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Abstract

In the group cross section libraries usually applied for reactor calculations, the energy dependent probabilities of interactions between neutrons and the materials existing in the reactor are represented by weighted average values over certain energy ranges with a neutron energy spectrum regarded as representative. The influence of the resonance structure of the cross sections via the neutron spectrum and the resultant effect on the averaged group cross sections is taken into account in an approximate way by so-called resonance self-shielding factors. The approximations indicated are of considerable importance for the elastic down scattering. They can be improved by the so-called REMO correction, which takes into account the neutron energy distribution existing in the reactor model. Because such detailed neutron distributions are very expensive to prepare, especially in multi-dimensional models, automatic program runs were established which, in some cases by simplifications of the model, allow collision densities to be made available at relatively little expenditure which permit many nuclear quantities to be calculated with a sufficient degree of accuracy. This report describes the program runs set up and the experience acquired in testing them by the examples of the MASURCA 3B experiment and the SNEAK 11B2 assembly. This report deals especially with the influence of the collision density used for the REMO correction on the k_{eff} value and other parameters of the reactor models considered.

Verbesserung des elastischen Ausstreugruppenquerschnittes für Neutronen durch die REMO-Korrektur

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Zusammenfassung

Bei der Bereitstellung von Gruppenwirkungsquerschnitten für die Durchführung von Reaktorberechnungen werden die energieabhängigen Wahrscheinlichkeiten für Wechselwirkungen der Neutronen mit den im Reaktor vorhandenen Materialien unter Wichtung mit einem als geeignet angesehenen Neutronenenergiespektrum über Energiebereiche gemittelt. Der Einfluß der Resonanzstruktur der Wirkungsquerschnitte auf das Neutronenspektrum und die dadurch hervorgerufene Rückwirkung auf die gemittelten Gruppenwirkungsquerschnitte wird näherungsweise durch sog. Resonanzselbstabschirmungsfaktoren berücksichtigt. Die angegebenen Näherungen machen sich besonders bei der elastischen Ausstreuung bemerkbar. Sie können mit der sogenannten REMO-Korrektur durch Berücksichtigung der im untersuchten Reaktormodell vorhandenen Neutronenverteilung verbessert werden. Da die Bereitstellung solcher Neutronenverteilungen vor allem bei mehrdimensionalen Modellen sehr aufwendig ist, wurden automatisierte Programmabläufen erstellt, die es - teilweise durch Vereinfachung des Modells - ermöglichen, mit relativ geringem Aufwand Stoßdichten bereitzustellen, die die Berechnung vieler nuklearer Kenngrößen mit ausreichender Genauigkeit zulassen. Dieser Bericht beschreibt die erstellten Programmabläufe sowie die bei ihrer Erprobung am Beispiel des MASURCA 3B-Experimentes und der SNEAK 11B2-Anordnung gewonnenen Erfahrungen über den Einfluß der zur REMO- Korrektur verwendeten Stoßdichten auf den k_{eff}-Wert und auf andere Parameter der betrachteten Reaktor-Modelle.

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Introduction to the REMO Correction

In reactor calculations the interaction between the neutrons and the materials*) existing in the reactor is considered and the neutron balance is calculated on this basis. The energy dependent probabilities of interactions of the neutrons, such as capture, fission or scattering into other energy ranges, with nuclei of fissile or fertile materials, structural materials, coolants, neutron absorbers and neutron moderators are described by group cross sections averaged over energy ranges, taking an appropriate weighting spectrum into account. In calculating the group cross sections for a mixture of materials, several approximations are made on the basis of the technique customary for 26-group sets and adapted from the Russian ABBN concept /1/:

1. In generating the material dependent group cross sections stored in group constant sets, a given neutron energy distribution is used for weighting of the energy dependent cross sections, which normally differs from that really existing in the reactor to be calculated.

2. The influence of the resonance structure of the cross sections via the neutron distribution, and the resultant effect on the averaged group constants of a mixture of materials, is taken into account by resonance self-shielding factors in accordance with the usual sigma0-concept /2/. However, in this way only the influence of the resonance structure of the cross sections of just the material considered will be taken into account; for the influence of the other materials in the mixture the approximate assumption is made that it can be taken into account by an energy independent background cross section, sigma0.

3. In most cases, the resonance self-shielding factors for elastic scattering within the whole group are also used for elastic down scattering into the adjacent group. However, down scattering in the usual 26-group scheme generally is encountered only in the low energy part (the size of which differs as a function of the material) of each of the 26 groups. In this way, for instance, the influence of the position of a scattering resonance within the respective group cannot be treated adequately.

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*) In the framework of this report the expression material means isotope or element and the expression mixture means a composition made up usually of several materials.

The approximations indicated have a particularly strong impact on calculating elastic down scattering. The REMO correction /3/ is an attempt to avoid most of the drawbacks mentioned above: The elastic down scattering cross section, SME, into the neighboring, energetically lower group is determined by weighting the energy dependent cross section for elastic down scattering into the adjacent group with a neutron energy distribution approximately corresponding to that which is to be expected in the corresponding region of the reactor to be calculated.

$$(1) \qquad SME(g->g+1,m) = N(m)*\frac{\int_g PHI(E)*SE(E,m)*PE(E,m)*dE}{\int_g PHI(E)*dE}$$

with

m	material index
N	particle number density
g	group index in the 26-group set (g increases with decreasing neutron energy)
E	energy within group g
int	symbol indicating integration
PHI	energy distribution of the neutrons
SE	cross section for elastic scattering
PE	transition probability for elastic scattering of neutrons of energy E within group g into group g+1.

This method is applied mainly to fast reactors. Normally it is not possible in practical application to work with data at sufficiently numerous energy grid points, because PHI(E) frequently cannot be represented with a sufficiently high energy resolution. For this reason, the first 14 groups in the 26-group set are subdivided into 14 fine groups, each with the same lethargy width. Each of the fine groups is subdivided into five intervals of the same energy width. The calculation can be further simplified by using for the weighting not the interval dependent neutron flux integral, but the quotient of the fine group dependent collision density integral and the interval dependent total cross section of the mixture. This substitution is justified, for the collision density can be regarded as largely constant within a fine group:

$$(2)\quad STD(i)/dE(i) = PHI(E)*\sum_{m}(N(m)*STOT(E,m)) = const \qquad \text{for E from fine group i}$$

The energy dependence of the neutron distribution within a fine group, which is important for the REMO correction, is determined largely by the interval dependent total cross section of the mixture. Accordingly, the following approximation is used:

$$(3)\quad int(PHI(E)) = STD(i)/\sum_{m}(N(m)*STOT(j,m))$$

with

m	material index
j	interval index for energy intervals in fine group i
i	fine group index
E	energy within fine group i
dE(i)	energy width of fine group i
int	symbol indicating integration
sum	symbol indicating summation
N	particle number density
STD	integral collision density, STOT*int(PHI), in fine group i
STOT	total cross section.

The fine group dependent collision density can be obtained from the neutron flux integrals calculated with a standard reactor code in a fine group structure by multiplication with the corresponding total cross sections of the mixture. For implementing the REMO correction it is regarded as being representative of the mixture occurring in a certain reactor zone. The interval dependent total cross sections required in implementing the REMO correction for finer energy resolution within a fine group, together with the interval dependent data for elastic scattering and for the transition probabilities for a number of materials particularly important for reactor calculations, are contained in the REMO-GRUBA file. The approximations described above, and substitution of (3) into (1), result in the elastic down scattering cross section, SME, into the adjacent group as:

$$(4)\qquad SME(g\to g+1,m) = N(m)\cdot\frac{\sum_i STD(i)\cdot\sum_j \frac{SE(j,m)\cdot PE(j,m)}{\sum_m N(m)\cdot STOT(j,m)}}{\sum_i STD(i)\cdot\sum_j \frac{1.0}{\sum_m N(m)\cdot STOT(j,m)}}$$

with E(g).GE.E(i).GT.E(j).GT.E(i+1).GE.E(g+1)

where

m	material index
g	group index in the 26-group set
i	fine group index
j	interval index for energy intervals in fine group i
E	energy; E(g), E(i) energy of a group boundary; E(j) energy of an energy interval
sum	symbol indicating summation
N	particle number density
STD	integral collision density, sum(m) (N(m)*STOT(i,m))*int(PHI) with int(PHI) flux integral over a fine group i, STOT(i) fine group dependent total cross section
SE	cross section for elastic scattering
PE	transition probability for elastic scattering into group g+1 from the energy interval j located within group g in fine group i
STOT(j)	interval dependent total cross section.

The energy distribution of the neutrons and thus the collision densities can be determined by calculations, sometimes for geometrically simplified reactor models, with 208 energy groups. In this approach, which is used at the Nuclear Research Center Karlsruhe, the energy limits of the first 196 (high energy) groups correspond to the energy group structure used in the REMO correction. The first 14 groups of the 26-group set (E>1keV) are subdivided into 14 fine groups, each of the same lethargy width, and each fine group is subdivided into five intervals of the same energy width. The energy boundaries of the last 12 (low energy) groups of the 26-group set (E<1keV) are adopted unchanged. The interval data within a fine group are

weighted with the weighting function int(PHI(E)) described above and summed up into fine group data during the calculation of the macroscopic cross sections in GRUCAL /5/. The approximations indicated can largely be avoided in calculations with 208 energy groups. However, because of the relatively high computation costs, especially in multi-dimensional problems, 26-group calculations cannot be replaced in routine applications as standard methods of computing k_{eff} by calculations with 208 energy groups. Because of the consequently reduced significance the 208-group cross section library does not contain all materials. The inaccuracies arising from the substitution of materials have no major influence on the energy distribution of the neutron fluxes and thus do not prevent the calculation of collision densities, whose accuracy is sufficient for execution of the REMO correction.

