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SPECTRUM – A computer code for prompt fission neutron spectrum and prompt neutron multiplicity calculation

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Abstract

The computer code SPECTRUM generates total prompt fission neutron spectrum, total prompt multiplicity, average energy of the spectrum and equivalent Maxwellian spectrum. Theoretical background employed in the calculations is that of Los Alamos model, with multiple chance fission, upgraded to allow a neutron incident energy dependence of the input parameters. The code handles the complete set of output data with a powerful graphical interface, allowing a comparison with reference data.

CODE SUMMARY

Title of the code: SPECTRUM (modules SPECTRUM and SPGRAPH)

Catalogue identifier: ADLH

Program Summary URL: http://cpc.cs.qub.ac.uk/summaries/ADLH

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland

Licensing provisions:

Computer: PC-Pentium 200 MHz

Installation: Bucharest University

Operating System: MS-DOS/Windows95

Programming languages used: Fortran77 and MS QuickBASIC 4.5

Memory required to execute with typical data: 500 kbyte

No. of bits in a word: 32

No. of lines in distributed program, including test data, etc.: 6618

No. of bytes in distributed program, including test data, etc.: 221 759 bytes

Distribution format: ASCII

PACS codes: 25.85.-w (Fission reactions); 25.85.Ca (Spontaneous fission); 25.85.Ec (Neutron-induced fission)

Keywords: Prompt fission neutron spectrum, average prompt neutron multiplicity, neutron emission in fission, post-scission, number of prompt neutrons per fission, energy distribution of secondary neutrons

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Nature of physical problem
Prompt fission neutron spectrum and average prompt neutron multiplicity are calculated

Method of solution
Prompt fission neutron spectrum and average prompt neutron multiplicity are calculated in the frame of Los Alamos model with multiple fission chances. Energy dependence of the compound nucleus cross sections of inverse process and incident neutron energy dependence of model parameters are considered.

Restriction of the complexity of the problem
Only the neutrons evaporated prior to scission are considered, the pre-equilibrium effects are neglected. The maximum number of compound nuclei undergoing fission (or fission chances) is four.

Typical running time: 5 minutes in the option of the energy dependence of the compound nucleus cross sections of the inverse process and less than 1 minute in the option of constant compound nucleus cross sections.

Unusual features of the code
Dependence on the incident neutron energy of model parameters, graphics and possibility to compare the results with data of external input files

References
[1] D.G. Madland, J.R. Nix, Nucl. Sci. Eng. 81 (1982) 213–271.
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[3] D.G. Madland, Post-scission fission theory, H4-SMR/1056-10,11, Workshop on Nucl. Reac. Data and Nucl. Reactors, Physics, Design and Safety, ICTP-Trieste, Italy (1998).

LONG WRITE-UP

1. Introduction

The early representations of the prompt fission neutron spectrum, which are still used today, are the Maxwellian and Watt spectrum representations with one and, respectively, two parameters that are adjusted to optimally reproduce the experimental spectrum for a given fissioning system at a given excitation energy. The two representations neglect many effects such as distribution of fission-fragment excitation energy, the energy dependence of the inverse process. The Maxwellian representation also neglects the motion of fission fragments emitting neutrons.

In recent years three new theoretical approaches have evolved for the calculation of the prompt fission neutron spectrum and correlated value of the average prompt neutron multiplicity.

The Los Alamos model [1] accounts for the above physical effects and also take into account multiple chance fission at high incident neutron energy.

The Dresden model [2], currently known as the Complex Cascade Evaporation Model (CCEM) accounts for the physical effects of the distribution of fission-fragment excitation energy in each step of the cascade, the energy dependence of the inverse process of compound nucleus formation, the center-of-mass motion of the fission fragments, the anisotropy of the center-of-mass neutron spectrum, the complete fission-fragment mass and kinetic energy distribution, and semi-empirical fission-fragment nuclear level densities.

The Hauser–Feshbach statistical model [3] accounts for the physical effects contained in the Los Alamos and Dresden models and, in addition, accounts for neutron and gamma-ray competition in the de-excitation of a given fission fragment, neutron transmission coefficients from an optical-model potential for each fragment considered, gamma-ray transmission coefficients for each fragment considered, and the angular momentum distribution for each fragment considered.

It is believed that, ultimately, the Hauser–Feshbach model will probably yield the most accurate results in the calculation of the prompt fission neutron spectrum and of the average prompt neutron multiplicity. This model, as well as the Dresden model, contains too many parameters and, consequently, in present, the Los Alamos model, which has a good predictive power with less input parameters, is largely used.

2. Physical model

The Los Alamos model [1,4,5] addresses both neutron-induced and spontaneous fission and accounts for the physical effects of:
(a) the distribution of fission-fragment excitation energy,
(b) the energy dependence of the inverse process of compound nucleus formation,
(c) the center-of-mass motion of the fission fragments, and
(d) the multiple chance fission at high incident neutron energy.

(a) To simulate the initial distribution of fission-fragment excitation energy and subsequent cooling as neutron is emitted, a triangular approximation is used to approximate the corresponding fission-fragment residual nuclear temperature distribution. This approximation has a maximum temperature T_{m} that is related to the initial total average fission-fragment excitation energy $\langle E^{*}\rangle$ by:

$$T_{\mathrm{m}} = \sqrt{\frac{\langle E^{*}\rangle}{a}}. \tag{1}$$

The average fission fragment excitation energy is given by:

$$\begin{aligned} &\langle E^{*}\rangle = \langle E_{\mathrm{r}}\rangle + E_x - \langle E_{\mathrm{f}}^{\mathrm{tot}}\rangle, \\ &E_x = B_{\mathrm{n}} + E_{\mathrm{n}}, \end{aligned} \tag{2}$$

here $\langle E_{\mathrm{r}}\rangle$ is the average energy release in fission, B_{n} is the separation neutron energy from the fissioning compound nucleus, E_{n} the incident neutron energy and $\langle E_{\mathrm{f}}^{\mathrm{tot}}\rangle$ is the total average fission-fragment kinetic energy. For spontaneous fission both E_{n} and B_{n} are zero.

The level density parameter a from (1) can be expressed in function of the mass number A of the fissioning compound nucleus:

$$a = \frac{A}{C_{\mathrm{f}}\ (\mathrm{MeV})}, \tag{3}$$

where the value usual used for the constant C_{f} is 11 MeV [1].

(b) The energy dependence of the inverse process is treated in the center-of-mass frame by calculating the compound nucleus formation cross section $\sigma_{\mathrm{c}}(\varepsilon)$ using an optical-model potential with explicit isospin dependence to describe neutron-rich fission fragments more correctly.

(c) The values of the average kinetic energy per nucleon of the average light fragment A_{L} and average heavy fragment A_{H} are obtained using momentum conservation and are given by:

$$E_{\mathrm{f}}^{\mathrm{L}} = \frac{A_{\mathrm{H}}}{A_{\mathrm{L}}}\frac{\langle E_{\mathrm{f}}^{\mathrm{tot}}\rangle}{A}, \qquad E_{\mathrm{f}}^{\mathrm{H}} = \frac{A_{\mathrm{L}}}{A_{\mathrm{H}}}\frac{\langle E_{\mathrm{f}}^{\mathrm{tot}}\rangle}{A}, \tag{4}$$

where A is the mass number of the compound nucleus undergoing fission.

