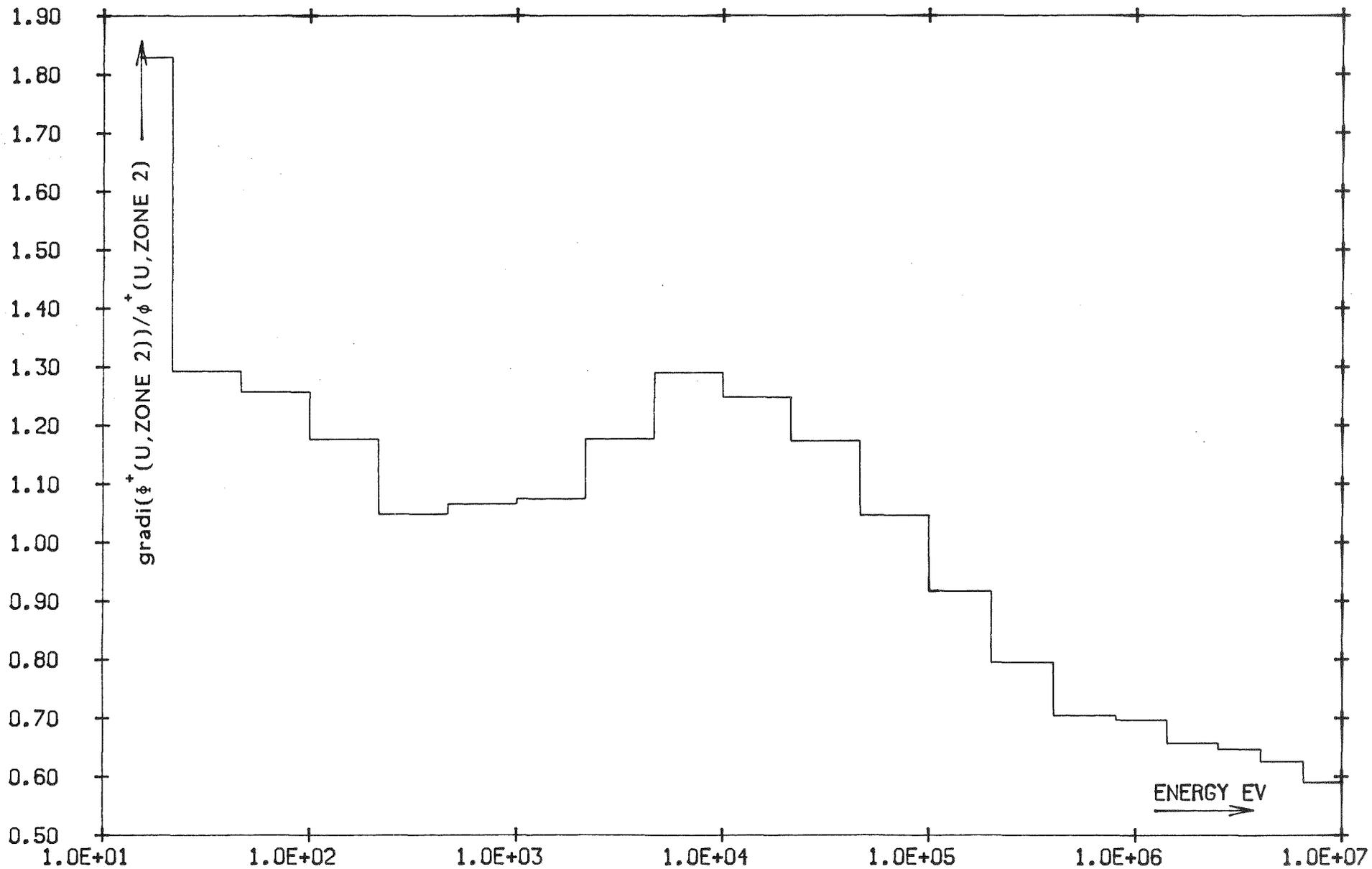
FIG. 10: ZPR III-48 SPHERICAL MODEL; RATIO OF NORMALIZED ADJOINT GRADIENT-
INTEGRAL TO NORMALIZED ADJOINT FLUX-INTEGRAL FOR ZONE 2