The collision densities required for execution of the REMO correction can be obtained by reactor calculations in 0-, 1- or multi-dimensional geometries. In order to minimize the computation expenditure, the reactor considered must be reduced to a model with the simplest possible geometry of the assembly considered, while still furnishing results of sufficient accuracy. This may require a new uniform mixture to be obtained from a number of mixing compositions; afterwards, the mixture input must be matched to the 208-group cross section data file containing fewer materials. In multi-dimensional models usually suitable reductions to a one-dimensional model must be made. For the simplified provision of collision densities within the framework of KAPROS /4/ the REMK1D and REMK2D KAPROS programs were set up /10/. This report contains a description of these programs and of the experience accumulated in testing them concerning the influence of the collision densities used for the REMO correction on the nuclear parameters in the assemblies considered.

Purpose of the Studies

Executing the REMO correction implies a certain amount of expenditure which, as a rule, increases with the complexity of the problem and, in particular, with the number of space dimensions for the geometric representation of the reactor model. Especially in two- and three-dimensional problems additional difficulties can arise from making available the appropriate collision densities for executing the REMO correction. However, in many cases studies of appropriately simplified reactor models are sufficient to provide a first impression of the influence of the REMO correction on the main parameters of interest. Very often the corrections obtained in this way can be transferred directly to the results of multi-dimensional calculations. Moreover, the collision densities found in this way can be used for further two- or three-dimensional calculations. In tests of the KAPROS programs /4/ for providing collision densities for the execution of the REMO correction in one-dimensional and two-dimensional reactor models /10/ comparative studies were conducted of the influence of the collision densities used in the REMO correction upon the criticality, k_{eff}, of the model considered and upon other nuclear parameters. Especially two problems were of interest:

1. What are the changes in the nuclear parameters of a reactor if, in executing the REMO correction, a reactor specific collision density is used instead of the standard collision densities provided in GRUCAL?

2. What error can be caused if, in a two-dimensional reactor model, instead of the collision densities obtained from expensive two-dimensional 208-group calculations those collision densities are used which were calculated from one-dimensional 208-group calculations (obtained from a section through the two-dimensional model)?

The studies were conducted during application tests of the newly formulated REMK1D and REMK2D KAPROS programs /10/ on the example of the MASURCA 3B experiment /7/ and the SNEAK 11B2 assembly in the normal case and the sodium void case /8/. From these two models neither a maximum influence of the REMO correction, nor an influence typical of a fast reactor can be expected, but its influence is sufficient to allow the questions above to be answered.

Computational Assistance by the Karlsruhe KAPROS Program System

The Karlsruhe KAPROS program system /4/ enables programs to be interconnected and calculated data to be passed on. This facilitates work on complex problems requiring several programs to be called. The programs can be called by routines of the KAPROS systems kernel in FORTRAN programs, which also allow the calculated data to be used to control the program sequence (e. g., accuracy checks during iterations). The data used as input or output quantities by the programs are managed as so-called data blocks by KAPROS. The existing core memory is used for storage as far as possible; if necessary, data blocks are stored on external disk memories. The occupancy of the core memory by programs and work fields is automatically adapted by KAPROS to the program lengths which changes as a consequence of program changes. Access to the data stored is provided by calling subprograms of the KAPROS systems kernel /4/, which then write, read or change data in data blocks.

For the understanding of some sections of this report it would be helpful, if the reader were familiar with details of KAPROS and some of the programs which are extensively used to carry out the REMO correction.

1. Description of the KAPROS Programs Set up for Execution of the REMO Correction

A number of programs were set up for execution of the REMO correction within the framework of KAPROS. Some of these programs can be applied also to problems not directly related to the REMO correction.

The programs set up can be subdivided into three groups:

1. Providing mixture input.
   - 1.1 MIMI for combining several individual mixtures (MIxing of MIxtures).
   - 1.2 SIMI for substituting materials of a mixture to match the modified mixture input to a group constant data file not containing all materials existing in the original mixture input (SImplifying of MIxtures).

2. Calculating collision densities.
   - 2.1 STD for calculating mixture dependent collision densities from neutron fluxes and macroscopic group constants.

3. Proividing collision densities for the REMO correction.
   - 3.1 REMK1D by 0- or 1-dimensional diffusion calculations.
   - 3.2 REMK2D by 1-dimensional diffusion calculations obtained as a section through a two-dimensional reactor model based on an input for the two-dimensional diffusion code DIXY code /11/.

The following sections are to provide a global overview of the functions of the programs listed above; a more detailed outline and a description of the necessary inputs can be found in /10/.

1.1 MIMI for Mixing Mixtures

The program serves for the generation of new mixtures from given fractions of starting mixtures.

The fractions of the starting mixtures for a new mixture are in normal case normalized to 1.0 before the beginning of the calculation. For all materials k occurring in the M starting mixtures, the particle number densities, N(k), of the materials in a new mixture and their temperatures, T(k), are calculated as

$$N(k) = \sum_{j=1}^{M} (F(j)*N(j,k)) / \sum_{j=1}^{M} F(j)$$

$$T(k) = \sum_{j=1}^{M} (F(j)*N(j,k)*T(j,k)) / \sum_{j=1}^{M} F(j)*N(j,k)$$

where

M	number of starting mixtures of the new mixture
N(j,k)	particle number density of material k in the starting mixture j
N(k)	particle number density of the material k in the new mixture
T(j,k)	temperature of the material k in the starting mixture j
T(k)	temperature of the material k in the new mixture
F(j)	fractions of the M starting mixtures.

In order to prevent changes, due to inaccuracies in calculation, in the frequently occurring standard temperatures 300 K, 900K and 2100 K, which would cause deviations in the results of the GRUCAL calculation, deviations in T(k) of less than 0.5 K are rounded to the corresponding standard temperature.

1.2 SIMI for Substituting Materials of a Mixture

The program serves for matching the mixing input for GRUCAL /5/ to a data file of group constants not containing all the materials occurring in the originally spezified mixtures; it is required, for instance, to simplify the transition from 26-group calculations to 208-group calculations. Materials not existing in the new group set are substituted by different materials in accordance with the rules found in a standard substitution table, which may be modified by input. For each material to be substituted an indication is made as to whether the material is to be deleted without substitution or by which fractions of other materials it is to be replaced. The fractions of the same material resulting from the substitution of several materials are added up to guarantee the adequate resonance self-shielding. The temperature chosen for one material is the temperature of the fraction of this material with the highest particle number density. The Annex lists the rules contained in the standard substitution table for matching mixtures to the 208-group constant data file, which contains fewer materials than, e. g., the 26-group KFKINR set /9/. In substituting it is attempted, as far as possible, to leave unchanged the respective particle number densities and the most important nuclear parameters of the materials substituted. Depending on the material, this relates to the total cross section, the absorption cross section, the elastic cross section, the slowing down power and, in fissile materials, the difference between the neutron production cross section and the absorption cross section (which is an approximate indication of the reactivity worth). As the total cross sections and the value of the average scattering cosine frequently show relatively little difference for nuclei with similar atomic weights, it is possible to ensure in many cases that, when making substitutions, not only the total particle number density but in most cases also the contribution to the macroscopic transport cross section remains almost unchanged (although in general this cannot be achieved in all energy groups at the same time). The reference values used are the group constants from 26-group data files containing additional materials and single-group cross sections averaged over a typical spectrum of a sodium cooled fast reactor.

1.3 STD for Calculating Mixture Dependent Collision Densities

The program serves for calculating mixture dependent collision densities, STOT*int(PHI), from group dependent integrals of neutron fluxes for partial regions of identical mixture compositions and the corresponding total cross sections. The neutron flux integrals must be calculated in a preceding 0-, 1- or multi-dimensional diffusion or transport calculation, while the total cross sections are taken from the cross section block set up by GRUCAL /5/.

1.4 REMK1D Supplying Collision Densities for Executing the REMO Correction by means of 0- or 1-dimensional Diffusion Calculations

The program provides collision densities for executing the REMO correction. The collision densities are obtained by 0- or 1-dimensional diffusion calculations. In 0-dimensional calculations a buckling iteration to k_{eff}=1.0 can first be carried out. The influence of the REMO correction on the k_{eff} value of a reactor can be estimated, if desired, by control calculations without and with the REMO correction. In this way, it is possible in many cases to obtain an impression about the significance of expensive multidimensional calculations. The control calculations are based on group cross section calculations, sometimes simplified, (e. g. without additional corrections such as the improvement of the fission spectrum) in order to preclude the influence of other corrections. The program sequence is controlled by the input data blocks transferred to REMK1D. If there is an input for the MIMI program (see 1.1), a new mixture block is generated by MIMI. The SIMI program (see 1.2) generates from the original mixture block, or the mixture block made available by MIMI, another mixture block enabling 208-group calculations to be performed. In the absence of an input for the 0-dimensional diffusion program DIFF0 /12/ or the one-dimensional diffusion program DIF1D /12/, a buckling iteration for k_{eff}=1.0 is first carried out with BUCITO /12/ for core mixtures. In the same process, an input is generated for the 0-dimensional diffusion program. The input blocks then available are used to calculate 208-group collision densities. If a control calculation is desired, the original mixture block or, if there had been an input for MIMI, the mixture block generated by MIMI, is used for group cross section calculations without and with REMO correction. Subsequently, 0- or 1-dimensional diffusion calculations are carried out from the results of which the user can recognize the influence of the REMO correction, for instance, on the criticality worth or the group dependent neutron fluxes.