With the inclusion of these physical effects, the total prompt fission neutron energy spectrum, in the laboratory system, at the incident neutron energy E_{n}, is given by the average of the spectra calculated for neutron emission from the light fragment L and from the heavy fragment H:

$$N(E) = \tfrac{1}{2}\big(N(E, E_{\mathrm{f}}^{\mathrm{L}}, \sigma_{\mathrm{cf}}^{\mathrm{L}}) + N(E, E_{\mathrm{f}}^{\mathrm{H}}, \sigma_{\mathrm{cf}}^{\mathrm{H}})\big), \tag{5}$$

where E is the energy of the emitted neutron and the prompt fission neutron spectrum for each fission fragment moving with the average kinetic energy per nucleon E_{f} is:

$$N(E, E_{\mathrm{f}}, \sigma_{\mathrm{cf}}) = \frac{1}{2T_{\mathrm{m}}^{2}\sqrt{E_{\mathrm{f}}}} \int_{(\sqrt{E}-\sqrt{E_{\mathrm{f}}})^{2}}^{(\sqrt{E}+\sqrt{E_{\mathrm{f}}})^{2}} \sigma_{\mathrm{cf}}(\varepsilon)\sqrt{\varepsilon}\, d\varepsilon \int_{0}^{T_{\mathrm{m}}} k_{\mathrm{f}}(T) T \exp(-\varepsilon/T)\, dT. \tag{6}$$

In this equation ε is the center-of-mass neutron energy and the normalization constant $k_{\mathrm{f}}(T)$ is given by:

$$k_{\mathrm{f}}(T) = \left[\int_0^\infty \sigma_{\mathrm{cf}}(\varepsilon)\varepsilon \exp(-\varepsilon/T)\, d\varepsilon \right]^{-1}. \tag{7}$$

The consideration of $\sigma_{\mathrm{cf}}(\varepsilon) = \text{constant}$ leads to a closed form solution for the fission neutron spectrum of each fission fragment:

$$\begin{aligned} N(E, E_{\mathrm{f}}) &= \frac{1}{2T_{\mathrm{m}}^2\sqrt{E_{\mathrm{f}}}} \int_{(\sqrt{E}-\sqrt{E_{\mathrm{f}}})^2}^{(\sqrt{E}+\sqrt{E_{\mathrm{f}}})^2} \sqrt{\varepsilon}\, d\varepsilon E1(\varepsilon/T_{\mathrm{m}}) \\ &= \frac{1}{3\sqrt{E_{\mathrm{f}}}T_{\mathrm{m}}}\big(u_2^{3/2}E1(u_2) - u_1^{3/2}E1(u_1) + \gamma(3/2, u_2) - \gamma(3/2, u_1)\big), \end{aligned} \tag{8}$$

where:

$$u_{1,2} = \frac{(\sqrt{E} \mp \sqrt{E_{\mathrm{f}}})^2}{T_{\mathrm{m}}}, \qquad E1(u) = \int_u^\infty \frac{\exp(-x)}{x}\, dx,$$

$$\gamma(a, u) = \int_0^u x^{a-1}\exp(-x)\, dx. \tag{9}$$

The average prompt fission neutron multiplicity $\overline{\nu}_{\mathrm{p}}$ is obtained from the energy conservation and can be calculated using the relationship:

$$\overline{\nu}_{\mathrm{p}} = \frac{\langle E^* \rangle - \langle E_\gamma^{\mathrm{tot}} \rangle}{\langle S_{\mathrm{n}} \rangle + \langle \varepsilon \rangle}, \tag{10}$$

where $\langle E_\gamma^{\mathrm{tot}} \rangle$ is the average prompt gamma energy, $\langle S_{\mathrm{n}} \rangle$ is the average fission fragment neutron separation energy and $\langle \varepsilon \rangle$ is the average center-of-mass energy of the emitted neutrons (first moment) that is calculated by:

$$\begin{aligned} \langle \varepsilon \rangle &= \frac{1}{2}\int_0^\infty \varepsilon\big(\Phi^{\mathrm{L}}(\varepsilon) + \Phi^{\mathrm{H}}(\varepsilon)\big)\, d\varepsilon \\ &= \frac{1}{T_{\mathrm{m}}^2}\int_0^\infty \varepsilon^2\sigma_{\mathrm{cf}}^{\mathrm{L}}(\varepsilon)\, d\varepsilon \int_0^{T_{\mathrm{m}}} k_{\mathrm{L}}(T) T \exp(-\varepsilon/T)\, dT \\ &\quad + \frac{1}{T_{\mathrm{m}}^2}\int_0^\infty \varepsilon^2\sigma_{\mathrm{cf}}^{\mathrm{H}}(\varepsilon)\, d\varepsilon \int_0^{T_{\mathrm{m}}} k_{\mathrm{H}}(T) T \exp(-\varepsilon/T)\, dT. \end{aligned} \tag{11}$$

In the case $\sigma_{\mathrm{cf}}(\varepsilon) = \text{constant}$ the first center-of-mass energy moment becomes:

$$\langle \varepsilon \rangle = \frac{4}{c}T_{\mathrm{m}}. \tag{12}$$

(*d1*) *Prompt fission neutron spectrum and average prompt fission neutron multiplicity*

At high incident neutron energy, above ≈6 MeV, the excitation energy of the compound nucleus is sufficiently large that fission is possible following the emission of one or more neutrons. Thus, at some excitation energy

the first-chance fission (n, f) reaction is in competition with the second-chance fission $(n, n'f)$ reaction; at some higher excitation energy these two reactions are in competition with each other and with the third-chance fission $(n, 2nf)$ reaction and so on.

In this case it is necessary to calculate the prompt fission neutron spectrum and the average neutron multiplicity for each compound nucleus that is formed in the process. If N is the number of fission chances (or N the number of fissioning compound nuclei with the mass numbers: $A, (A-1), (A-2), \ldots, (A-N+1)$) the expressions (1)–(12) must be used for each compound nucleus undergoing fission and each corresponding central fragmentation $\{H, L\}$.

The total prompt fission neutron spectrum $N(E)$ and the total average prompt neutron multiplicity $\overline{\nu}_{\mathrm{p}}$ at the incident neutron energy E_{n}, due to first-, second-, third- and fourth-chance fission events (for instance) are given, in the laboratory system, by the expressions:

$$
\begin{aligned}
N(E) &= S_1 + S_2 + S_3 + S_4,\\
S_1 &= \frac{R_1\overline{\nu}_{\mathrm{p1}}N_1(E)}{R_1\overline{\nu}_{\mathrm{p1}} + R_2(1+\overline{\nu}_{\mathrm{p2}}) + R_3(2+\overline{\nu}_{\mathrm{p3}}) + R_4(3+\overline{\nu}_{\mathrm{p4}})},\\
S_2 &= \frac{R_2(\varphi_1(E) + \overline{\nu}_{\mathrm{p2}}N_2(E))}{R_1\overline{\nu}_{\mathrm{p1}} + R_2(1+\overline{\nu}_{\mathrm{p2}}) + R_3(2+\overline{\nu}_{\mathrm{p3}}) + R_4(3+\overline{\nu}_{\mathrm{p4}})},\\
S_3 &= \frac{R_3(\varphi_1(E) + \varphi_2(E) + \overline{\nu}_{\mathrm{p3}}N_3(E))}{R_1\overline{\nu}_{\mathrm{p1}} + R_2(1+\overline{\nu}_{\mathrm{p2}}) + R_3(2+\overline{\nu}_{\mathrm{p3}}) + R_4(3+\overline{\nu}_{\mathrm{p4}})},\\
S_4 &= \frac{R_4(\varphi_1(E) + \varphi_2(E) + \varphi_3(E) + \overline{\nu}_{\mathrm{p4}}N_4(E))}{R_1\overline{\nu}_{\mathrm{p1}} + R_2(1+\overline{\nu}_{\mathrm{p2}}) + R_3(2+\overline{\nu}_{\mathrm{p3}}) + R_4(3+\overline{\nu}_{\mathrm{p4}})},
\end{aligned}
\tag{13}
$$

