Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew
Gatlinburg, Tennessee, April 6-11, 2003, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2003)

EXTENDED PROBABILITY TABLES FOR APPROXIMATING NEUTRON MULTIGROUP CROSS-SECTIONS

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ABSTRACT

A modification of the probability table (subgroup) technique for approximating neutron multigroup cross-sections in the resonance energy range is presented. This approach can be applied for computing composition-dependent macroscopic cross-sections from isotope-wise multigroup cross-section data. The extended probability tables include additional parameters and can be obtained in a more simplified (compared to the traditional probability tables) manner from multigroup parameters computed on the basis of evaluated nuclear data files.

Key Words: Nuclear data, resonance self-shielding, f-factor, probability table, subgroup method, multiband method, multigroup cross-sections

1. INTRODUCTION

Safety analyses of advanced nuclear reactor concepts require use of modern safety codes that include sophisticated neutronics and thermal-hydraulics models. A safety code - developed at FZK/IKET in cooperation with other partners - includes a neutronics model that employs (for neutron flux and reactivity calculations) multigroup composition-dependent cross-sections. They are computed for each reactor node at each shape/reactivity step during a transient simulation, the fluid-dynamics model of the code providing mesh-wise temperatures and densities for the fertile and fissile fuel components, structure, coolant, and control materials, their isotopic composition being constant during the transient.

The cross-section processing part of the neutronics model of the code is currently under revision and extension. In particular, we consider a problem of preparing multigroup cross-section parameters (including those for taking into account resonance self-shielding effects) for isotope mixtures on the basis of isotope-wise multigroup data libraries computed in advance from evaluated nuclear data files. In the paper we briefly discuss advantages and disadvantages of the traditional f-factor and probability table (subgroup, multiband) methods with respect to this problem and describe a new technique for solving it. This technique is similar to the probability table method, but takes into account simultaneously a smaller number of equations for computing parameters of probability distributions of neutron cross-sections that facilitates calculations of these parameters compared to the traditional treatment.

2. COMPARISON OF F-FACTOR AND PROBABILITY TABLES TECHNIQUES

The f-factor [1] and probability table techniques [2, 3] were developed to take into account in a fairly easy way the resonance structure of neutron cross-sections while preparing "effective" group cross-section parameters employed in neutron transport codes. The f-factor tables are computed on the basis of the group-averaged cross-sections and "moments" of the total (*t*) and partial (*x*) cross-sections of the following type (for simplicity we omit group indices and temperature dependence):

$$m_t(\sigma_0) = < 1/(\sigma_t(E) + \sigma_0) >, \tag{1}$$

$$m_x(\sigma_0) = < \sigma_x(E)/(\sigma_t(E) + \sigma_0) >, \tag{2}$$

$$m_{t2}(\sigma_0) = < 1/(\sigma_t(E) + \sigma_0)^2 >, \tag{3}$$

where <> means energy group averaging, E is neutron energy, $\sigma_t(E)$, $\sigma_x(E)$ are the total and partial (e.g. fission) cross-sections, σ_0 is so-called dilution or background cross-section. The moments (3) may not be needed if only "flux-weighted" f-factors [4] are employed.

For preparing "effective" macroscopic group cross-section parameters for isotope mixtures, the group averaged isotope cross-sections are multiplied by f-factor values. These values are obtained from f-factor tables by interpolation, an "effective" dilution cross-section used in the interpolation procedure representing the total cross-section of all other isotopes of the mixture (this dilution cross-section may include additional components if f-factor tables for the isotope mixture are computed or a heterogeneity model is employed). Thus, an interpolation procedure and a certain technique of iteration type [1] for computing "effective" σ_0 values are used. Both these interpolation- and (especially) σ_0-iteration-techniques are potential sources of uncertainties, but the f-factor technique is widely used due to a fairly straightforward manner of computing f-factors from evaluated data files by employing available software packages like NJOY [5].