1.5 REMK2D for Supplying Collision Densities on the Basis of an Input for the Two-dimensional Diffusion Code DIXY

On the basis of a two-dimensional reactor model, the program makes available suitable collision densities for carrying out the REMO correction for the two-dimensional diffusion calculations with DIXY /11/. First of all REMK2D by calling the KAPROS program DX6731 /12/, produces a section through the two-dimensional reactor model and carries out a one-dimensional diffusion calculation in the sectional plane by means of DIF1D /12/. For this purpose, the input for REMK2D contains an indication of the direction of the section (horizontal or vertical) and the number of the mesh line in the two-dimensional grid through which the section is to be made. For the geometry defined in this way, DX6731 on the basis of the input for DIXY, sets up the input for DIF1D. In the input for MIMI, the user defines a new mixture block starting from the original mixture block for the DIXY calculation. For this purpose, mixtures can be adopted unchanged or several mixtures can be put together into a new mixture as described before. Each zone of the one-dimensional model is assigned the number of the mixture in the new mixture block. The mixture number indicated in the input is included in the geometry block for DIF1D set up by DX7631. The SIMI program (see 1.2) is used to transform the mixture block for 208-group calculations; the GRUCAL program finally generates a 208-group cross section block. The user has the possibility to provide a buckling block for the one-dimensional calculation or to carry out, by means of IBUCK1 /12/, a one-dimensional buckling iteration with a group set with 26 or 208 groups. The data blocks made available in accordance with the program sequence described above are used to carry out a one-dimensional 208-group diffusion calculation; the flux integrals obtained are converted into collision densities by means of STD (see 1.3). Collision densities newly calculated, e. g., by multiple calling of REMK2D for sections in various planes and/or directions, are added to an existing block of collision densities so that a single block of collision densities is available at the end of the calculation of collision densities. Allocating the collision densities obtained in this way to the original mixture block for the DIXY calculation requires special care to be exercised: The numbering of the collision densities generated by the application of MIMI and by writing in a sequential order must be taken into account; moreover, the proper choice of the collision density used for the REMO correction of the

respective mixture necessitates a certain amount of experience and physical touch (not every mixture is necessarily contained in a one-dimensional section, while other mixtures may occur several times). The program sequence and the allocation of mixtures and collision densities becomes clearer when considering the example given for the SNEAK 11B2 assembly (see Chapter 3 and Fig. 2 to 5).

2. Studies of a One-dimensional Model of the MASURCA 3B-Experiment

The one-dimensional model of the MASURCA 3B experiment /7/ was used to study the influence of the REMO correction and the influence of the collision densities used for the REMO correction upon the k_{eff} of the experiment considered. Figure 1 shows the structure of the experiment and the used mixture.

2.1 Calculations Performed

The 26-group cross sections to be used for one-dimensional diffusion calculation were calculated

(a) without REMO correction and

(b) with REMO correction with two different types of collision densities the collision density stored in GRUCAL, which is typical of the SNR-2 /6/, and the collision densities derived with REMK1D, which are typical of the MASURCA 3B experiment.

The calculations were performed with an accuracy in k_{eff} of 0.0001. In the sequence of this program, a one-dimensional diffusion calculation with 26-group cross sections without REMO correction is carried out first to calculate an initial estimate of the source distribution with an accuracy in k_{eff} of 0.05. The composition of the mixture is adapted to the materials existing in the 208-group GRUBA file by internal call of SIMI (see 1.2). In a subsequent 208-group GRUCAL run followed by a diffusion calculation the collision densities for the REMO correction are derived. Diffusion calculations in 26 groups, with cross sections without and with REMO correction, represent the influence of REMO correction on the calculated k_{eff} value of the experiment. Compared to the original k_{eff} of 0.99361, the REMO correction reduced k_{eff} by 0.0024 to 0.99122. The values found for the REMO correction constitute a reliable indication of the corresponding values to be expected in studies carried out in two- and three-dimensional geometries, respectively.

2.2 Results of Calculations

The table below contains a summary of the k_{eff} values resulting from the calculations performed.

REMO corr.	Collision density used	k_{eff}
Without		0.99361
With	SNR-2	0.99440
With	from REMK1D	0.99122

It has thus been found for the MASURCA 3B experiment that the use of a collision density stored in GRUCAL results in a change in k_{eff} in the wrong direction (+0.0008 as against -0.0024, when using a collision density typical of an experiment). In this case, the application of the stored collision densities should be avoided and the use of a collision density typical of the experiment is indispensable; its calculation is greatly facilitated by the REMK1D program (see 1.4).

3. Studies of a Two-dimensional Model of the SNEAK 11B2 Assembly

The model of the SNEAK 11B2 R/Z assembly /8/ (see Fig. 2 and Fig. 3) was used to study, for the normal case and the sodium void case, the error produced by different ways of performing the REMO correction, explained in the following section 3.1. The influence of the various collision densities used for the REMO correction on the calculated k_{eff} of the assembly and on the fission rate traverses of U-235 and Pu-239 was investigated.

3.1 Calculations Performed

DIXY calculations /11/ with evaluations were carried out subsequent to the calculations of cross sections without and with REMO corrections with various collision densities. Their results allowed to derive the influence of the collision densities used for the REMO correction on the k_{eff} and on the fission rate traverses. All 26-group DIXY calculations were carried out with a source accuracy of 1.0E-4 and a flux accuracy of 1.0E-4. For comparison, the calculations were performed first without the REMO correction. In the further calculations, the REMO correction was carried out for all 25 mixtures for the materials C, Cr, Fe, Mo, Na, Ni, O, as far as they were present in the mixtures, in the energy groups 1 to 14. The collision densities used for the REMO correction were obtained in the following way:

1. The CHIETCON collision density stored in GRUCAL was used. The use of CHIETCON (composed of a fission spectrum, CHI (U) above 2.5 MeV and a constant below 2.5 MeV, see Fig. 6) for the collision density in the approximate execution of the REMO correction (see /8/) appeared to be acceptable, because the SNEAK 11B2 assembly contained mixtures with a relatively high hydrogen content, which was assumed to lead to a rather soft neutron spectrum.

2. The collision densities were calculated with the REMK2D program by means of three one-dimensional diffusion calculations for sections through the two-dimensional model. The REMK2D program was used to make two horizontal sections in the DIXY grid lines 18 and 35 and one vertical section in the reactor axis (see Fig. 4). Two horizontal sections were found to be necessary for ascertaining with sufficient

accuracy both the mixture 3 (core + absorber) and the mixture 4 (core + follower) (see Fig. 2 to Fig. 4). In the horizontal sections, the mixtures penetrated by the sections were incorporated unchanged in the one-dimensional diffusion calculation. For the vertical section, the core mixtures adjacent to the section plane in the horizontal direction were averaged. The averaging factors used were the flux integrals in group 10 (an energy range known to give a comparably large contribution to important reaction rates) from the DIXY reference calculation (REMO correction with the CHIETCON collision density) (see Fig. 6). The group independent axial and radial bucklings for the one-dimensional diffusion calculations were computed approximately from the geometry data of the reactor. The attribution of the collision densities calculated by means of the one-dimensional diffusion calculations to the mixtures of the two-dimensional model can be seen from Fig. 4 and Fig. 5. Other attributions are probably also possible, but the approach selected appears to be physically plausible.

3. The collision densities were calculated from a two-dimensional 208-group DIXY calculation. A two-dimensional 208-group calculation constitutes the most precise possibility feasible at tolerable expenditure to determine the collision densities required for the REMO correction. This avoids the approximations and corresponding errors associated with the use of the REMK2D program due to simplification of the geometry. As only the energy distribution of the fine groups within one coarse group is important for the REMO correction, the 208-group DIXY calculation was carried out with relatively moderate accuracy. The source distribution of the preceding 26-group calculation without REMO correction was used for a source estimate. The 208-group calculation was terminated after three iterations; the accuracy achieved was 5.E-3 for the source, 6.5E-3 for the flux. Calculating the collision density took some 14 minutes of computation time on the Siemens 7890 computer, approx. one minute of this for the 208-group GRUCAL calculation and some 13 minutes for the 208-group DIXY calculation. The REMO correction was carried out with collision densities from calculations with two iterations and with three iterations, the 26-group DIXY calculations carried out subsequently resulted in a k_{eff} of 0.9878805 with the collision density from two iterations and a k_{eff} of 0.9878865 with the collision density from three iterations, which is only a minor difference. This proves that a

small number of iterations with fairly low source and flux accuracy are sufficient to obtain reasonably reliable collision densities for carrying out the REMO correction (given a sufficiently accurate source estimate, which can be obtained from a 26-group calculation).

3.2. Results of calculations

The collision densities resulting from the calculations are shown in Fig. 7 to Fig. 10. It can be seen from the diagrams that the core region and the radial blanket and reflector regions are described relatively well by the collision densities calculated in REMK2D, while the more heterogeneous axial blanket and reflector regions are represented badly by the corresponding collision densities from REMK2D. This means that the application of REMK2D is less useful when more precise data are required, for instance, for reaction rates in the blanket and reflector regions; in those cases, collision densities should be used from a 208-group DIXY calculation with low accuracy requirements. The k_{eff} values achieved with the different collision densities in DIXY are summarized in the Table below:

REMO corr.	Collision density used	k_{eff} normal	k_{eff} Na void
Without		0.989299	0.952531
With	CHIETCON	0.990135	0.952564
With	from REMK2D	0.988070	0.951132
With	from DIXY 208 groups	0.987920	

The relative change in the sodium void effect brought about by the REMO correction was relatively slight in SNEAK-11B2. This was to be expected for the small core because, with a highly negative sodium void effect, only the small fraction of the degradation term is influenced by the REMO correction, but not the diffusion term, which is larger in absolute amounts. In larger reactors, however, the negative diffusion term (largely unaffected by the REMO correction) and the then positive degradation term will partially compensate each other. As a consequence, a change in the

degradation term by the REMO correction in such reactors produces a larger relative change in the sodium void effect. Because of the relatively slight importance of the REMO correction for the sodium void effect in this case, no sophisticated 208-group DIXY calculations were performed for the sodium void case. Fig. 11 shows the axial fission rate traverses along the core axis for U-235 and Pu-239. The relatively good agreement is seen between the data calculated by means of the collision densities from REMK2D and from DIXY, while the data calculated without REMO correction and with the help of the CHIETCON collision density stored in GRUCAL, respectively, differ in various directions.