$$
\overline{\nu}_{\mathrm{p}} = R_1\overline{\nu}_{\mathrm{p1}} + R_2(1+\overline{\nu}_{\mathrm{p2}}) + R_3(2+\overline{\nu}_{\mathrm{p3}}) + R_4(3+\overline{\nu}_{\mathrm{p4}}) \tag{14}
$$

with:

$$
R_1 = \frac{\sigma_{n\mathrm{f}}}{\sigma_{\mathrm{ftot}}}; \quad R_2 = \frac{\sigma_{nn'\mathrm{f}}}{\sigma_{\mathrm{ftot}}}, \quad R_3 = \frac{\sigma_{n2n\mathrm{f}}}{\sigma_{\mathrm{ftot}}}, \quad R_4 = \frac{\sigma_{n3n\mathrm{f}}}{\sigma_{\mathrm{ftot}}}, \tag{15}
$$

where σ_{ftot}, $\sigma_{n\mathrm{f}}$, $\sigma_{nn'\mathrm{f}}$, $\sigma_{n2n\mathrm{f}}$, $\sigma_{n3n\mathrm{f}}$ are total and ith chance fission cross sections (with $i = 1$, 2, 3 and 4) and the quantities $N_i(E)$ and $\overline{\nu}_{\mathrm{p}i}$ are the prompt fission neutron spectrum and the average prompt fission neutron multiplicity for each "i" indexed fissioning compound nucleus.

In Eq. (13) the quantities $\varphi_1(E)$, $\varphi_1(E) + \varphi_2(E)$ and $\varphi_1(E) + \varphi_2(E) + \varphi_3(E)$ are the emitted neutron spectra: for the neutron of the $(n, n'\mathrm{f})$ reaction, the first and second neutron of the $(n, 2n\mathrm{f})$ reaction and the first, second and third neutron of the $(n, 3n\mathrm{f})$ reaction, respectively, calculated with Weisskopf–Ewing evaporation model, given by the relations:

$$
\begin{aligned}
\varphi_i(E) &= k(\theta_i)\sigma_{\mathrm{c}}(E)E\exp(-E/\theta_i),\\
k(\theta_i) &= \left[\int_0^\infty E\sigma_{\mathrm{c}}(E)\exp(-E/\theta_i)\,dE\right]^{-1},
\end{aligned}
\tag{16}
$$

$\sigma_{\mathrm{c}}(E)$ in this equation is the compound nucleus formation cross section of the fissioning nucleus calculated from an actinide optical potential. Because an actinide nucleus is on kinetic point of view a good approximation of an infinite mass nucleus, the distinction between center-of-mass and laboratory system for the neutrons emitted prior to fission can be neglect. Consequently E (in the relations (16)) is the laboratory neutron energy.

For the case $\sigma_{\mathrm{c}}(E) =$ constant,

$$
\varphi_i(E) = \frac{1}{\theta_i^2}E\exp(-E/\theta_i). \tag{17}
$$

The spectrum constructed in this way gives unit normalization when integrated from zero to infinity.

For $N_i(E)$ and $\overline{\nu}_{pi}$ calculation it is necessary to use the equations (1)–(12) in which the model parameters $\langle E_{ri}\rangle$, $\langle E_{fi}^{tot}\rangle$, $\langle S_{ni}\rangle$, $\langle E_{\gamma i}\rangle$, the level density parameter a_i and the neutron separation energy B_{ni} are necessary for each "i" indexed compound nucleus and the total average fission-fragment excitation energy $\langle E^*\rangle$ from Eq. (2) for the ith chance ($i = 1, 2, 3, 4$) are given by:

$$\langle E_i^*\rangle = \langle E_{ri}\rangle + E_{xi} - \langle E_{fi}^{tot}\rangle, \tag{18}$$

where the quantities E_{xi} corresponding at each compound nucleus undergoing fission are given by the following relations:

$$E_{xi+1} = E_{xi} - B_{ni} - \varepsilon_{evi} \quad \text{with} \quad E_{x1} = B_{n1} + E_n \quad \text{and} \quad \varepsilon_{ev0} = 0. \tag{19}$$

Here the energy ε_{evi} represents the mean kinetic energy of the evaporated neutrons calculated using the relation:

$$\varepsilon_{evi} = k(\theta_i)\int_0^\infty E^2\sigma_c(E)\exp(-E/\theta_i)\,dE \tag{20}$$

and the evaporation temperatures θ_i are computed using the expression:

$$\theta_i = \sqrt{\frac{E_{xi} - B_{ni}}{a_{i+1}}}. \tag{21}$$

In the case of $\sigma_c(E) =$ constant this energy is calculated with the formula:

$$\varepsilon_{evi} = 2\theta_i. \tag{22}$$

(*d2*) *Energy moments of the spectrum*

The first and second order laboratory energy moments of the spectrum for each compound nucleus (indexed i) are:

$$\langle E_i\rangle = \int_0^\infty E N_i(E)\,dE, \qquad \langle E_i^2\rangle = \int_0^\infty E^2 N_i(E)\,dE. \tag{23}$$

In the case $\sigma_{cf}(\varepsilon) =$ constant there are closed forms for this energy moments:

$$\begin{aligned}\langle E_i\rangle &= \tfrac{1}{2}\left(E_{fi}^{L} + E_{fi}^{H}\right) + \tfrac{4}{3}T_{mi}\\ \langle E_i^2\rangle &= \tfrac{1}{2}\left[\left(E_{fi}^{L}\right)^2 + \left(E_{fi}^{H}\right)^2\right] + \tfrac{20}{9}\left(E_{fi}^{L} + E_{fi}^{H}\right)T_{mi} + 3(T_{mi})^2.\end{aligned} \tag{24}$$

The total laboratory energy first moment of the spectrum for multiple fission chances is given by the expression:

$$\begin{aligned}\langle E\rangle &= W_1 + W_2 + W_3 + W_4,\\ W_1 &= \frac{R_1\overline{\nu}_{p1}\langle E_1\rangle}{R_1\overline{\nu}_{p1} + R_2(1+\overline{\nu}_{p2}) + R_3(2+\overline{\nu}_{p3}) + R_4(3+\overline{\nu}_{p4})},\\ W_2 &= \frac{R_2(\varepsilon_{ev1} + \overline{\nu}_{p2}\langle E_2\rangle)}{R_1\overline{\nu}_{p1} + R_2(1+\overline{\nu}_{p2}) + R_3(2+\overline{\nu}_{p3}) + R_4(3+\overline{\nu}_{p4})},\\ W_3 &= \frac{R_3(\varepsilon_{ev1} + \varepsilon_{ev2} + \overline{\nu}_{p3}\langle E_3\rangle)}{R_1\overline{\nu}_{p1} + R_2(1+\overline{\nu}_{p2}) + R_3(2+\overline{\nu}_{p3}) + R_4(3+\overline{\nu}_{p4})},\\ W_4 &= \frac{R_4(\varepsilon_{ev1} + \varepsilon_{ev2} + \varepsilon_{ev3} + \overline{\nu}_{p4}\langle E_4\rangle)}{R_1\overline{\nu}_{p1} + R_2(1+\overline{\nu}_{p2}) + R_3(2+\overline{\nu}_{p3}) + R_4(3+\overline{\nu}_{p4})},\end{aligned} \tag{25}$$

in which the first, second, third and fourth term represents the contribution of the first-, second-, third- and fourth-chance respectively, to the mean energy of the prompt fission neutrons.