The mentioned disadvantages of the f-factor technique can be avoided if the probability table method is applied. This method assumes that a set of certain probabilities (subgroup weights) $a_i, i = 1,...,N$ and corresponding values $\sigma_{t,i}, \sigma_{x,i}$ (the total and partial subgroup cross-sections) can "effectively" represent the resonance cross-section structure within an energy group. It is assumed that

$$\sum_{i=1}^{N} a_i = 1, \tag{4}$$

$$\sum_{i=1}^{N} a_i \sigma_{x,i} = < \sigma_x >, \tag{5}$$

$$\sum_{i=1}^{N} a_i \sigma_{t,i} = < \sigma_t >, \tag{6}$$

$$\sum_{x} \sigma_{x,i} = \sigma_{t,i}, i = 1,..., N, \tag{7}$$

all parameters being positive. This method is free from the mentioned disadvantages of the f-factor technique, but calculations of the subgroup parameters [6, 7] are more complicated. These calculations may be based on the preservation of the cross-section moments (under the constraints defined by Eqs. (4 -7), which are approximated as follows:

$$m_t(\sigma_0) \approx \sum_{i=1}^{N} a_i /(\sigma_{t,i} + \sigma_0), \tag{8}$$

$$m_x(\sigma_0) \approx \sum_{i=1}^{N} a_i \sigma_{x,i} /(\sigma_{t,i} + \sigma_0). \tag{9}$$

One may note that the same subgroup parameters $a_i, \sigma_{t,i}$ are used in Eqs. (8, 9), i.e. they are not reaction dependent that is an attractive feature. However, all "total" and "partial" moments should be taken into account *simultaneously* for computing probability tables. This condition poses a certain numerical problem and makes preparation of the multigroup cross-section isotope-wise data libraries more difficult compared to the f-factor method.

3. EXTENDED PROBABILITY TABLES

If probability table parameters are available, calculation of the cross-section parameters for a mixture of isotopes is quite straightforward (in the following we consider an infinite medium consisting of two isotopes for simplicity, use capital letters for the macroscopic parameters, assume that isotope k is approximated by N_k subgroups, k=1,2). Let us consider a case of computing macroscopic moments for a set of σ_0^M values (to get then macroscopic f-factors), the σ_0^M values being parameters for taking into account background cross-sections for the mixture:

$$M_x(\sigma_0^M) = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} a_{1,i} a_{2,j} (\rho_1 \sigma_{1,x,i} + \rho_2 \sigma_{2,x,j}) /(\rho_1 \sigma_{1,t,i} + \rho_2 \sigma_{2,t,j} + \sigma_0^M), \tag{10}$$

where ρ_k is the atomic number density for isotope k. Eq. (9) can be rewritten as $M_x(\sigma_0^M) = M_{1,x}(\sigma_0^M) + M_{2,x}(\sigma_0^M)$ where

$$M_{k,x}(\sigma_0^M) = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} a_{1,i} a_{2,j} \rho_k \sigma_{k,x,i} /(\rho_1 \sigma_{1,t,i} + \rho_2 \sigma_{2,t,j} + \sigma_0^M), k = 1,2. \tag{11}$$

One may note that even if the probability table parameters for isotope k were obtained without taking into account Eqs. (6 - 8), the values defined by Eq. (11) would still be computed correctly. In other words, if a table of (microscopic) moments is given for isotope k and a probability table

is given for the other isotope, then any accurate interpolation procedure for the "microscopic" table of moments will give accurate macroscopic values. Thus, one may introduce additional parameters: "conditional" total subgroup cross-sections $\sigma_{tx,i}$. They can be obtained by preserving (instead of considering Eq. (9)) the following tabulated functions (as earlier, for a representative set of background cross-sections):

$$m_x(\sigma_0) \approx \sum_{i=1}^{N} (a_i \sigma_{x,i}) / (\sigma_{tx,i} + \sigma_0) \tag{12}$$

and excluding Eq. (7) from consideration, the original meaning being kept only for $a_i, \sigma_{t,i}$ (see Eqs. (4, 6)). The "extended" set of probability table parameters includes: $a_i, (a_i \sigma_{x,i}), \sigma_{tx,i}, \sigma_{t,i}$. Thus, $\sigma_{k,tx,i}$ may replace $\sigma_{k,t,i}$ in Eq. (11). The main advantage of this approach is that this extended set can be obtained by approximating Eqs. (8, 12) independently from each other: since Eqs. (5, 12) contain $\sigma_{tx,i}$ and the products $a_i \sigma_{x,i}$ (the very products are obtained and used) do not "interfere" with Eqs. (4, 6, 8). Thus, the problem of approximating several tabulated functions at the same time is reduced to the problem of approximating each function independently. The latter problem is solved more easily since partial cross-sections may have different shapes (see Fig. 1).