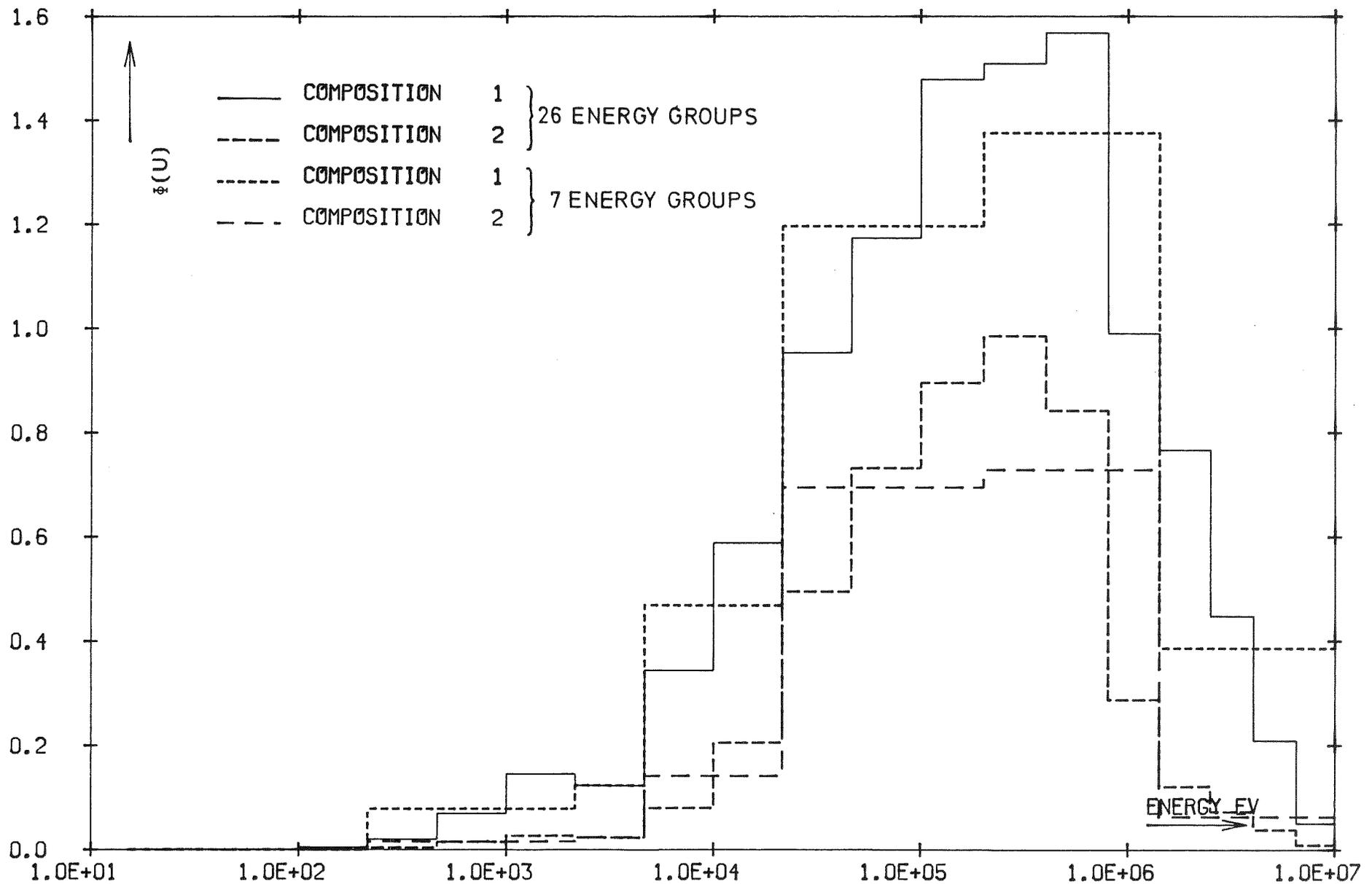
FIG. 11: ZPR III-48 SPHERICAL MODEL; $\Phi(U)$ IN 26 and 7 ENERGY GROUPS
(7-GROUP-Σ OBTAINED USING REAL WEIGHTING)
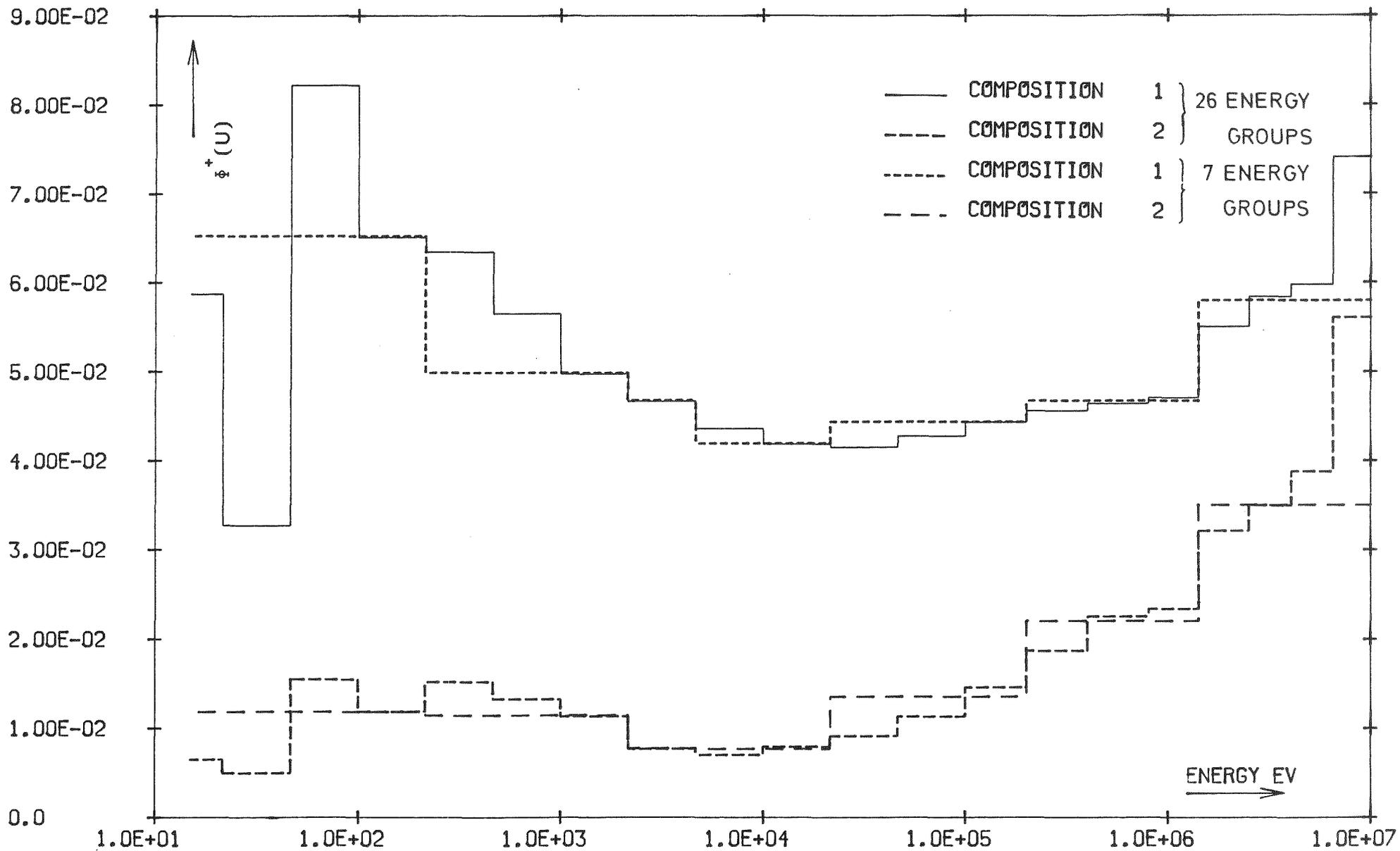