4. Conclusions

Executing the REMO correction was greatly facilitated by the KAPROS programs, REMK1D for zero- or one-dimensional reactor models and REMK2D for two-dimensional models, which provide the appropriate collision densities for the REMO correction. The MIMI and SIMI programs called by REMK1D and REMK2D relieve the need for the user to make input modifications which formerly had to be carried out largely manually. Consequently, the REMO correction, which so far has been carried out infrequently and, if at all, with sometimes unsatisfactory collision densities because of the expenditure involved in calculating suitable collision densities, can now also be applied routinely. However, especially when using the REMK2D program, a careful approach must be considered in choosing the sections through the two-dimensional model and attributing the collision densities to the original mixtures.

The following conclusions can be drawn from the results of the recalculation of the MASURCA 3B experiment and the SNEAK 11B2 assembly with regard to calculations of the collision densities and their use for REMO correction:

- Using a collision density which is not typical of a reactor, such as CHIETCON, may furnish unsatisfactory results.
- Using collision densities typical of a reactor from one-dimensional approximations and from two-dimensional calculations will produce a large amount of agreement, especially in the criticality value.
- Collision densities from two-dimensional 208-group calculations should be used to calculate reactions rates etc., especially in very heterogeneous reactor regions.
- If collision densities are obtained from two-dimensional 208-group calculations, normally a small number of iterations of relatively low accuracy are sufficient.

The procedure to be adopted in carrying out the REMO correction must be determined by the user in the light of the assembly considered, the nuclear parameters to be determined, and the accuracy desired.

The author would like to express his gratitude to Dr. E. Kiefhaber for numerous suggestions concerning the execution of the calculations and the support, given in many discussions including the compilation of this report. He also would like to thank Mr. R. Friese for translating a draft of this report which originally was written in German and Mrs. Duffner for her expert and patient typing of several versions of this report.

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Annex

Standard Substitution Rules for SIMI

At the time of this writing it was not possible to indicate useful substitution rules for some materials in the standard substitution table, e. g., because of the absence of suitable single-group cross sections. In this case, NMN=-1 was assumed, which means that the user will have to indicate his own rules, when such materials occur in his mixtures.

NAMOLD	NMN	NAMNEW	FACTOR	BASIS
AG	2			SABS
		NB	0.47	
		GD	0.53	
AG107	2			SABS
		NB	0.5	
		GD	0.5	
AG109	2			SABS
		NB	0.4	
		GD	0.6	
AL1/E	1			
		AL	1.0	
AM241	2			NUSF-SABS
		PU239	0.05	
		U 238	0.95	
AM243	1			NUSF-SABS
		U 238	1.0	
ANTI	-1			PSEUDOMATERIAL
AU	2			SABS
		TA	0.8	
		PB	0.2	
B10/E	1			
		B 10	1.0	
B11/E	1			
		B 11	1.0	
BE1/E	1			
		BE	1.0	
C1/E	1			
		C	1.0	
CD	2			SABS
		NB	0.95	
		GD	0.05	
CF252	-1			
CM242	-1			
CM244	2			NUSF-SABS
		PU239	0.25	
		PU240	0.75	
CO	2			SABS
		MN	0.6	
		NI	0.4	
CS	2			SABS
		NB	0.6	
		GD	0.4	

CU	2			SABS
		MN	0.8	
		NI	0.2	
D	2			SLOWING DOWN POWER, SELSC
		H	0.087	
		HE 4	2.25	
D1/E	2			SLOWING DOWN POWER, SELSC
		H	0.087	
		HE 4	2.25	
DPA	-1			PSEUDOMATERIAL
DPA70	-1			PSEUDOMATERIAL
DPA81	-1			PSEUDOMATERIAL
EAVER	-1			PSEUDOMATERIAL
EU151	-1			
EU153	-1			
F	2			SABS
		AL	0.95	
		N	0.05	
FAFLU	-1			PSEUDOMATERIAL
FE1/E	1			
		FE	1.0	
FPP35	1			
		SPP 9	1.0	
FPP38	1			
		SPP 9	1.0	
FPP39	1			
		SPP 9	1.0	
FPP40	1			
		SPP 9	1.0	
FPP41	1			
		SPP 9	1.0	
FPP42	1			
		SPP 9	1.0	
GA	2			SABS
		NB	0.45	
		NI	0.55	
H1/E	1			
		H	1.0	
HE 3	2			
		HE 4	0.15	SLOWING DOWN POWER, SABS
		B 10	1.25	
HE3/E	2			
		HE 4	0.15	SLOWING DOWN POWER, SABS
		B 10	1.25	
HE4/E	1			
		HE 4	1.0	
I	2			SABS
		NB	0.6	
		GD	0.4	
I 129	2			SABS
		NB	0.85	
		GD	0.15	
IN115	-1			
LA139	2			SABS
		NI	0.997	
		GD	0.003	
LI6/E	1			
		LI 6	1.0	

```
LI  7     2                                  SLOWING DOWN POWER, SELSC
             HE  4    0.35
             BE       0.13
LI7/E     2                                  SLOWING DOWN POWER, SELSC
             HE  4    0.35
             BE       0.13
MG1/E     1
             MG       1.0
MN1/E     1
             MN       1.0
N1/E      1
             N        1.0
NA1/E     1
             NA       1.0
ND       -1
NI1/E     1
             NI       1.0
NP237     1                                  NUSF-SABS
             TH232    1.0
O1/E      1
             O        1.0
P         2                                  SABS
             CL       0.63
             SI       0.37
PA233     1                                  NUSF-SABS
             TH232    1.0
PD       -1
PR        2                                  SABS
             NI       0.80
             HF       0.20
PU238     2                                  NUSF-SABS
             PU239    0.45
             PU240    0.55
RH        2                                  SABS
             NB       0.5
             GD       0.5
SM       -1
SP233     1
             SPP 9    1.0
SP235     1
             SPP 9    1.0
TH1/E     1
             TH232    1.0
U33/E     1
             U 233    1.0
U 234     2                                  NUSF-SABS
             U 238    0.95
             PU239    0.05
W         2                                  SABS
             HF       0.7
             PB       0.3
XY       -1                                  PSEUDOMATERIAL
XY1/E    -1                                  PSEUDOMATERIAL
ZR1/E     1
             ZR       1.0
END
```

with

NMN	number of materials used for substitution
SABS	SIGMA (absorption)
NUSF	NUE x SIGMA (fission)
SELSC	SIGMA (elastic scattering)

Buckling B**2 = 6.5E-4 cm**-2

CORE		BLANKET		REFLECTOR	
U 235	0.189394-2	U 235	0.753337-4		
U 238	0.641852-2	U 238	0.176938-1		
K	0.507117-6	FE	0.863468-2		
FE	0.119932-1	CR	0.233604-2		
CR	0.324629-2	NI	0.116204-2		
NI	0.196474-2	MO	0.170708-4	FE	0.572255-1
MO	0.165357-4	AL	0.177894-5	CR	0.154564-1
AL	0.619493-5	ZR	1.052370-6	NI	0.822061-2
ZR	0.433342-6	O	0.355383-1	MO	0.299472-4
NB	0.885287-6	C	0.338493-4	NB	0.162207-5
B 10	0.230813-6	N	0.143926-4	PB	0.146066-6
B 11	0.936091-6	NA	6.149900-6	C	0.153218-3
O	0.119214-1	W	0.222879-5	W	0.965310-5
C	0.327326-4	TI	0.135704-5	TI	0.370652-5
NA	0.913500-2	CU	0.192700-3	CU	0.151251-2
W	0.181887-5	H	0.124275-5	H	0.124460-5
TI	0.189750-5	SI	0.131351-3	SI	0.922670-3
LI 6	0.131460-5	CA	0.239513-5	V	0.246142-4
CU	0.124341-3				
H	0.580228-5				
SI	0.870679-4				
CA	0.123694-5				
MG	0.224186-5				
V	0.201556-5				

atomic number densities in 10**-24 cm**3

0.0 — 54.155 — 78.432 — 88.0 — 108.40 r(cm)

19 — 8 — 3 — 5

Number of intervals

Fig. 1: Structure of the MASURCA 3B experiment as a cylindrical model.