(*d3*) *Equivalent Maxwellian spectrum*

Equating the average energy $\langle E\rangle$ of the Maxwellian spectrum to that of the expression (25) it is possible to find the Maxwell temperature T_{M}:

$$T_{\mathrm{M}} = \frac{2}{3}\langle E\rangle \tag{26}$$

and to calculate the equivalent Maxwellian spectrum:

$$N_{\mathrm{Maxw}}(E) = \frac{2}{\sqrt{\pi}T_{\mathrm{M}}^{3/2}}\sqrt{E}\exp(-E/T_{\mathrm{M}}). \tag{27}$$

(*d4*) *Effective level density parameter*

From the above formulae it was obviously that the computation is easier when compound nucleus formation cross section is *constant*. An approximate way to simulate the energy dependence of the compound nucleus cross section is possible. This simulation can be performed by a slight readjustment of the nuclear level density parameter a which is described here by Eq. (3). This simulation allows the prompt fission neutron spectrum and the average prompt neutron multiplicity to be expressed in closed form and therefore easily calculated.

The method of adjusting the level density parameter, proposed in [1], is to equate the first moment or mean energy of the constant cross section spectrum to that of the more nearly exact energy-dependent cross section spectrum. Using the expressions (23), (24), (1), (2) the effective level density parameter for each compound nucleus i is given by:

$$a_{\mathrm{eff}i} = \frac{16\langle E_i^*\rangle}{9[\langle E_i\rangle - \frac{1}{2}(E_{\mathrm{f}i}^{\mathrm{L}} + E_{\mathrm{f}i}^{\mathrm{H}})]^2}. \tag{28}$$

Applying the same method, but equating second moments or mean square energies, the agreement between simulated energy-dependence spectra and exact spectra at high neutron energy is improved [1]. In this case the effective level density parameter for each fissioning compound nucleus can be calculated using the following expressions:

$$\begin{aligned} T_{\mathrm{m}i} &= \tfrac{1}{3}\big(\sqrt{z_{1i}^2 - 3(z_{2i} - \langle E_i^2\rangle)} - z_{1i}\big),\\ z_{1i} &= \tfrac{10}{9}\big(E_{\mathrm{f}i}^{\mathrm{L}} + E_{\mathrm{f}i}^{\mathrm{H}}\big),\\ z_{2i} &= \frac{(E_{\mathrm{f}i}^{\mathrm{L}})^2 + (E_{\mathrm{f}i}^{\mathrm{H}})^2}{2},\\ a_{\mathrm{eff}i} &= \frac{\langle E_{\mathrm{r}i}\rangle + E_{xi} - \langle E_{\mathrm{f}i}^{\mathrm{tot}}\rangle}{T_{\mathrm{m}i}^2}. \end{aligned} \tag{29}$$

In terms of the formula (3) we can express the effective coefficient $C_{\mathrm{eff}i}$ that allows the use of the closed form to simulate energy dependence of the compound nucleus cross section:

$$C_{\mathrm{eff}i} = \frac{A_i}{a_{\mathrm{eff}i}}, \tag{30}$$

where A_i are the mass numbers of the compound nuclei i undergoing fission and $a_{\mathrm{eff}i}$ are the level density parameters of these nuclei given by the expressions (28) or (29).

(*d5*) *Energy dependence of the input parameters*

The experimental data prove that the parameters $\langle E_{\mathrm{f}}^{\mathrm{tot}}\rangle$ and $\langle E_{\gamma}^{\mathrm{tot}}\rangle$ have a slight dependency on the incident neutron energy E_{n}. Thus the total average fission-fragment kinetic energy $\langle E_{\mathrm{f}}^{\mathrm{tot}}\rangle$ is diminished (enhanced) with increasing excitation energy and therefore with the incident neutron energy. This dependence on the incident neutron energy can be estimated from experimental data for certain cases or from a theoretical approach [6]. Similarly, the measurements [7] showed that the total average prompt gamma-ray energy $\langle E_{\gamma}^{\mathrm{tot}}\rangle$ increases with the average prompt neutron multiplicity $\overline{\nu}_{\mathrm{p}}$ and therefore with the incident neutron energy. Similarly the average energy release $\langle E_{\mathrm{r}}\rangle$ and the average fission-fragment neutron separation energy $\langle S_{\mathrm{n}}\rangle$ must be depended on the incident neutron energy due to the slight dependence of the mass and charge distributions on excitation energy.

The variation of the quantities mentioned above versus the incident energy is expressed, in the computer code, by the relations:

$$\begin{aligned}
&\langle E_{\mathrm{r}i}\rangle = \langle E_{\mathrm{r}i}^{0}\rangle + q_{\mathrm{r}i}\,E_{\mathrm{inc}i}\,,\\
&\langle E_{\mathrm{f}i}^{\mathrm{tot}}\rangle = \langle E_{\mathrm{f}i}^{\mathrm{tot}0}\rangle + q_{\mathrm{f}i}^{(1)}E_{\mathrm{inc}i} + q_{\mathrm{f}i}^{(2)}E_{\mathrm{inc}i}^{2}\,,\\
&\langle S_{\mathrm{n}i}\rangle = \langle S_{\mathrm{n}i}^{0}\rangle + q_{\mathrm{s}i}\,E_{\mathrm{inc}i}\,,\\
&\langle E_{\gamma i}^{\mathrm{tot}}\rangle = \langle E_{\gamma i}^{\mathrm{tot}0}\rangle + q_{\gamma i}^{(1)}E_{\mathrm{inc}i} + q_{\gamma i}^{(2)}E_{\mathrm{inc}i}^{2}\,,
\end{aligned} \tag{31}$$

where the $\langle E_{\mathrm{r}i}^{0}\rangle$, $\langle E_{\mathrm{f}i}^{\mathrm{tot}0}\rangle$, $\langle S_{\mathrm{r}i}^{0}\rangle$ and $\langle E_{\gamma i}^{\mathrm{tot}0}\rangle$ are the values at thermal incident neutron energy and the coefficients q_{r}, $q_{\mathrm{f}}^{(1)}$, $q_{\mathrm{f}}^{(2)}$, q_{s}, $q_{\gamma}^{(1)}$ and $q_{\gamma}^{(2)}$ are input quantities for each "i" fissioning compound nucleus. The corresponding incident energy for each compound nucleus undergoing fission is calculated by:

$$E_{\mathrm{inc}i} = E_{xi} - B_{\mathrm{n}i}\,, \qquad E_{\mathrm{inc}1} = E_{\mathrm{n}}. \tag{32}$$

The inclusion of the dependency of the model parameters versus the incident neutron energy can lead to considerable modifications of prompt neutron multiplicity and spectrum evaluations in comparison with the situation without this dependency as can be seen in the Fig. 6.

3. The code structure

The SPECTRUM code contains two programs (modules): SPECTRUM and SPGRAPH, each of them having the possibility to run independently. The two codes work in BATCH mode with the creation of a temporary file STEMPO that contains the name of the output file. The two modules are created fully bound executables.

The code calculates all the quantities described above, also having the possibility to allow the dependence of the model parameters with the incident neutron energy. The calculated data are processed in graphical form.

The SPECTRUM module is written in Fortran77 using only the standard features of the Fortran language in order to assure the portability of the program.

This module calculates, for a given incident neutron energy E_{n}, the prompt fission neutron spectra and average prompt fission neutron multiplicities for each fissioning compound nucleus formed in the process as well as the corresponding total quantities in multiple-chance fission, the first and second laboratory energy momentum. Optionally the program computes the equivalent Maxwellian spectrum, the ratio to an evaluated fission spectrum (input from an external file) and the average prompt fission neutron multiplicities at many incident neutron energies.

The SPECTRUM program can run on two ways:

Option "variab": with the consideration of the energy dependence of the compound nucleus cross section for the inverse process. In this option the code also calculates the effective level density parameter in order to simulate the energy dependence of the compound nucleus cross section.

Option "const": with the consideration of *constant* compound nucleus cross section for the inverse process. In this option the program can calculate (optionally) the average prompt neutron number at many incident neutron energy.