FIG. 12: ZPR III-48 SPHERICAL MODEL; Φ^+(U) IN 26 and 7 ENERGY GROUPS
(7-GROUP-Σ OBTAINED USING REAL WEIGHTING)
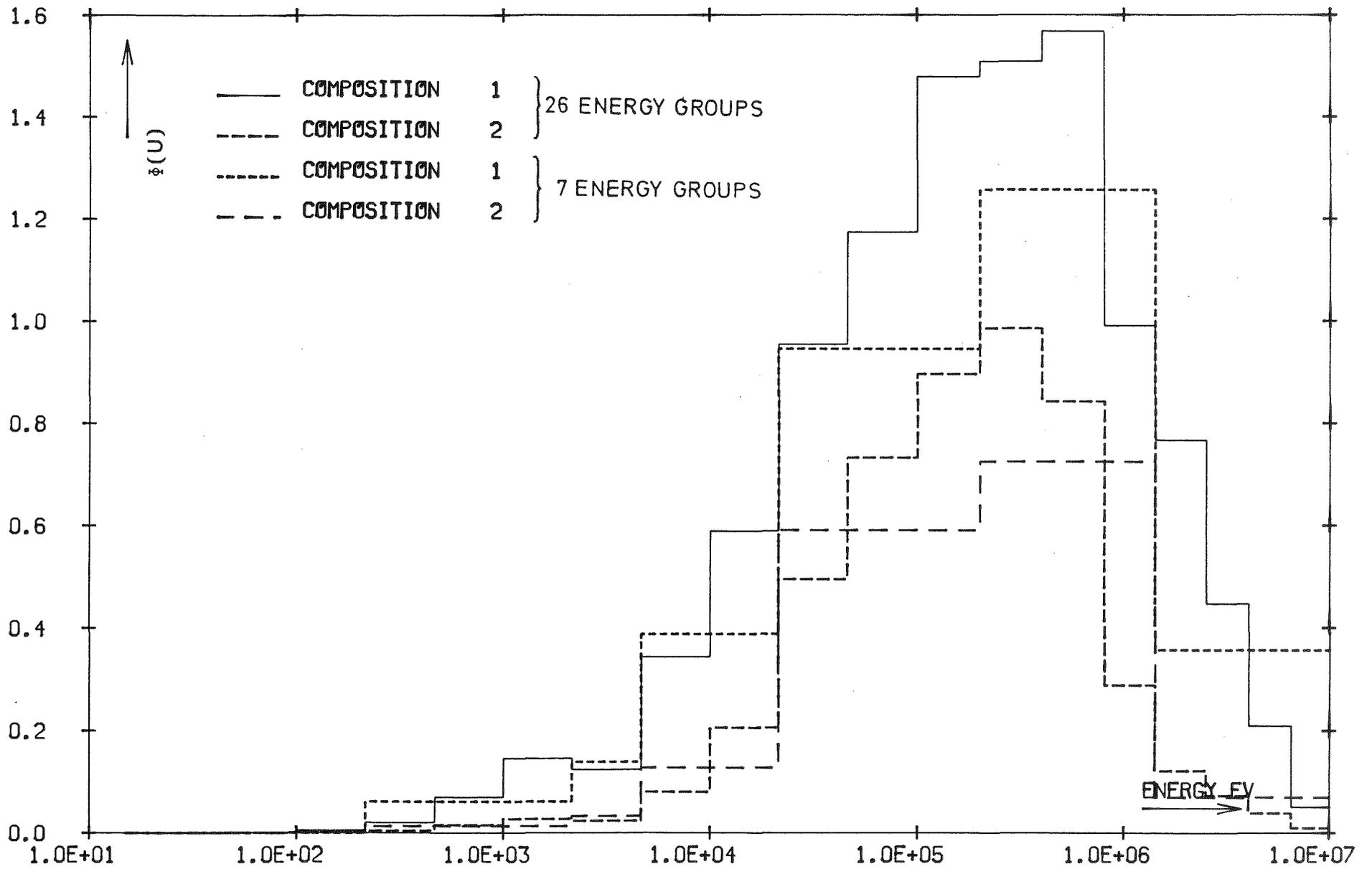
FIG. 13: ZPR III-48 SPHERICAL