The new approach involves more parameters. Their physical meaning differs from those of the traditional method: the partial $\sigma_{x,i}$ and corresponding conditional total $\sigma_{tx,i}$ subgroup cross-sections are defined with respect to each other and should be used together for computing probabilities of the $\sigma_x / (\sigma_t + ...)$ type, while the total $\sigma_{x,i}$ subgroup cross-sections are related to probabilities of the $1/(\sigma_t + ...)$ type.

We have not yet tried to modify a deterministic cell or a Monte-Carlo neutron transport model to process the extended probability tables: we are not yet so far in extending the cross-section processing module of our safety code system. However, for computing cross-sections for isotope mixtures, the new technique combines all advantages of the probability table method (no interpolation of tabulated f-factors vs. σ_0, no σ_0-iteration) with a relatively simple way of computing required parameters, this way being not much more complicated than calculations of f-factor tables.

4. NUMERICAL RESULTS

For testing the new technique, we have processed more than 300 files (isotopes or their natural mixtures), mainly from the ENDF/B6.7 nuclear data library that was downloaded from the LANL website. We employed a 172-group structure [8], 90 energy groups being in the energy range above 5 eV. The cross-section moments were computed using NJOY for 16 dilution cross-sections, 9 temperatures (from 300K to 6000K) with an error tolerance of 0.1%.

Calculations of the extended probability table parameters from the moments (Eqs. (8, 12)) were performed by employing Padé approximation techniques described in [9]. The code looks for sets of 4, or a greater even number of dilution cross-sections in each group so that the related set

of moments used in the approximation procedure provides the most accurate approximation of Eqs. (8, 12), the related normalization equations being satisfied, only positive parameters being accepted. The search is finished when the desired accuracy of 0.1% is reached or when increasing the number of subgroups N (related to 2N dilution cross-sections) does not improve the accuracy. Thus, this scheme automatically selects "relevant" dilution cross-section values for each energy group. Since the employed method does not need "non-relevant" moments for obtaining the approximation parameters, the size of the stored f-factor array (from which moments can be reconstructed for computing then "on-the-fly" the extended probability tables) can be made relatively small (if the dilution cross-section set can be isotope- and group-dependent).

To give a better impression about the introduced technique, a particular case is presented in more details in the following: approximation of U-238 cross-sections in group 64 (near 200 eV). In Fig. 1, the cross-sections (at T=300K) are shown. The corresponding f-factors for U-238, and the error of their approximation by extended probability tables (for N=6) are shown in Figs. 2, 3.

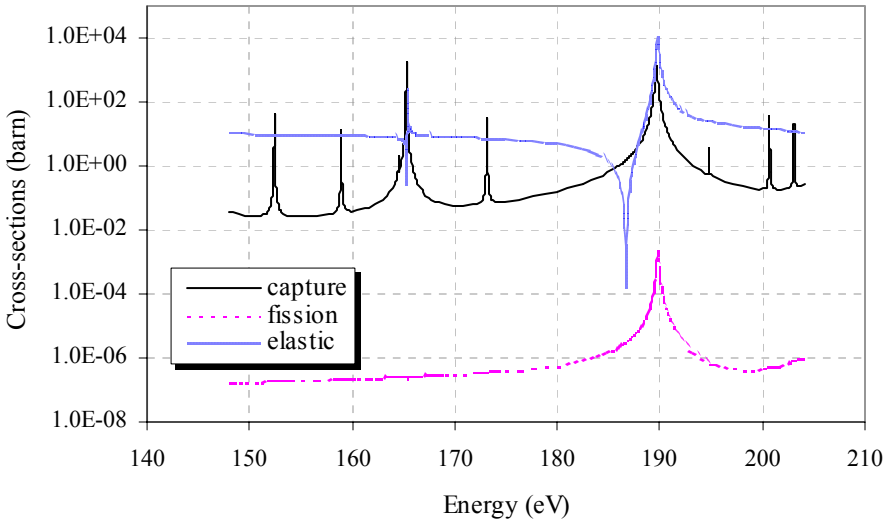

Figure 1. U-238 cross-sections in energy group 64

For computing the error, we have taken into account f-factor values at 32 dilution cross-sections (though only 16 were taken into account while selecting 12 "relevant" ones). A very small approximation error is reached in this case.