For the fission neutron energy range three options are given: (1) $E = 0.001$–15 MeV, (2) $E = 0.001$–20 MeV and (3) $E = 0.001$–40 MeV with an energy grid that assures the possibility to calculate the integrals of energy moments.

The SPGRAPH module, written in Quick-Basic language, helps the user to fast process the output data in a convenient way.

3.1. Input files

3.1.1. The main input file required by the SPECTRUM module, includes: the model parameters for all fissioning compound nuclei as well as the names of the auxiliary input files necessary in the computation.

The syntax of the main input file is the following:

– The first line is a free space (format A60) in order to allow the user to write comments, information, etc.

– The second line (in free format) contains the model parameters for the main compound nucleus in the order

$$Z,\ A_1,\ B_{\mathrm{n}1},\ \langle E^0_{\mathrm{r}1}\rangle,\ \langle E^{\mathrm{tot}0}_{\mathrm{f}1}\rangle,\ A_{\mathrm{H}1},\ \langle S^0_{\mathrm{n}1}\rangle,\ \langle E^{\mathrm{tot}0}_{\gamma 1}\rangle,$$

where Z is the atomic number. The quantities indexed with 0 are for thermal incident neutron energy.

– The third line, in free format, contains the names of four auxiliary input files:

$$file^{\mathrm{L}}_1, file^{\mathrm{H}}_1, fileR, fileCN$$

where $file^{\mathrm{L}}_1$ and $file^{\mathrm{H}}_1$ contain the $\sigma^{\mathrm{L}}_{\mathrm{cf}}(\varepsilon)$, $\sigma^{\mathrm{H}}_{\mathrm{cf}}(\varepsilon)$ for the central light fragment and heavy fragment corresponding to the main compound nucleus, *fileR* is the name of the file containing the fission ratios R_i versus the incident neutron energy and *fileCN* is the name of the file containing the compound nucleus cross section of the main fissioning nucleus. In the option "const" the auxiliary files $file^{\mathrm{L}}_1, file^{\mathrm{H}}_1, fileCN$ are not necessary and any fictive names can be written.

– The next six lines of the input file, written in free format, contain the data for the other three fissioning compound nuclei:

$$Z,\ A_i,\ B_{\mathrm{n}i},\ \langle E^0_{\mathrm{r}i}\rangle,\ \langle E^{\mathrm{tot}0}_{\mathrm{f}i}\rangle,\ A_{\mathrm{H}i}, \langle S^0_{\mathrm{n}i}\rangle,\ \langle E^{\mathrm{tot}0}_{\gamma i}\rangle$$
$$file^{\mathrm{L}}_i,\ file^{\mathrm{H}}_i$$

with i running from 2 to 4.

– The last four lines of the input file (also in free format) contain the coefficients from the Eq. (31) that express the variation of model parameters versus the incident neutron energy. If this variation it is not considered, these coefficients are zero. The syntax of these lines is:

$$q_{\mathrm{r}1},\ q_{\mathrm{r}2},\ q_{\mathrm{r}3},\ q_{\mathrm{r}4},$$
$$q^{(1)}_{\mathrm{f}1}, q^{(2)}_{\mathrm{f}1},\ q^{(1)}_{\mathrm{f}2}, q^{(2)}_{\mathrm{f}2},\ q^{(1)}_{\mathrm{f}3}, q^{(2)}_{\mathrm{f}3},\ q^{(1)}_{\mathrm{f}4}, q^{(2)}_{\mathrm{f}4},$$
$$q_{\mathrm{s}1},\ q_{\mathrm{s}2},\ q_{\mathrm{s}3},\ q_{\mathrm{s}4},$$
$$q^{(1)}_{\gamma 1}, q^{(2)}_{\gamma 1},\ q^{(1)}_{\gamma 2}, q^{(2)}_{\gamma 2},\ q^{(1)}_{\gamma 3}, q^{(2)}_{\gamma 3},\ q^{(1)}_{\gamma 4}, q^{(2)}_{\gamma 4}.$$

3.1.2. The auxiliary input files are the following:

– The file *fileR* containing the fission ratios R_i (expression (15)) versus the neutron incident energy E_{n}, in free format, in the order $E_{\mathrm{n}},\ R_1(E_{\mathrm{n}}),\ R_2(E_{\mathrm{n}}),\ R_3(E_{\mathrm{n}}),\ R_4(E_{\mathrm{n}})$. These ratios can be calculated using the data from the evaluated nuclear data libraries: the file MF = 3, sections MT = 18, 19, 20, 21 and 38.

– The files $file_i^{\mathrm{L}}$, $file_i^{\mathrm{H}}$, $fileCN$ containing the energy dependent compound nucleus cross sections for the central light and heavy fission fragments corresponding to each fissioning compound nucleus and for the main compound nucleus. All these files are in free format with the syntax ε $\sigma_{\mathrm{c}}(\varepsilon)$. The cross sections $\sigma_{\mathrm{c}}(\varepsilon)$ can be calculated using direct interaction models with phenomenological optical potential with strong isospin dependence.
  The first line of all the auxiliary input files contains the number of data in the file.
  The names of these auxiliary input files are at the free choice of the user.

3.1.3. External input files: some options of the code require external input files which names typed by the user (on the keyboard). There are three types of external files with the names at the free users choice:
– the file containing evaluated prompt fission neutron spectra (in free format) with the syntax: E N(E), the number of data in the file being on the first line.
– the file containing experimental average prompt neutron multiplicities (in free format too) with the syntax: $\mathrm{E_n}$ $\nu_{\mathrm{p}}(\mathrm{E_n})$ (+)$\delta_\nu(\mathrm{E_n})$ (-)$\delta_\nu(\mathrm{E_n})$, where δ_ν is the absolute error of the ν_{p}.
– the file containing evaluated average prompt neutron number (in free format) having the syntax $\mathrm{E_n}$ $\nu_{\mathrm{p}}(\mathrm{E_n})$.

3.2. The SPECTRUM module

The SPECTRUM program has a main part and 19 subroutines.

MAIN part: here the input data are read and the most important quantities (such as prompt fission neutron spectra and average neutron multiplicities) are calculated.

SECTSANSE: in this subroutine the fission probability ratios (formulae (15)) are read and the number of chances, at the incident neutron energy E_{n}, is determined.

EXCI subroutine calculates the quantities E_{xi} (from the expression (19)) and the evaporation temperatures (according to the relation (21)).

EVMEDIA: in this subroutine the mean evaporation energies (expression (20)) are calculated, the normalization constant $k(\theta_i)$ being computed by the subroutine **KTINTEG** (called by the subroutine Evmedia).

PARAM subroutine computes the model parameters taking into account their variation with the neutron incident energy (according to the relations (31) and (32)).

KTE subroutine calculates the normalization constants (according to the relation (7)) for the central light and heavy fragments corresponding at each fissioning compound nucleus.

EPSIL: in this subroutine the average center-of-mass energies of the emitted neutrons (according to the expression (11)) corresponding to each fissioning compound nucleus are computed.

TINTEG subroutine assures the integration over the temperature T (see the formulae (6), (11)) being called by Main and by the subroutine Epsil.

INTERPOL and INTERP subroutines assure the linear interpolation of the auxiliary input file data. They are called by Main and by other subroutines (such as Evmedia, Ktinteg, Epsil, Evap and respectively Sectsanse, Nu, etc.)

SPSCONST subroutine computes the prompt fission neutron spectra (according to the expressions (8) and (9)) for each fissioning nucleus in the option “const”. The functions E1 and γ-incomplete are calculated by the subroutines **FE1** and **GAM**, respectively.

EVAP subroutine: here the evaporation spectra from the expressions (16)–(17) are done.