MODEL; $\Phi(U)$ IN 26 and 7 ENERGY GROUPS
(7-GROUP-Σ OBTAINED USING ADJOINT WEIGHTING)
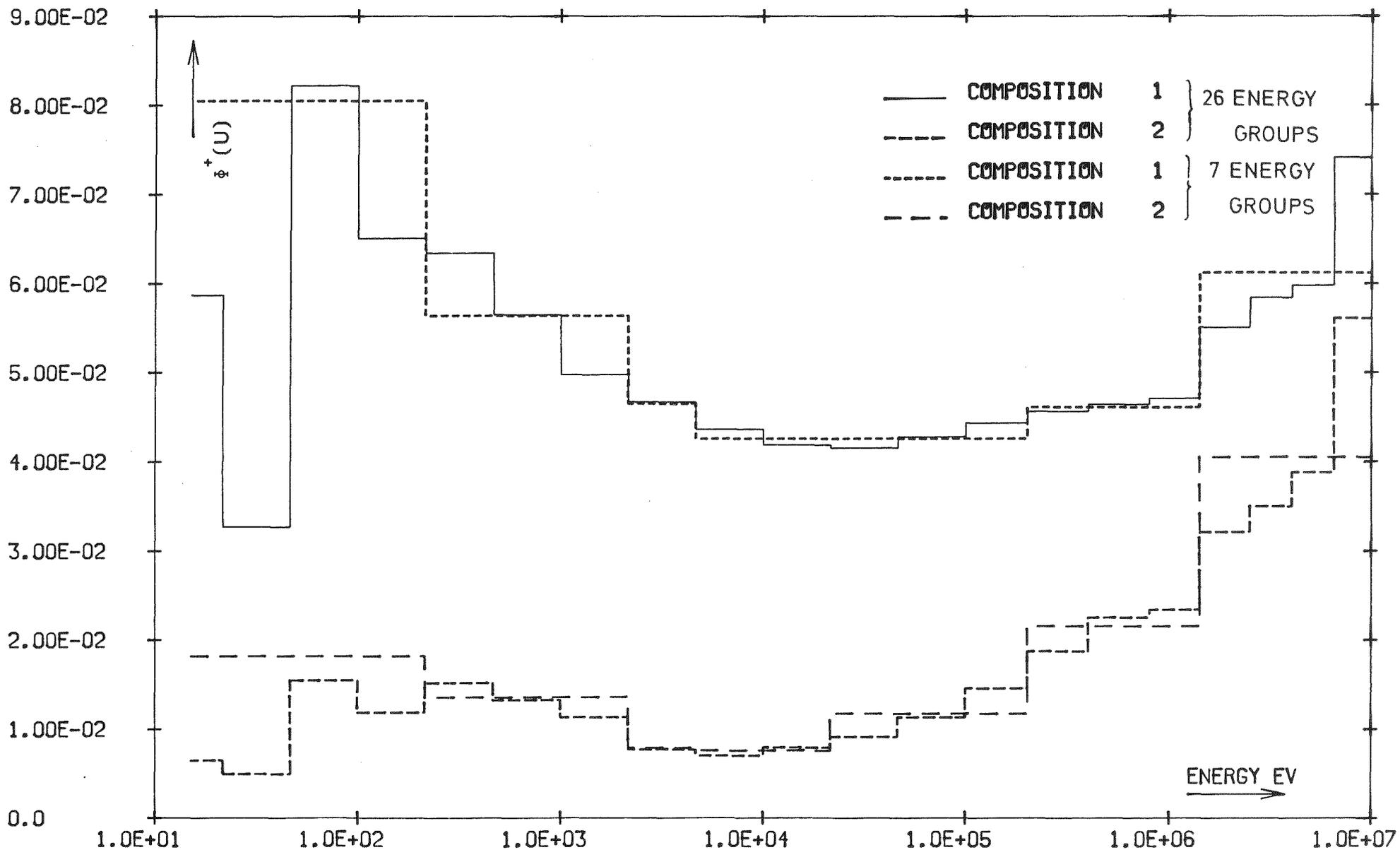
FIG. 14: ZPR III-48 SPHERICAL MODEL; $\Phi^+(U)$ IN 26 and 7 ENERGY GROUPS