In Fig. 4 the corresponding conditional total subgroup cross-sections $\sigma_{tx,i}$ are shown. On one hand, they are similar (for different partial cross-sections) because they represent in a certain sense the same total cross-section. On the other hand, they are not completely the same, because they were obtained by approximating (independently and using as few parameters as possible) the different ratios containing total and different partial cross-sections.

In Fig. 5 the maximum approximation error for U-238 cross-sections in all energy groups are shown. These values were obtained by comparing approximation errors for the total and all partial cross-sections, data at all temperatures being considered. One may see that in this case all

moments can be approximated as required, i.e. not exceeding the 0.1% criterion. The f-factor and moment approximation errors are different because the f-factors are computed from moment ratios.

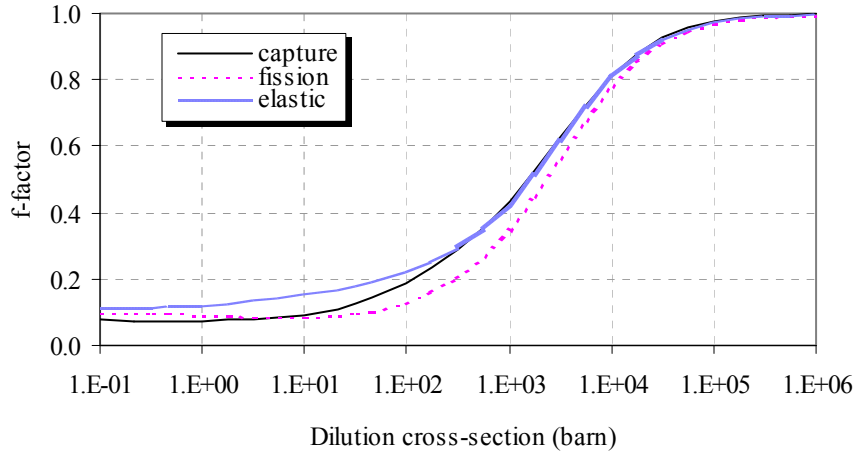

Figure 2. U238 f-factors in energy group 64

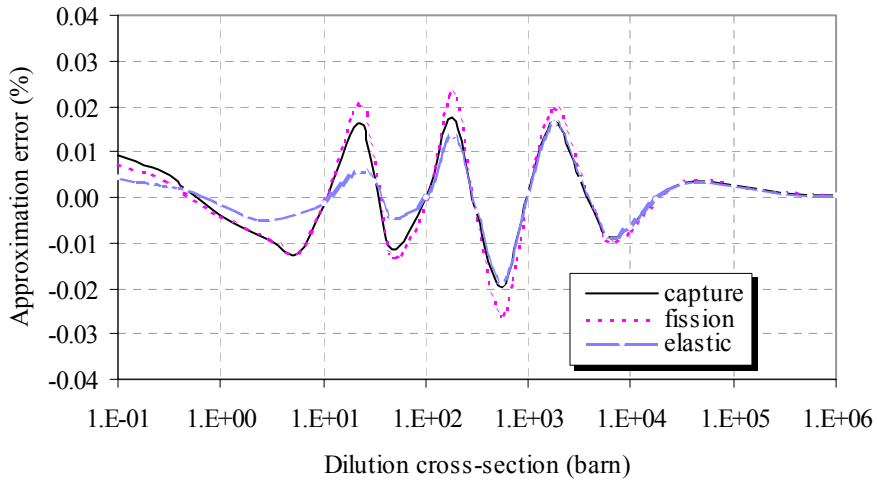

Figure 3. Approximation error in energy group 64 for U-238

For the total cross-section, we considered the accuracy of the "flux-weighted" f-factors only. The approximation error for "current-weighted" f-factors is usually several times larger because the moments defined by Eq. (3) were not directly taken into account while obtaining the extended probability table parameters. This larger error seems to be acceptable, however, taking into account other approximations for computing "effective" total/transport cross-sections usually employed in the frame of the multigroup method.

In Fig. 6, numbers of subgroups for each energy group are shown. The results are given for the Fe-56, U-238 and Pu-239 cross-sections. Only in few groups more than 4 subgroups are needed.