EMEDIE: in this subroutine first and second order laboratory energy moments of the spectrum for each nucleus undergoing fission are integrated (according to the expressions (23) and (24)).

MAXW subroutine computes the equivalent Maxwellian spectrum (expressions (26) and (27)) if this option is chosen.

RAP subroutine provides the ratio

$$r(E) = \frac{N(E)}{N_{\text{eval}}(E)} \tag{33}$$

if the user has made the option to compare the calculated total prompt fission neutron spectrum with an other spectrum $N_{\text{eval}}(E)$ (for example, an evaluated spectrum from a nuclear data library) that is given on an external input file.

AEFF subroutine calculates the effective level density parameter to simulate the energy dependence of the compound nucleus cross section, using the relations (28) and (29) and the corresponding coefficients (the expression (30)) for each fissioning nucleus, of course in the "variab" option.

NU subroutine, called by Main in the option "const", calculates the average prompt fission neutron multiplicities in the incident neutron energy range (0–15) MeV.

All the integrals in the code are computed using the Simpson method. The big areas are in common blocks. The mean running time of this module is few minutes in the option "variab" and less than one minute in the option "const", the running time being dependent, of course, on the number of fission neutron energies.

3.3. The output file

The quantities of interest calculated by the SPECTRUM module are printed on a single output file with the name at the free choice of the user.

The output file contains information about the options used, the auxiliary input files used, the incident neutron energy, the number of fission chances, the number of emitted fission neutron energies, same intermediate quantities calculated (such as E_{fi}^{HF}, E_{fi}^{LF}, $T_{\text{m}i}$, evaporation temperatures etc.), the average prompt neutron multiplicities for each fissioning compound nucleus, the total average fission neutron multiplicity, the tabulated fission neutron spectra for each compound nucleus, the tabulated total prompt fission neutron spectrum and the multiple-chance spectrum components, the first and second momentum, the average fission neutron energy.

Optionally the output file can contain the tabulated equivalent Maxwellian spectrum, the tabulated ratio to an external input spectrum, the effective level density parameter and the tabulated average prompt fission neutron number versus the incident neutron energy.

3.4. The SPGRAPH module

This module is organized in a main part and five subroutines (called by Main).

In the Main part, the data of the output file are read and processed.

INFO subroutine makes the first screen page containing a summary of the results.

GRAFSP subroutine displays the second screen page that contains the graphic representation of the total prompt fission neutron spectrum, the only one chance neutron spectrum and the equivalent Maxwellian spectrum (if this option was made). On this second screen the user has also the option to represent an other neutron spectrum from an external input file, in order to make comparisons.

GRAFSP1 subroutine shows the third screen page that displays the graphics of the multiple fission chance spectra. Here the user has also the possibility to represent a spectrum from an external file. This screen page is switch off if only one fission chance is involved.

RATIOMAXW subroutine: if the option to calculate the equivalent Maxwellian spectrum was chosen, this subroutine calculates the ratio to Maxwellian spectrum and displays it on the fourth screen page, the graphic representation being accompanied by information about the maximum and minimum deviations.

RATIOEV subroutine runs if the option to calculate the ratio to an other spectrum (for an external input file) was done. Then, the fifth screen page will display the graphic representation of this ratio and auxiliary information about the maximum and minimum deviations.

NU subroutine displays on the last screen page the graphic representation of the calculated average prompt neutron multiplicity versus the incident neutron energy. Here the user has the option to represents other data too, such as experimental data and/or evaluated data from external input files, in order to make comparisons.

4. Conclusions

The code takes into account all the possibilities of the Los Alamos model upgraded to allow the dependencies of the input parameters on the incident neutron energy.

The main input quantities and the calculated quantities are printed on a single output file. These quantities are then represented graphically helping the user to process efficiently the data and (optionally) compared with other corresponding spectra (reference spectra) from an external input file. This option allows a slight modification of the input parameters in order to obtain model parameters which give a good agreement with the reference data (experimental or calculated).

All quantities generated are important data required in the evaluated nuclear data libraries. The tabulated data of the output file can be easily processed in the ENDF-6 format of these libraries.

The use of standard features of Fortran language ensures the portability of the program.

An earlier version of this code, with only one fission chance, was used by the authors to evaluate prompt fission neutron spectrum of the n+^{242}Pu process [8,9].

5. Sample problems

The run test problems presented here refers to n + ^{235}U process in two cases.

5.1 The first main input file is the following:

```
---- n+U-235 ----(Madland parameters)---
92  236   6.546   186.98   171.8   140   4.998   6.71
sr-96.opt   xe-140.opt  rpfmad.dat  u-235.opt
92  235   5.298   188.946  171.95  139   5.151   6.67
sr-96.opt   xe-139.opt
92  234   6.844   188.971  172.1   139   5.274   6.69
sr-95.opt   xe-139.opt
92  233   5.743   0.       0.      0.    0.      0.
dummy     dummy
0.   0.   0.   0.
```

```
0.   0.   0.   0.   0.   0.   0.   0.
0.   0.   0.   0.
0.   0.   0.   0.   0.   0.   0.   0.
```

The parameters B_{ni}, $\langle E_{ri}^{0}\rangle$, $\langle E_{fi}^{tot0}\rangle$, A_{Hi}, $\langle S_{ni}^{0}\rangle$, $\langle E_{\gamma i}^{tot0}\rangle$ are taken from [1].

In this case the variation of the model parameters versus the incident neutron energy is not taken into account, consequently the coefficients from Eq. (31) are zero.

The auxiliary input files involved in this sample problem are:

(a) The file "rpfmad.dat" containing the fission probability ratios $R_i(E_n)$ taken from [1].
(b) The files "*.opt" containing the compound nucleus cross sections for the inverse process, versus the center-of-mass neutron energy, for the central light and heavy fragments corresponding to each fissioning compound nucleus. These data were calculated using the Becchetti-Greenlees optical model potential and an optical model code [10] for the processes $n + {}^{96}Sr$, $n + {}^{140}Xe$, $n + {}^{95}Sr$, $n + {}^{139}Xe$, in the energy range (10^{-6}–40) MeV.
(c) The file "u-235.opt" containing the compound nucleus cross section for the $n+{}^{235}U$ process calculated using an optical model code with the Madland actinide optical model potential [10].

5.2. The second main input file is the following:

```
n + U-235: Madland Parameters, En dependency for Er, Eftot
92  236   6.546   186.98   171.8   140   4.998   6.71
sr-96.opt   xe-140.opt  rpfmad.dat  u-235.opt
92  235   5.298   188.946  171.95  139   5.151   6.67
sr-96.opt   xe-139.opt
92  234   6.844   188.971  172.1   139   5.274   6.69
sr-95.opt   xe-139.opt
92  233   5.743   0.       0.      0.    0.      0.
dummy     dummy
0.   0.   0.   0.
0.045233  -0.012     -0.015    -0.0085     0.026301  -0.01      0.  0.
0.   0.   0.   0.
0.12863   0.   0.112      0.  0.10856   0.     0.    0.
```

The data of this input file are the same that above one but the variation of the model parameters $\langle E_{fi}^{tot}\rangle$ and $\langle E_{\gamma i}^{tot}\rangle$ versus the incident neutron energy is taken into account.