(7-GROUP-Σ OBTAINED USING ADJOINT WEIGHTING)
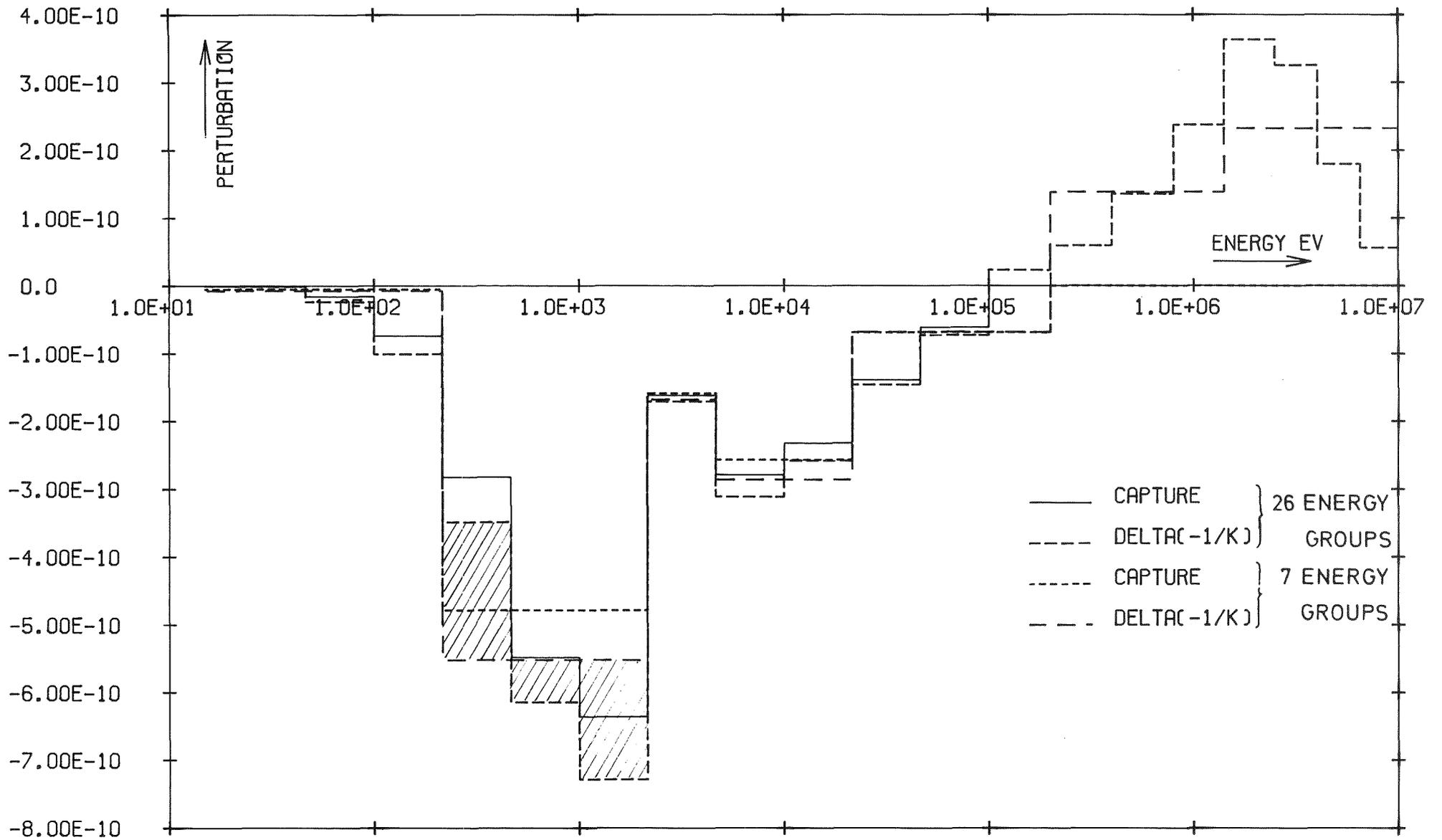
FIG. 15: ZPR III-48 SPHERICAL MODEL; CENTRAL DOPPLER COEFFICIENT: RESULTS FROM