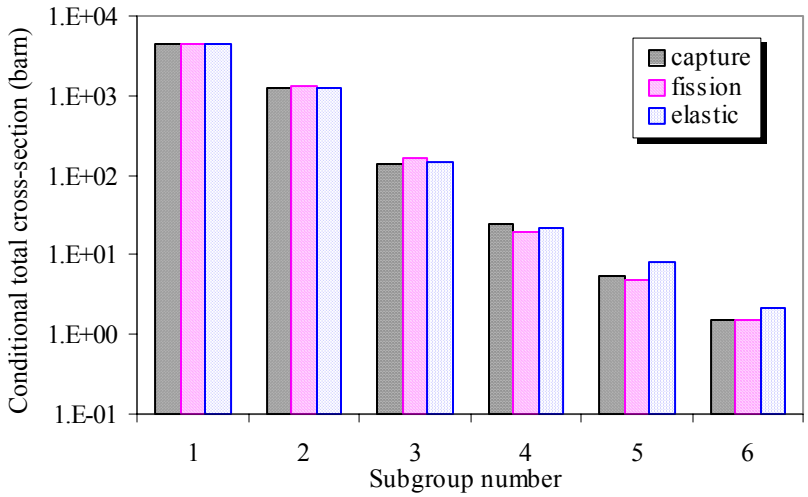

Figure 4. U-238 additional parameters in group 64

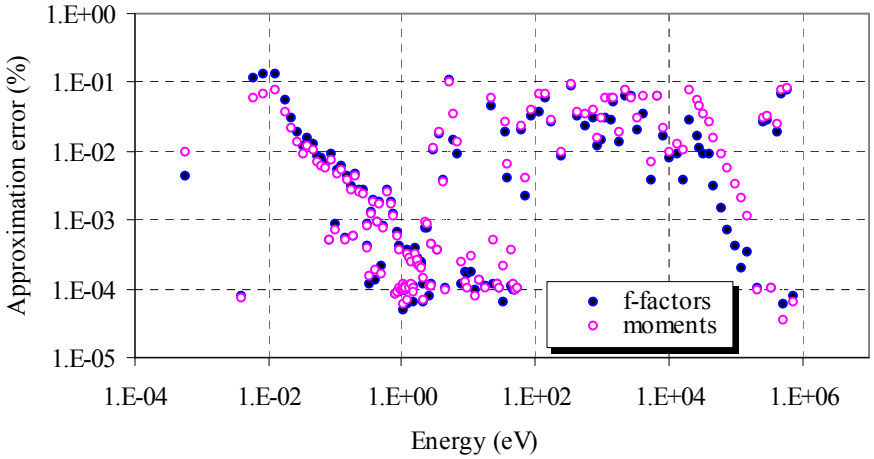

Figure 5. Maximum approximation error in energy groups for U-238

The maximum approximation errors and numbers of subgroups for all nuclides of the obtained library are shown in Figs 7, 8. The nuclides are specified by their ZA number: Z+A/1000 where Z is the number of protons, A is the number of neutrons and protons together. By now the described technique failed to meet our accuracy criteria in 2 cases (in total we tried to process data for 320 isotopes of the ENDF/B6.7 libraries and for many nuclides from other libraries) only: for Hf-Nat (natural mixture of Hf isotopes) and W-Nat of ENDF/B6.7. In these cases, the maximum error reached a level of few percents. These cases are not shown in Figs. 7 and 8: since all Hf and W isotopes of ENDF/B6.7 were processed successfully (contrary to their natural mixtures), we decided to use the corresponding isotope-wise data in our multigroup library.

One may see that the maximum error for all f-factors (for which the results are presented in Fig. 8) does not exceed 0.25%, while for heavy nuclides (Z>90) this error is less than 0.18%. The number of subgroups employed to get this accuracy is fairly low. We never were able to