Using the two main input files described above we present some Test Run Inputs and Outputs:

For the first main input file (named in this example "input1") the options chosen are the following:

MASTER INPUT FILE NAME #5: **input1**

OPTION: CN C.S. (type const or variab) = **variab**

INCIDENT NEUTRON ENERGY = **14**

Coeff for a = **11**

1.Emax=15 MeV 2.Emax=20 MeV 3.Emax=40 MeV **2**

OUTPUT FILE NAME #6 **sp14v.out**

Equivalent Maxwell Spect. on output file -y/n **y**

Eval. Spectrum input file name #7/n **evu35_14.dat**

```
   ---- n+U-235 ----(Madland parameters)---
   OUTPUT FILE sp14v.out
Incident Neutron Energy =  14  MeV        Number of chances =  3
Number of Fission Neutron Energies =  205
                              Equivalent Maxwell Spectrum calculation
                              Ratio to Evaluation calculation
                              NOT Av.Pr.Neut.Multip.in En range calculation
   Average Prompt Neutron Multiplicities
   -------------------------------------
   1-st Comp.Nuc.  4.393917
   2-nd Comp.Nuc.  3.436759
   3-rd Comp.Nuc.  2.456437
   Total           4.431491

First Moments (MeV)                  Second Moments (MeV)
-------------------                  --------------------
1-st Comp.Nuc.  2.38697              1-st Comp.Nuc.  9.31231
2-nd Comp.Nuc.  2.24203              2-nd Comp.Nuc.  8.16719
3-rd Comp.Nuc.  2.07686              3-rd Comp.Nuc.  6.95023
Average Fission Neutron Energy =  2.08383  MeV


                -------for graphics press any key-------------
```

Fig. 1. The first screen image.

For the second main input file (named in this example “input2”) the options chosen are the following:

MASTER INPUT FILE NAME #5: **input2**

OPTION: CN C.S. (type const or variab) = **const**

INCIDENT NEUTRON ENERGY = **14**

Coeff for a = **10**

1.Emax=15 MeV 2.Emax=20 MeV 3.Emax=40 MeV **2**

OUTPUT FILE NAME #6 **sp14c1.out**

Equivalent Maxwell Spect. on output file -y/n **y**

Eval. Spectrum input file name #7/n **evu35_14.dat**

NU CALCULATION AT MANY En - y/n **y**

The external input file “evu35_14.dat” is the prompt fission neutron spectrum from the ENDF/B-VI evaluation [11].

The most important data for the output file “sp14v.out” are processed on the first five screen pages presented in Figs. 1–5.

In the second Test Run case the first 5 screen pages are similar, consequently only the sixth screen page, which contents the calculation of the prompt fission average multiplicity versus the neutron incident energy, is given in Fig. 6 (the lower curve).

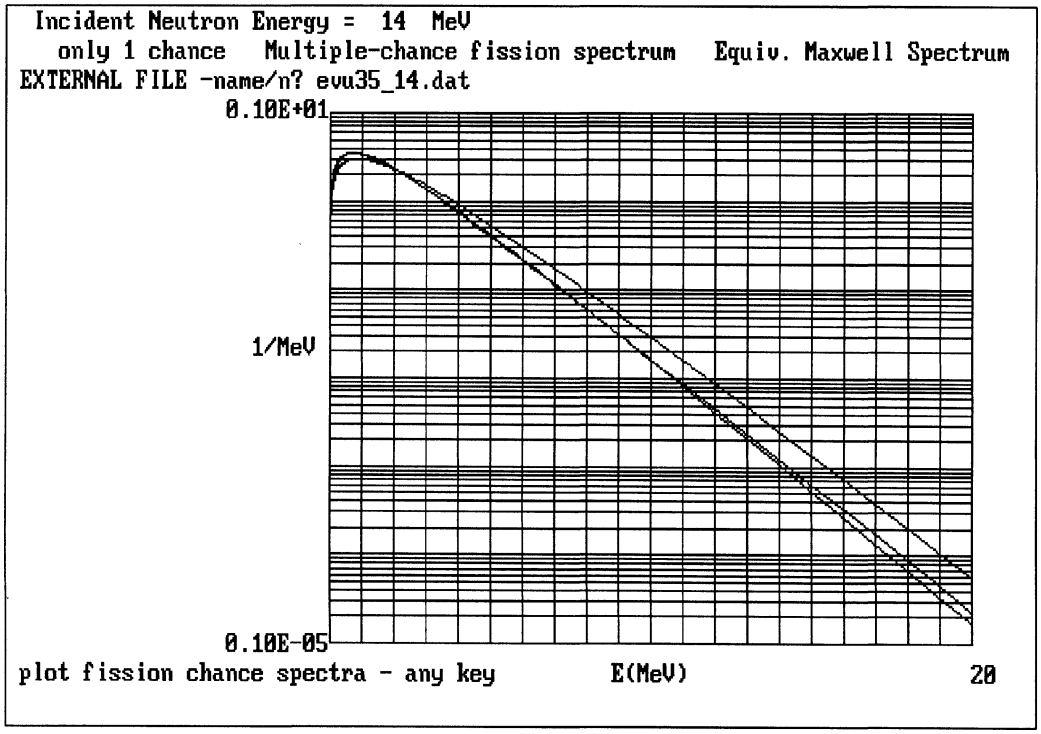

Fig. 2. The second screen image.

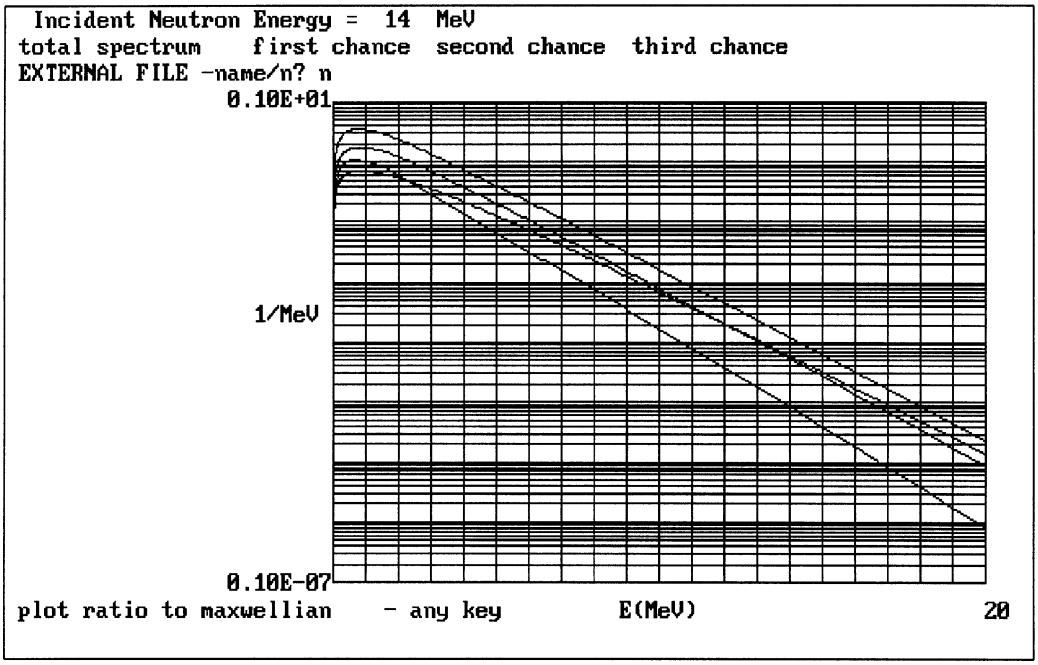

Fig. 3. The third screen image.