26-GROUP AND CONSISTENT 7-GROUP LOCAL PERTURBATION CALCULATIONS
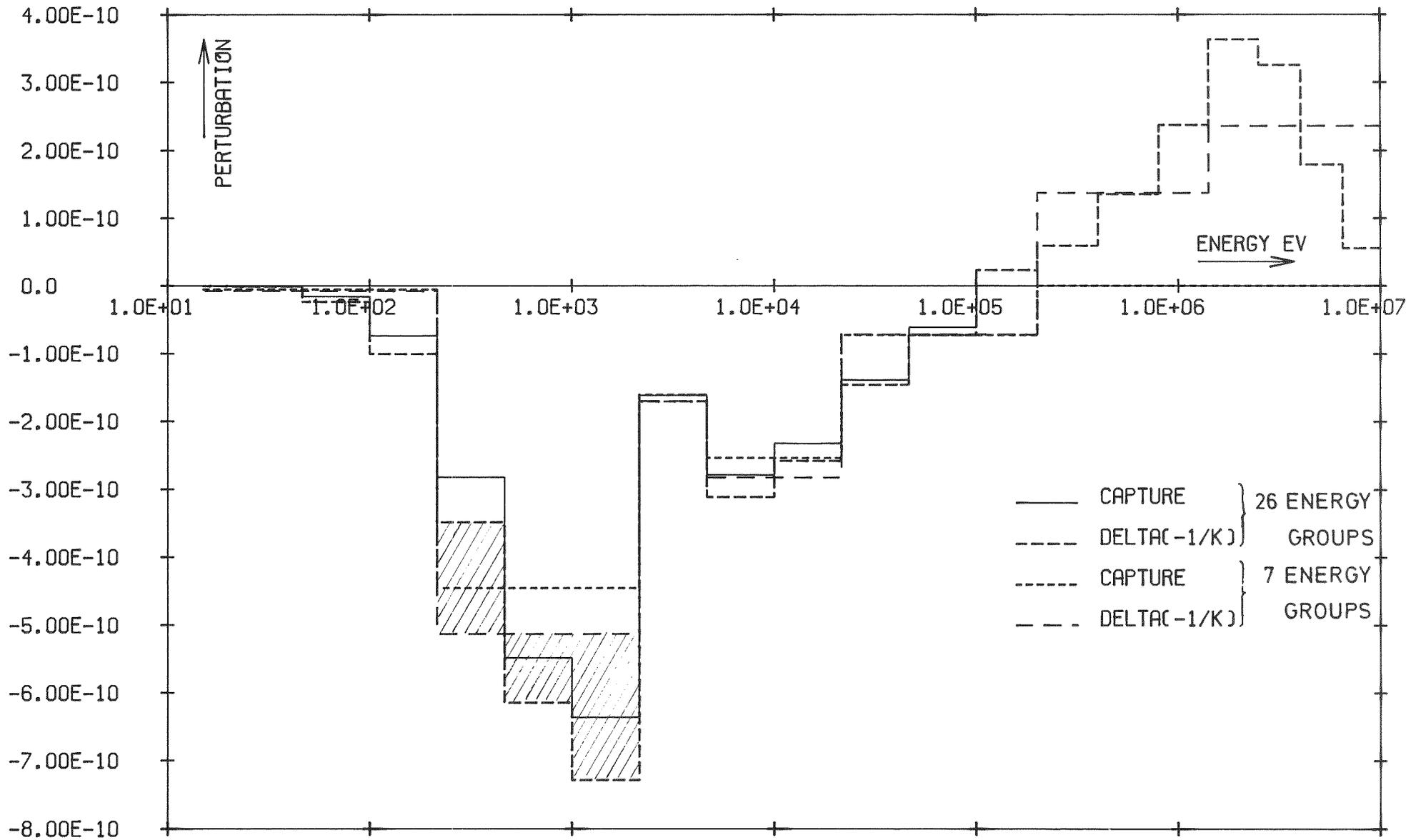
FIG. 16: ZPR III-48 SPHERICAL MODEL; CENTRAL DOPPLER COEFFICIENT: RESULTS FROM