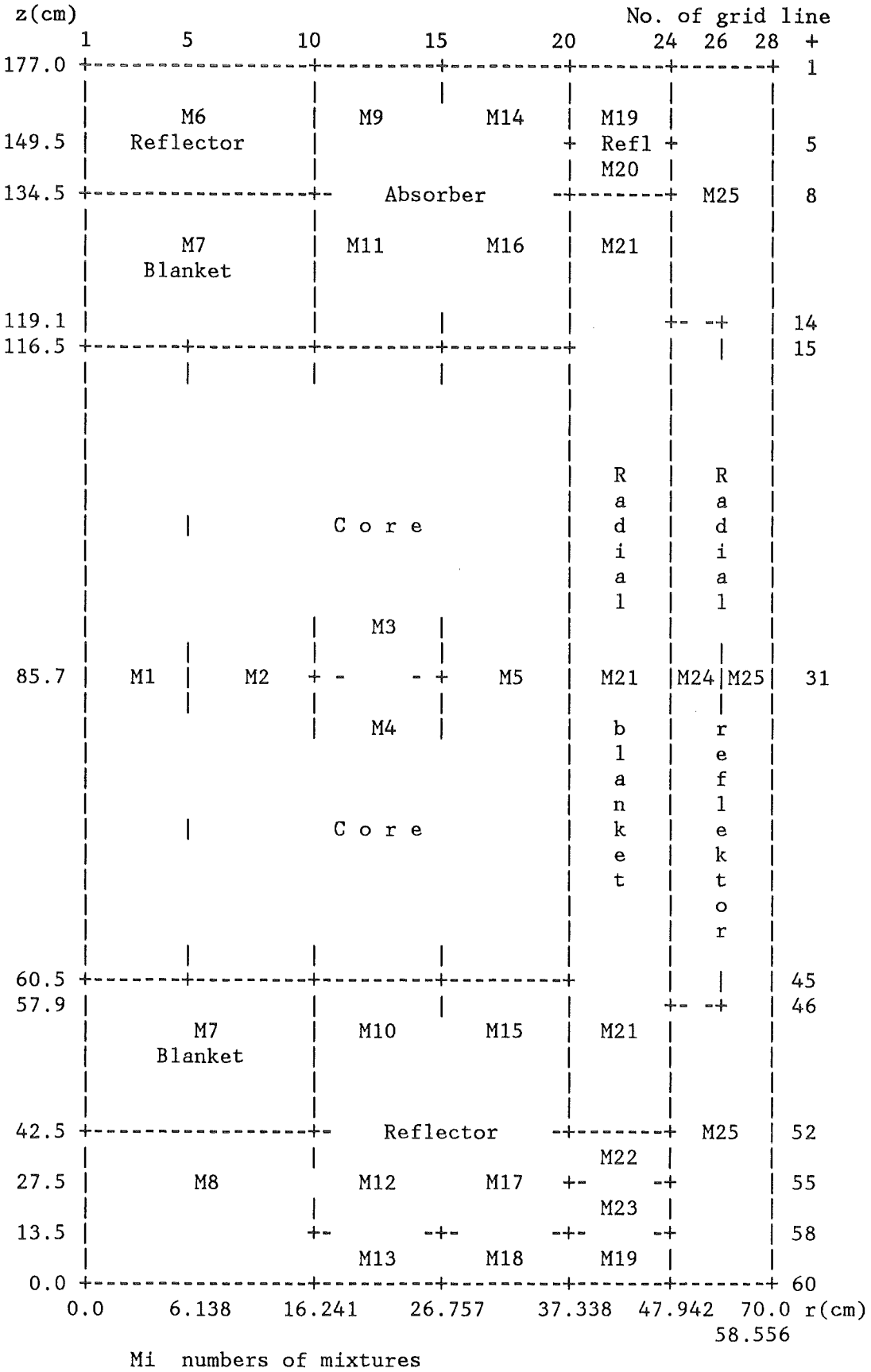
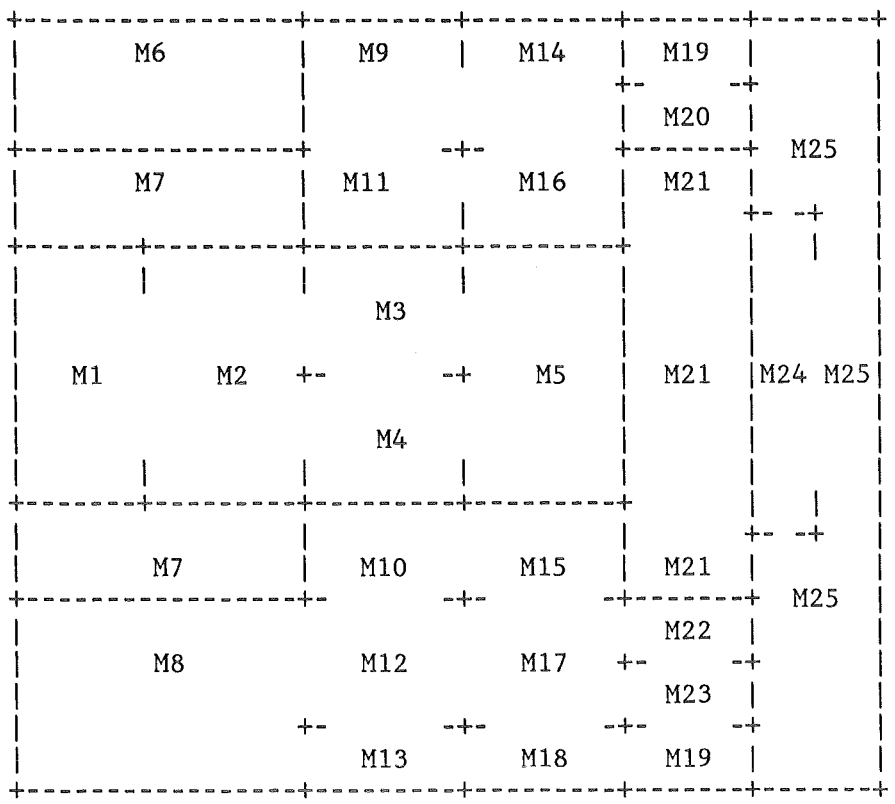
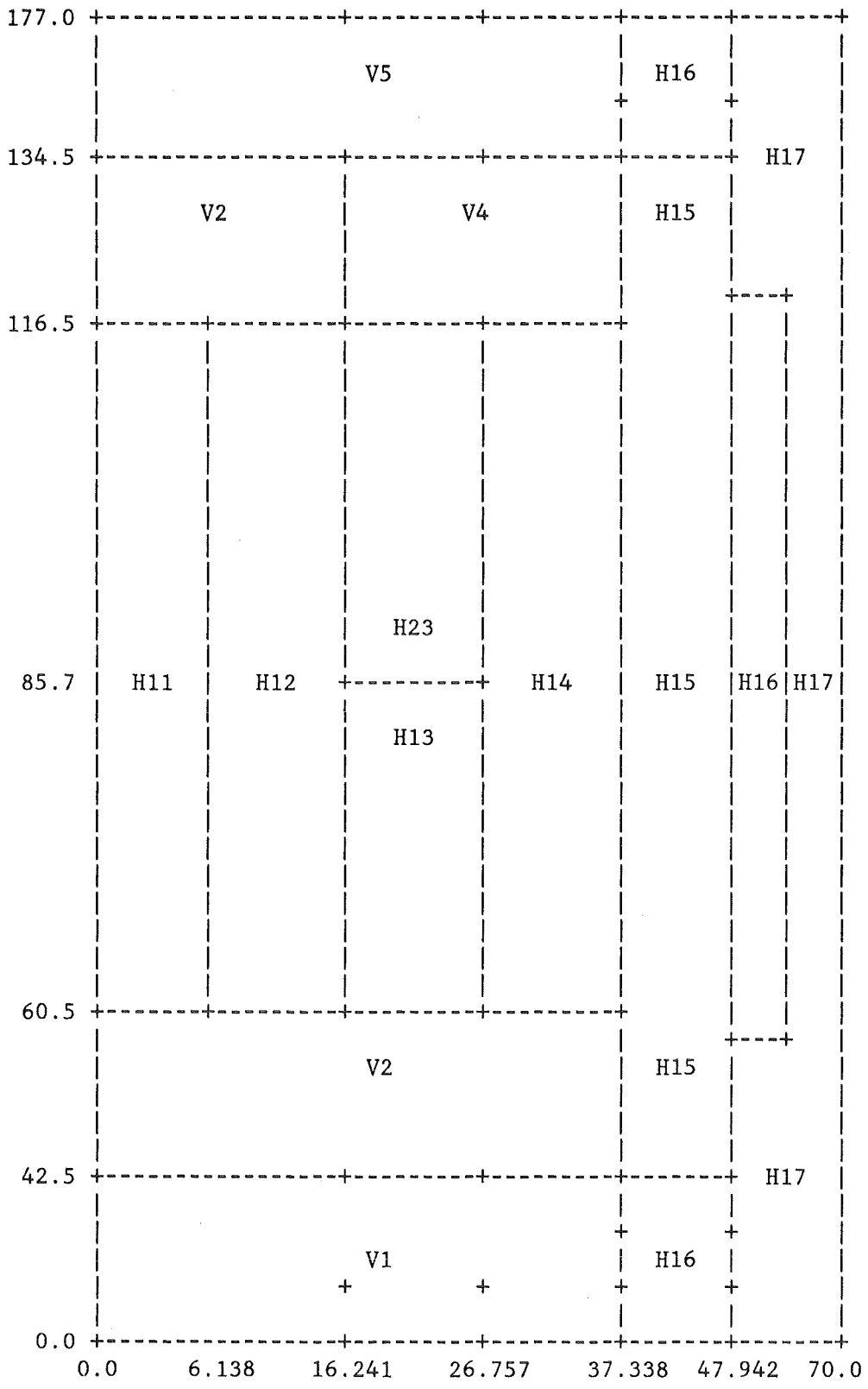


Fig.2: Structure of the SNEAK 11B2 assembly (RZ geometry)