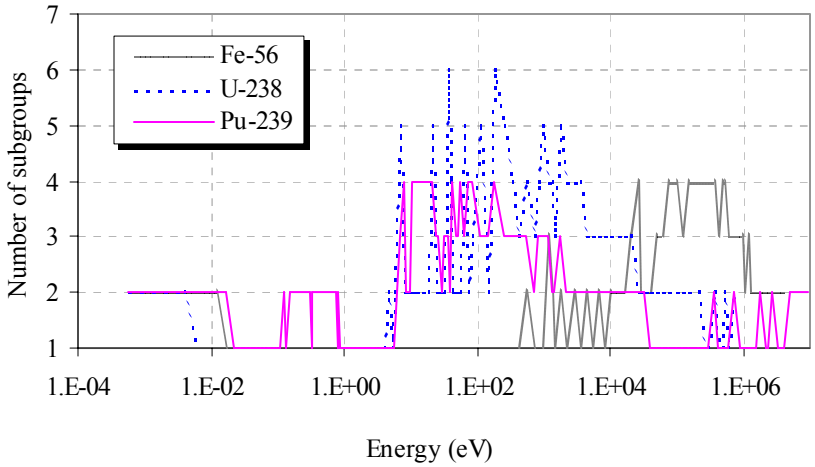

Figure 6. Number of subgroups in energy groups

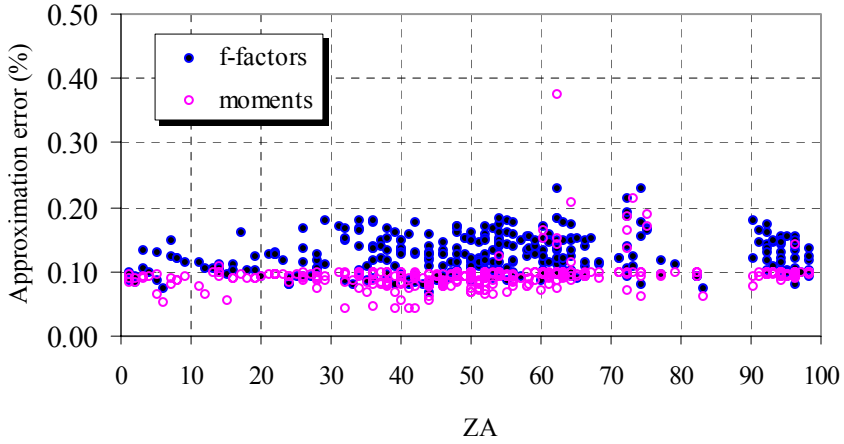

Figure 7. Approximation errors for nuclides

reach this level of performance in the past with traditional probability tables (though different techniques were tried).

5. CONCLUSIONS

The use of probability tables provides an accurate and rather straightforward way of computing effective macroscopic multigroup cross-sections that are employed by deterministic neutron transport codes. In the paper, an extended formulation of the probability table scheme is proposed providing the capability of computing probability parameters in a more simple and efficient manner compared to the traditional approach. The numerical results show an excellent performance of the technique of generating the extended tables. The new technique retains all advantages of the traditional approach while used for computing effective cross-sections or f-factors for isotope mixtures. The potential of using the extended probability tables in cell and Monte-Carlo models (directly employing the probability tables for simulating neutron transport) is currently investigated and may become a subject of future research activities.

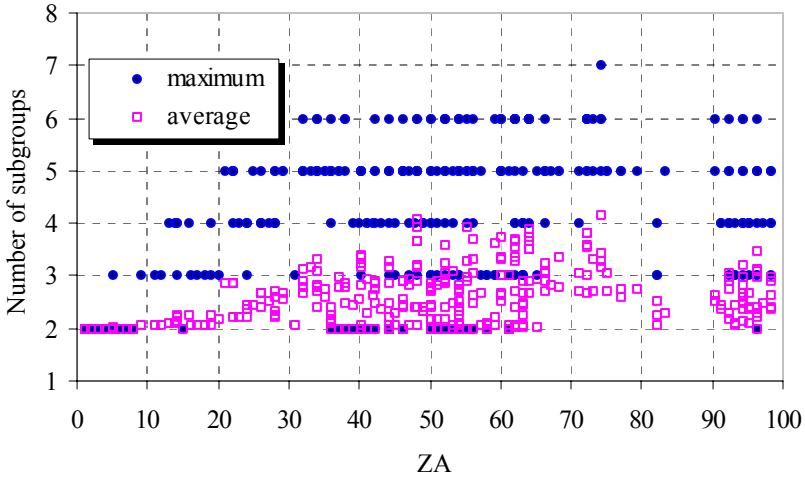

Figure 8. Maximum and average number of subgroups for nuclides

ACKNOWLEDGMENTS

The authors are grateful to Dr. E. Kiefhaber for useful suggestions and comments. The second author also thanks Prof. T. Schulenberg, Dr. W. Maschek, and other colleagues for supporting his stay as a guest scientist at FZK/IKET while performing this study.

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