26-GROUP AND USUAL 7-GROUP LOCAL PERTURBATION CALCULATIONS
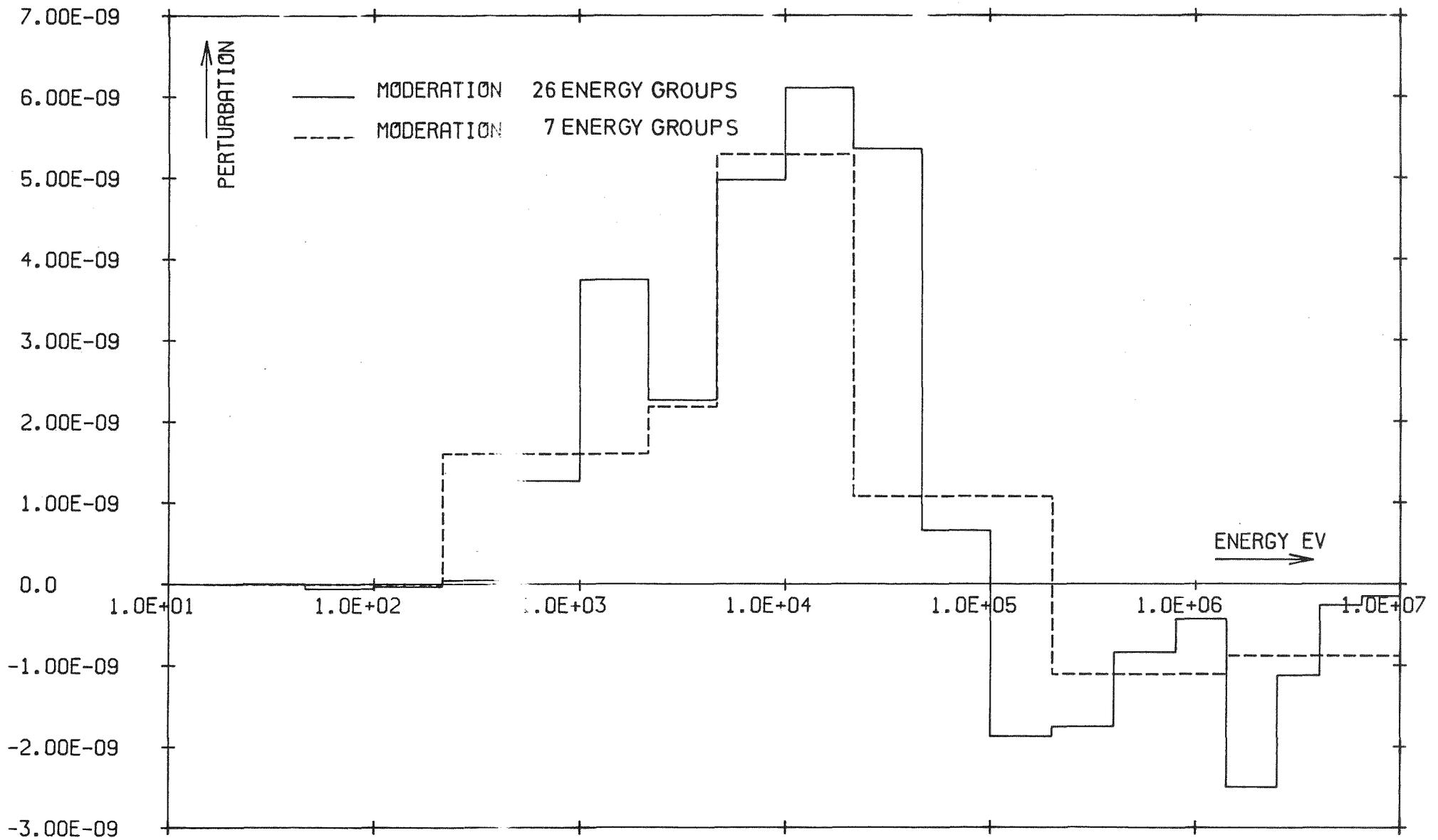
FIG. 17: ZPR III-48 SPHERICAL MODEL; CENTRAL H-MAT. WORTH: MODERATION TERM
FROM 26-GROUP AND CONSISTENT 7-GROUP LOCAL PERTURB. CALCULATIONS

FIG. 18: ZPR III-48 SPHERICAL MODEL; CENTRAL H-MAT. WORTH: MODERATION TERM
FROM 26-GROUP AND USUAL 7-GROUP LOCAL PERTURBATION CALCULATIONS