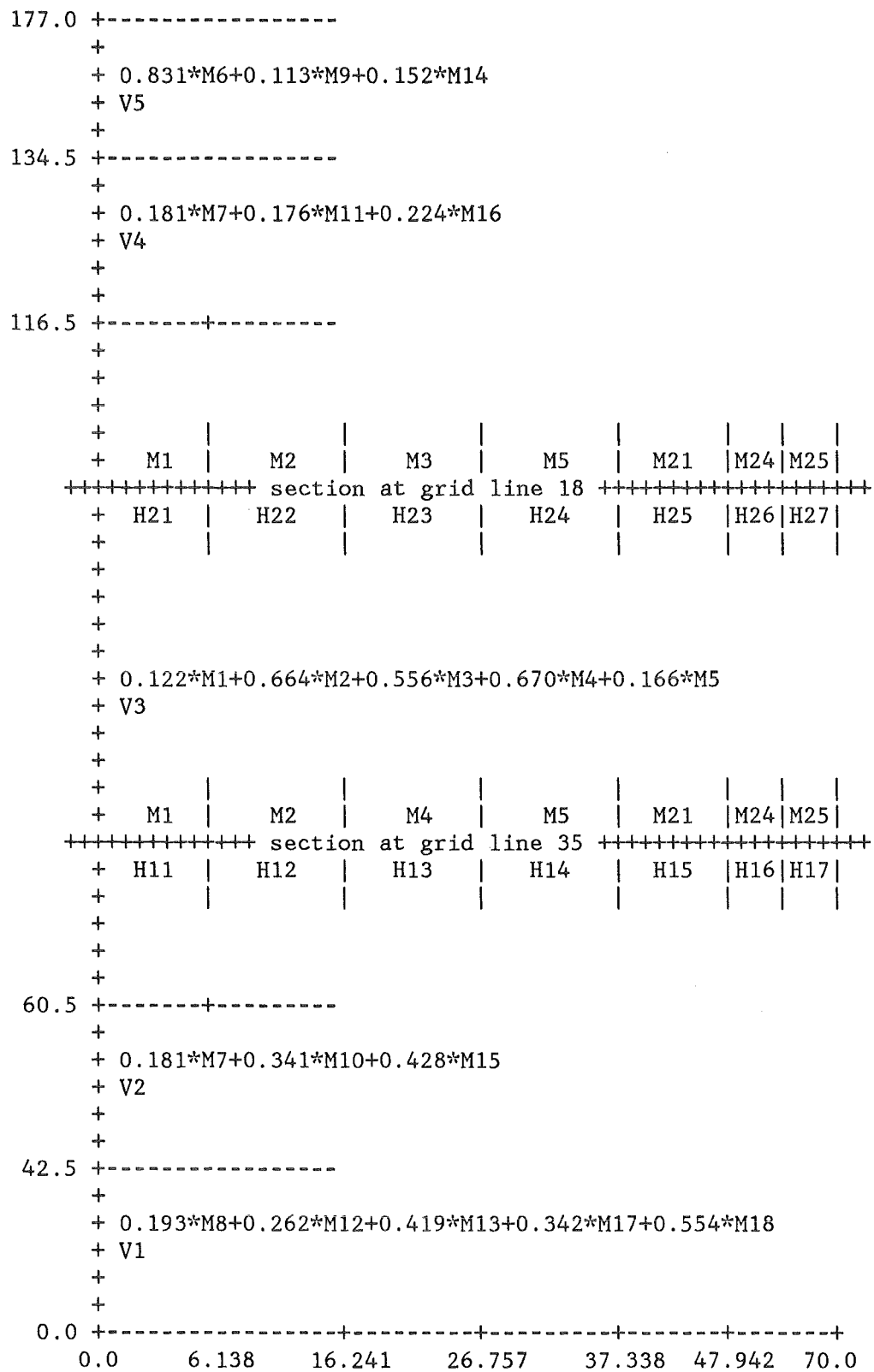
Mixture	Explanation	Characteristic materials
M1	Core 1, inner zone	UO_2/PuO_2
M2	Core 1, outer zone	UO_2/PuO_2
M3	Core + absorber	UO_2/B_4C
M4	Core + follower	UO_2/Na
M5	Core 2	UO_2/steel/CH
M6	Upper axial reflector	Steel/Na
M7	Upper + lower axial blankets	$U_{nat}O_2$/steel/Na
M8	Lower axial reflector	Steel/Na
M9	Upper outer absorber (strong)	B_4C/steel/Na
M10	Lower inner follower	Steel/Na
M11	Upper inner absorber (strong)	B_4C/steel/Na
M12	Lower central follower	Steel/Na
M13	Lower outer follower	Steel/Na
M14	Upper outer absorber (weak)	B_4C/steel/Na
M15	Lower inner reflector	Steel/Na
M16	Upper inner absorber (weak)	B_4C/steel/Na
M17	Lower central reflector	Steel/Na
M18	Lower outer reflector	Steel/Na
M19	Upper + lower outer reflectors of rad. bl.	Steel/Al
M20	Upper inner reflector of rad. bl.	Steel
M21	Radial blanket	$U_{nat}O_2$/steel/Na
M22	Lower inner reflector of rad. bl.	Steel/Na
M23	Lower central reflector of rad. bl.	Steel/Na
M24	Inner radial reflector	Steel/Na
M25	Outer radial reflector	Steel/Na

Fig. 3: Characterization of mixtures.



H1i collision densities from calculation along horizontal grid line 35
H2i collision densities from calculation along horizontal grid line 18
Vi collision densities from calculation in the vertical direction
Mi numbers of starting mixtures

Fig. 4: Attribution of mixtures and collision densities to the one-dimensional diffusion calculations.



H1i collision densities from calculation along horizontal grid line 35
H2i collision densities from calculation along horizontal grid line 18
Vi collision densities from calculation in the vertical direction

Fig. 5: Attribution of collision densities to the mixtures.