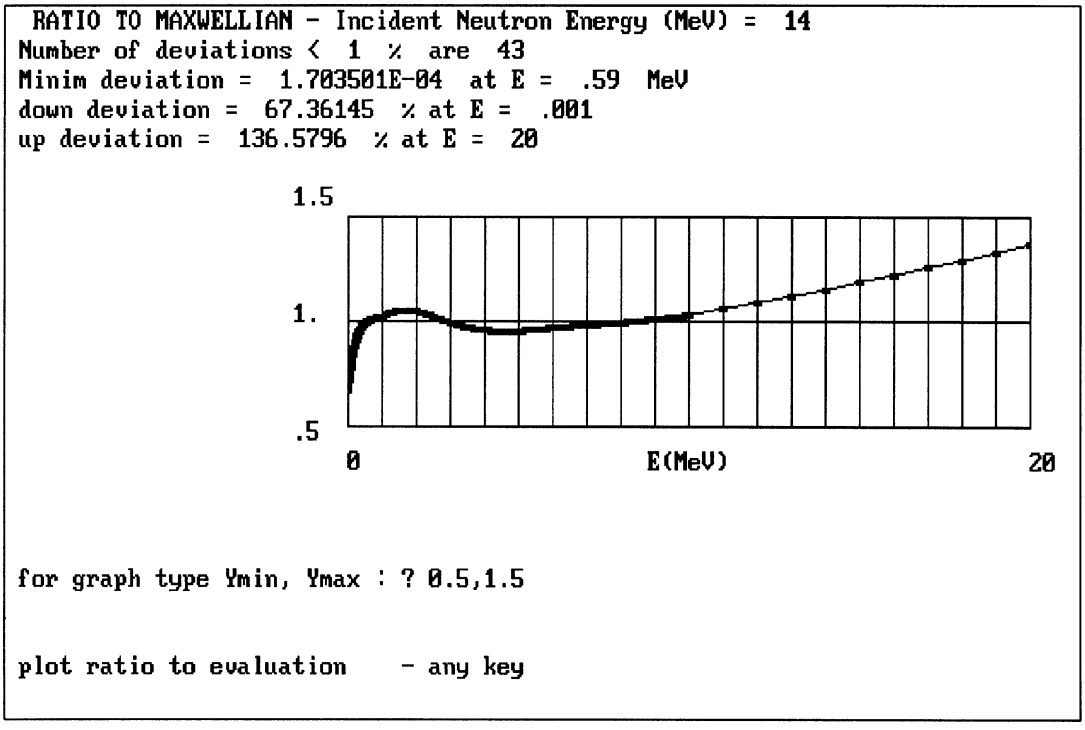

Fig. 4. The fourth screen image.

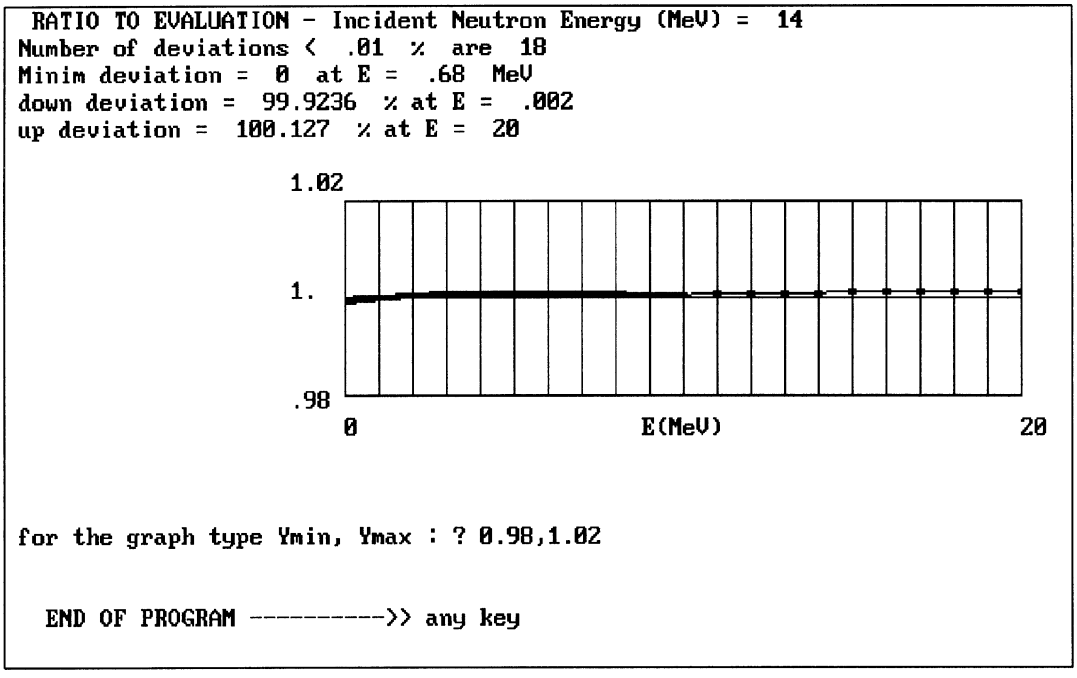

Fig. 5. The fifth screen image.

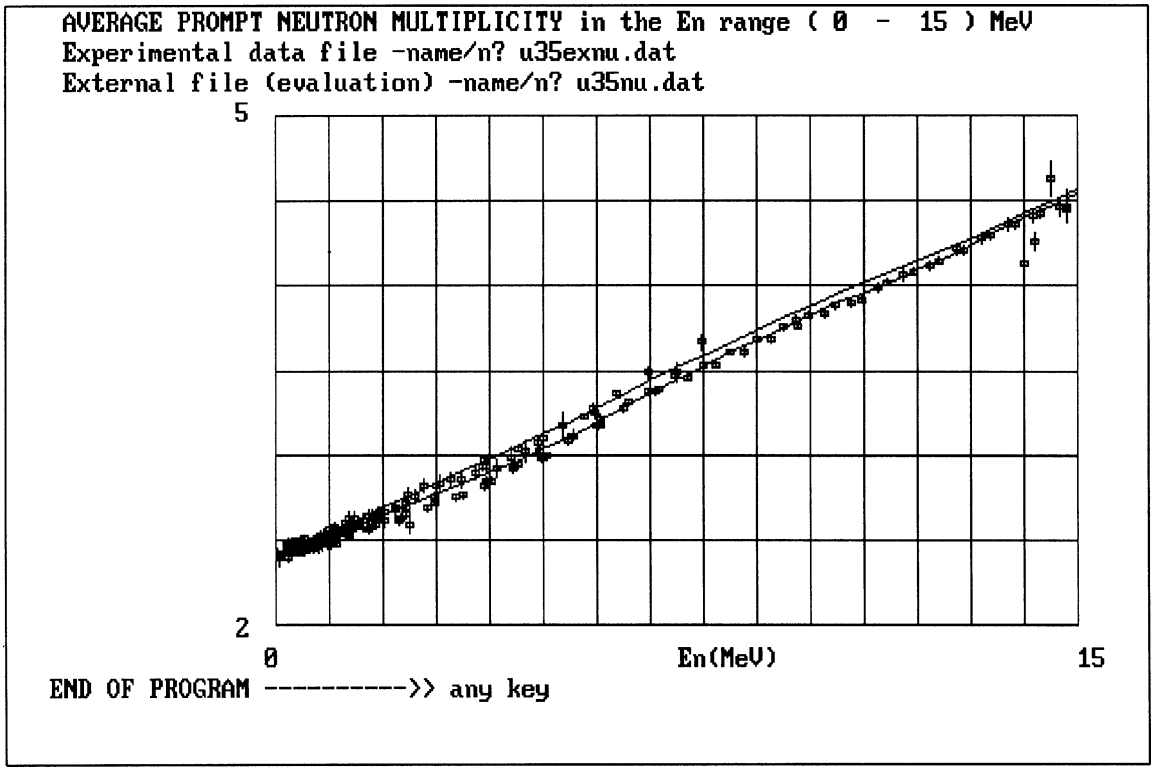

Fig. 6. The sixth screen image.

In the last screen page the external files “u35exnu.dat” and “u35nu.dat” contain respectively the experimental data taken from EXFOR library [12] and the average prompt neutron multiplicity evaluated using the input file INPUT1 and the option “const” (the upper curve).

In the figures a monochrome representation is used but the display terminal of the SPGRAPH module produces output curves in different colors.

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