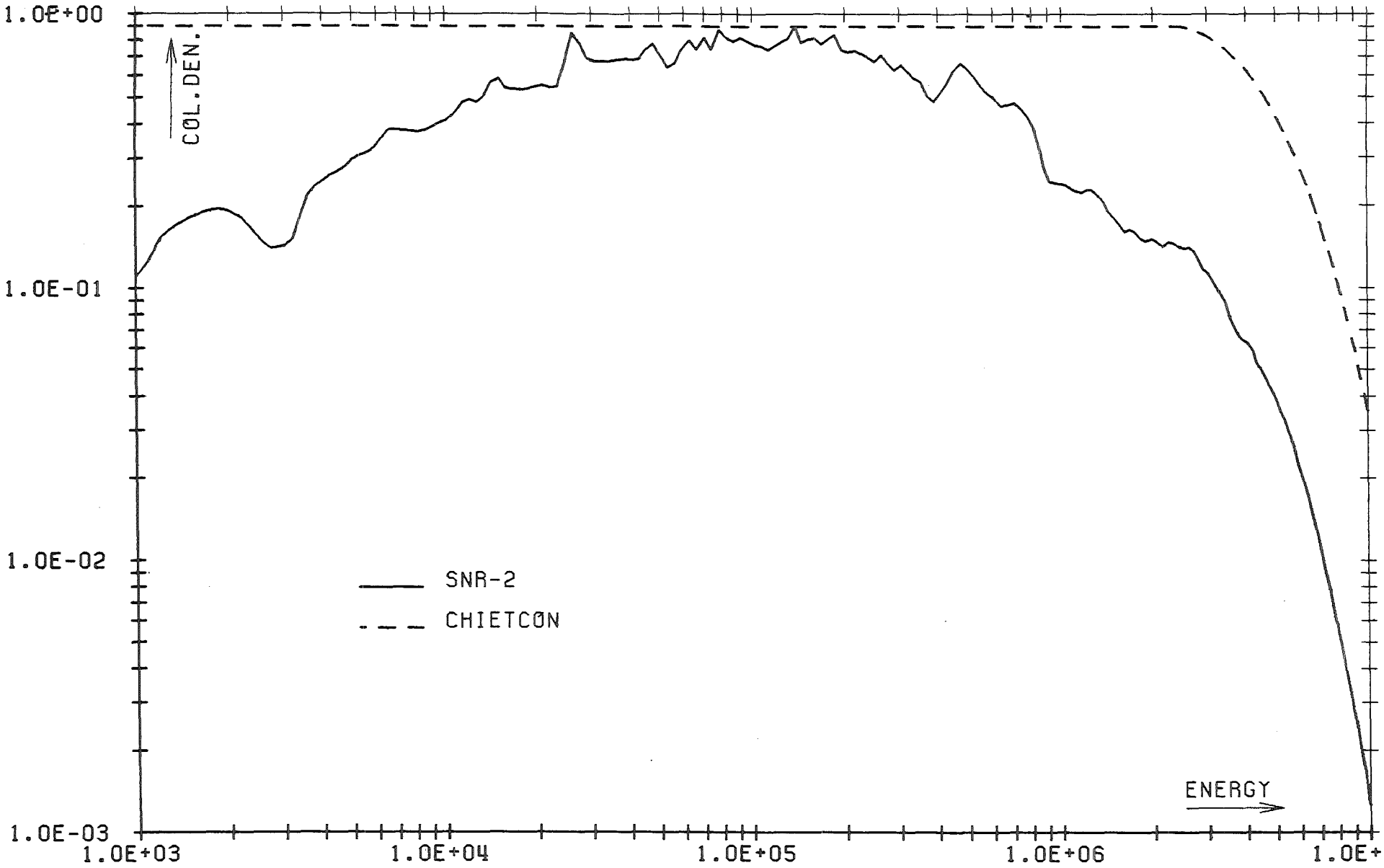


FIG. 6 STANDARD COLLISION-DENSITIES AVAILABLE IN GRUCAL

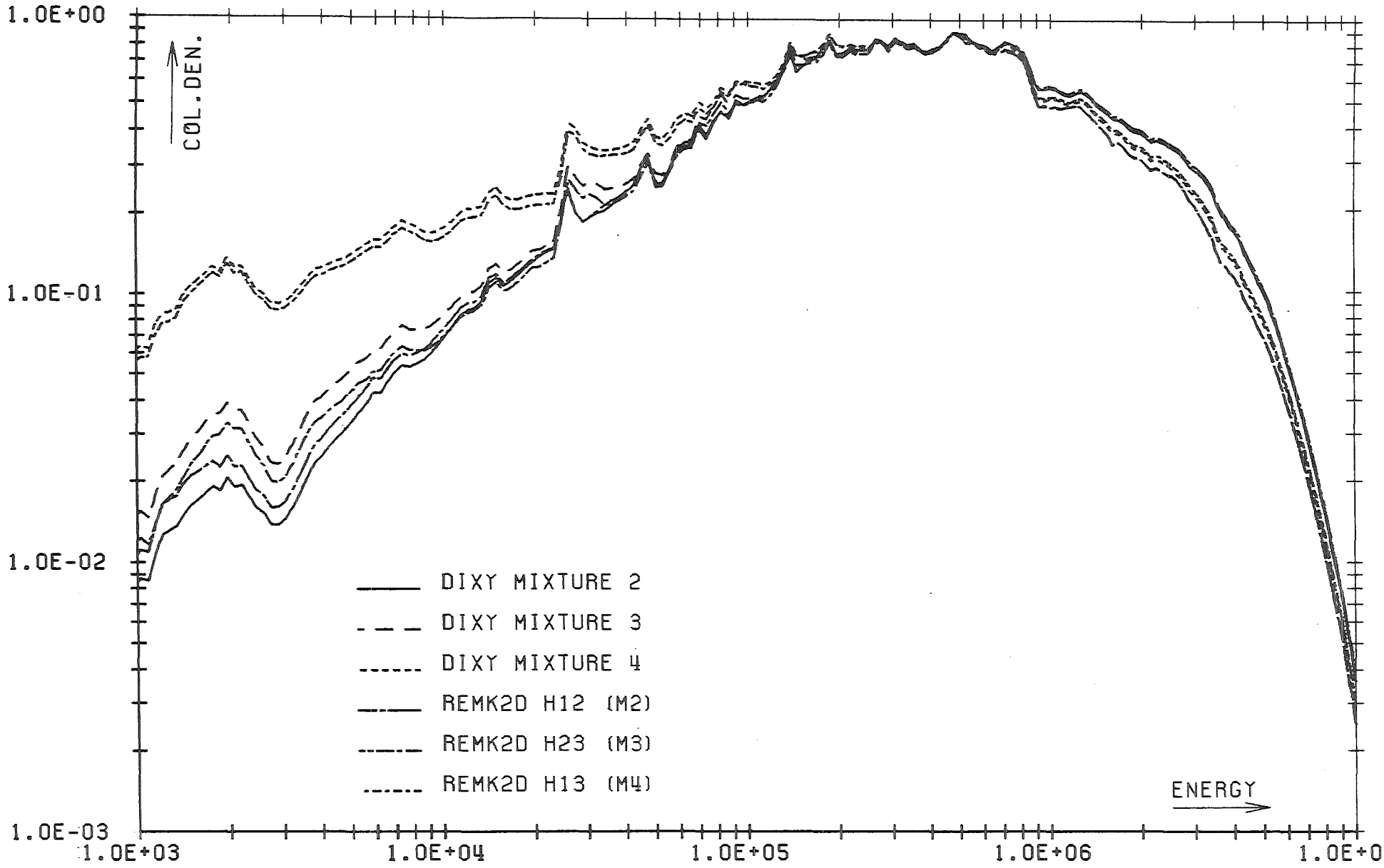


FIG. 7 COMPARISON OF CORE COLLISION DENSITIES

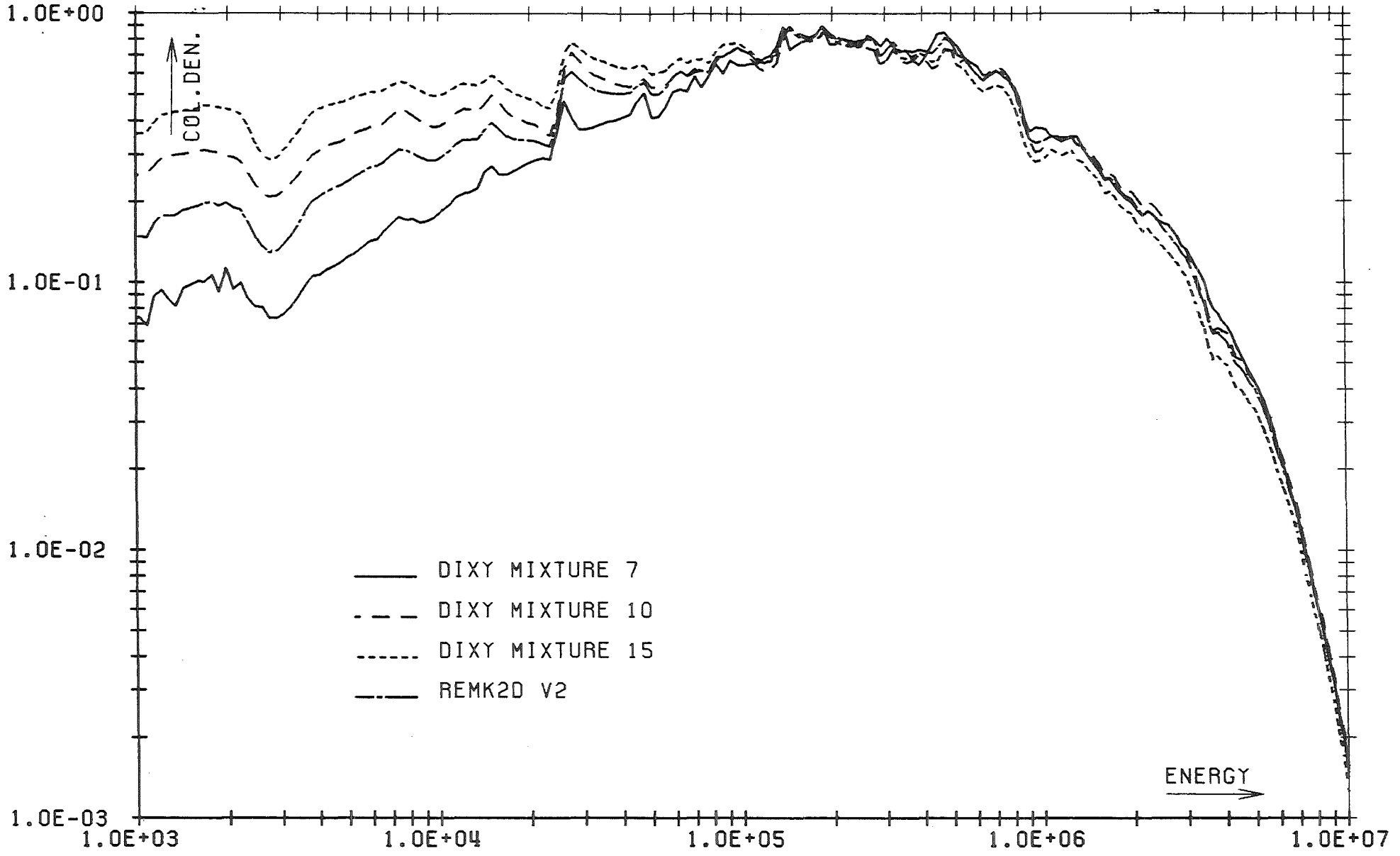


FIG. 8 COMPARISON OF BLANKET COLLISION DENSITIES

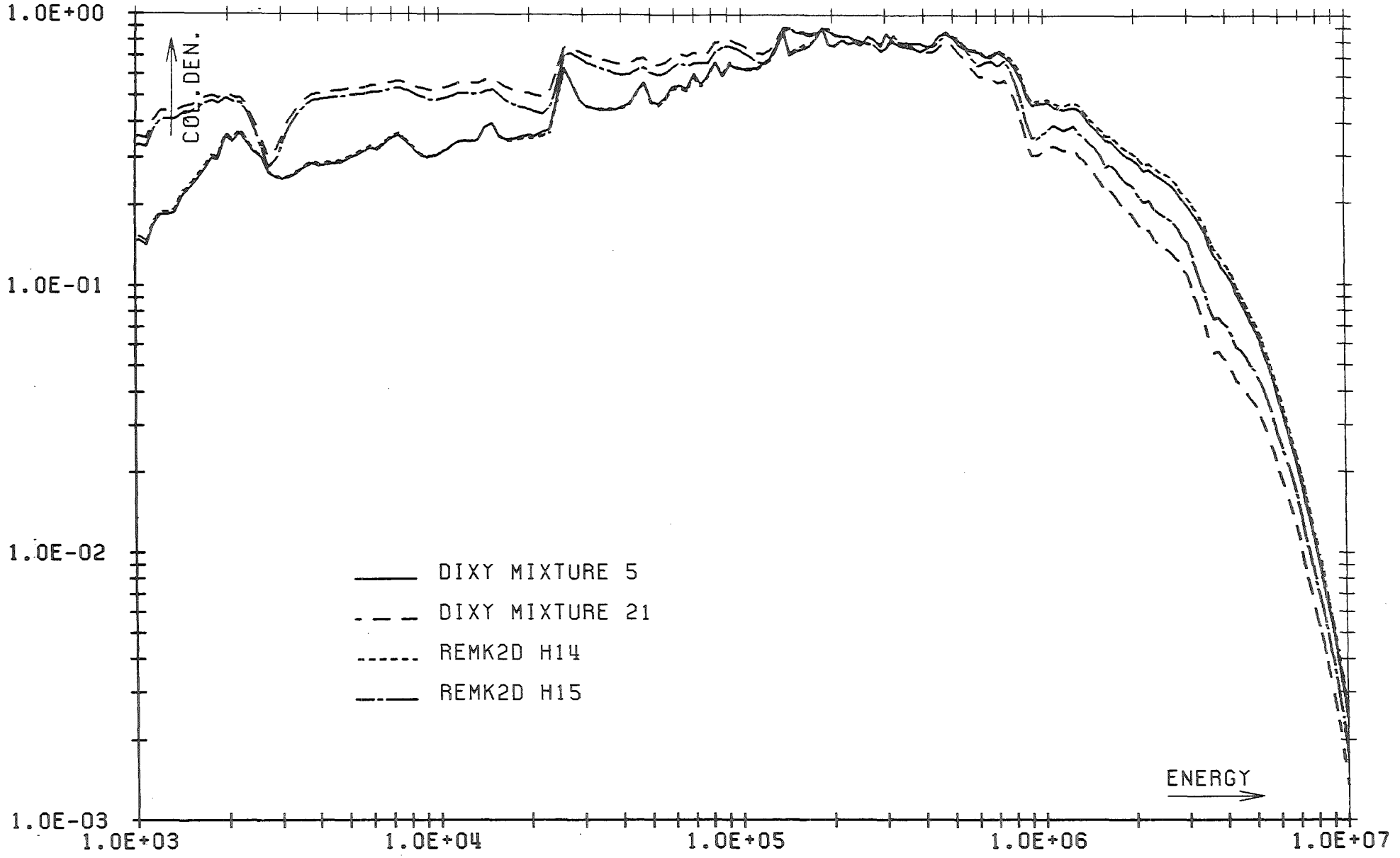


FIG. 9 COMPARISON OF CORE AND BLANKET COLLISION DENSITIES

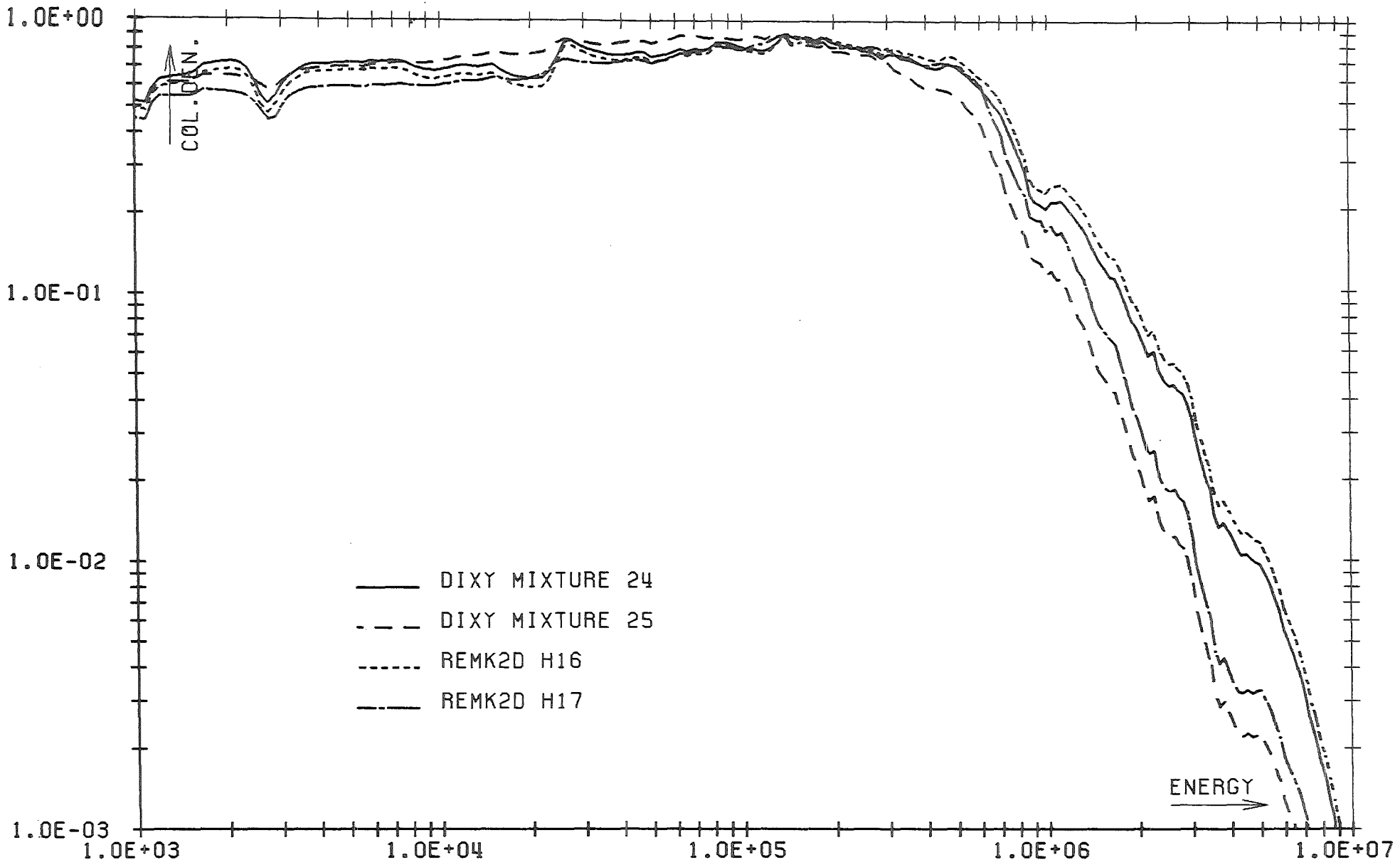


FIG. 10 COMPARISON OF REFLECTOR COLLISION DENSITIES

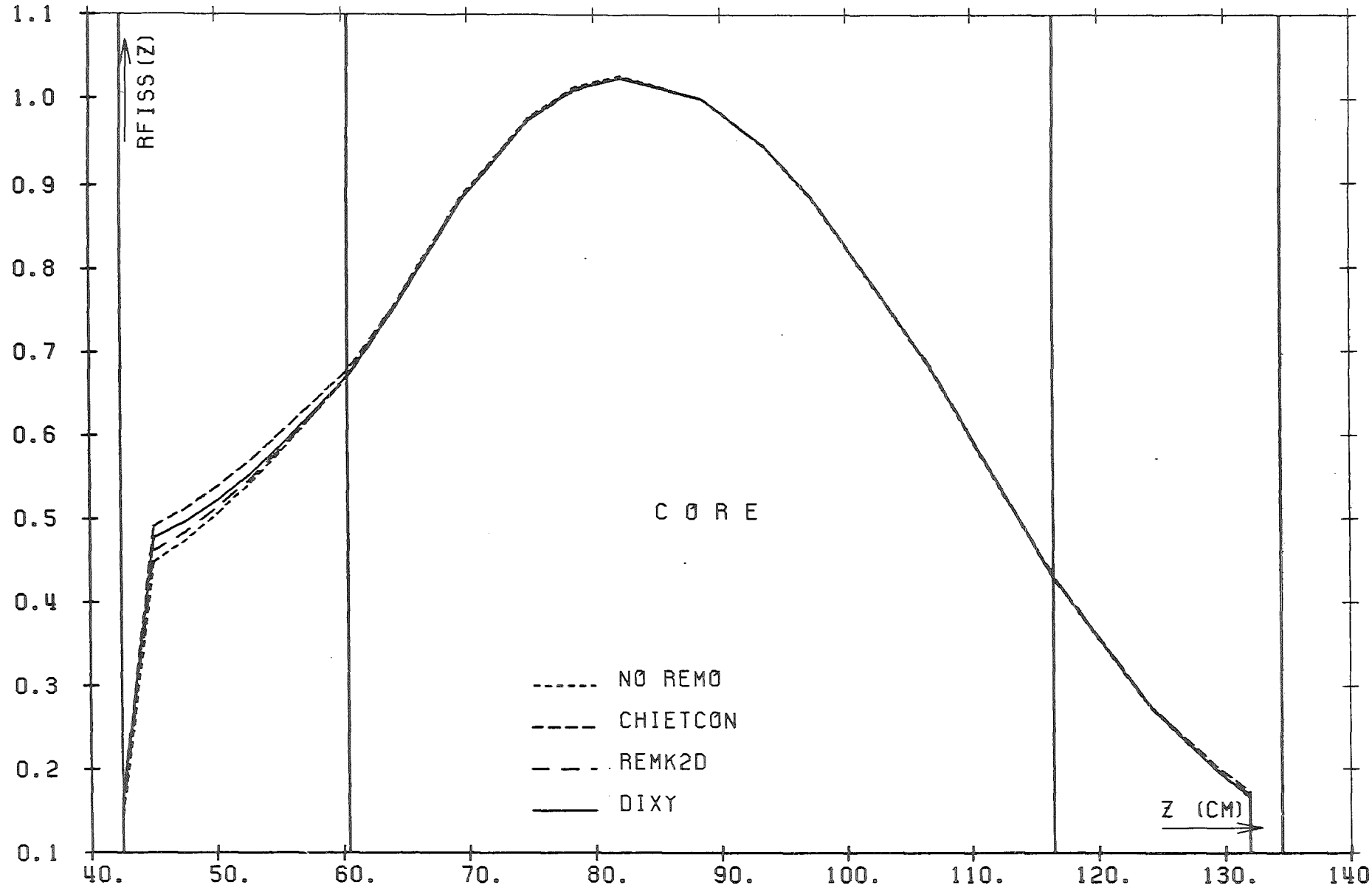


FIG. 11 PU239 FISSION RATE TRAVERSE ALONG THE CORE-AXIS