KfK 4867
Juli 1991

Nuclear Data Libraries for the Treatment of Sequential (x, n) Reactions in Fusion Materials Activation Calculations

S. Cierjacks, P. Obložinský, B. Rzehorz
Institut für Materialforschung

Kernforschungszentrum Karlsruhe

KERNFORSCHUNGSZENTRUM KARLSRUHE
Institut für Materialforschung

KfK 4867

Nuclear Data Libraries for the Treatment of Sequential (x,n) Reactions in Fusion Materials Activation Calculations

S. Cierjacks , P. Obložinský[1] and B. Rzehorz

Diese Arbeit wurde im Rahmen der Zusammenarbeit auf dem Gebiet der Kernfusion zwischen dem Kernforschungszentrum Karlsruhe und Euratom durchgeführt.

[1] On leave from the Institute of Physics, SAS, 842 28 Bratislava, Czechoslovakia

Kernforschungszentrum Karlsruhe GmbH, Karlsruhe

Als Manuskript gedruckt

Kernforschungszentrum Karlsruhe GmbH
Postfach 3640, 7500 Karlsruhe 1

ISSN 0303-4003

Die Erstellung von Kerndatenbibliotheken für die Einbeziehung von sequentiellen (x,n) Reaktionen in Aktivierungsrechnungen für Fusionsmaterialien

Kurzfassung

Es werden verschiedene, neu erstellte Kerndatenbibliotheken beschrieben, mit denen in Aktivierungsrechnungen für Fusionsmaterialen auch die sog. "sequentiellen (x, n) Reaktionen" einbezogen werden können. Mit den jetzt vorhandenen Kerndaten ist es möglich, alle sequentiellen (p, n), (d, n) und (α, n) Reaktionen an stabilen und radioaktiven Kernen mit Halbwertszeiten von $\geq$ 1 Tag im Bereich der Elemente von H bis Mo zu erfassen. Die vorhandene Datenbasis überdeckt den Energiebereich von 0-20 MeV für Primär-Neutronen und von 0-24 MeV für alle sekundär emittierten, geladenen Teilchen. Bezüglich der notwendigen Anregungsfunktionen für die Produktion geladener Teilchen aus den primären neutroneninduzierten Reaktionen konnte auf die vorhandene Bibliothek REAC-ECN-5 zurückgegriffen werden, die alle erforderlichen Neutronenreaktionen (teilweise sogar in evaluierter Form) enthält. Für die zusätzlich notwendigen normierten Spektren der emittierten geladenen Teilchen wurde eine neue Datenbibliothek, KFKSPEC, erstellt. Diese enthält derzeit ca. 12 300 Spektren mit etwa 300 000 Datenpunkten. Ähnliche Kernmodellrechnungen wurden auch für die Erstellung der neuen Datenbibliothek, KFKXN, durchgeführt, welche die Anregungsfunktionen für die sekundären (x, n) Reaktionen (1025 verschiedene Reaktionen mit ca. 24 600 Datenpunkten) enthält. Ein vollständiger Satz von differentiellen Reichweiten geladener Teilchen wurde mit Hilfe des Ziegler-Formalismus berechnet. Die entsprechende Datenbibliothek, KFKSTOP, mit 11 040 Datenpunkten ist vollständig bzgl. p, d, t, $^3He-$ und $\alpha-$Teilchen und deren Reichweiten in allen Elementen von H bis U.

Abstract

The current status of nuclear data libraries produced or under development for the kinematically complete treatment of sequential (x,n) reactions in fusion materials activation calculations is discussed. The existing libraries allow complete treatment virtually of all isotopes from Z = 1 through 42 ($A \leq 100$) with half-lifes exceeding 1 day for primary neutron energies $E_n < 20MeV$ and secondary charged particles x = p, d and α with energies $E_x < 24MeV$. Production cross sections of charged particles for primary (n,x) reactions are derived from the evaluated activation file REAC-ECN-5. For the corresponding normalized charged particle spectra we created the starter file KFKSPEC, fully based on nuclear-reaction model calculations and presently containing 12 300 spectra with about 300 000 data points. The same approach was adopted to create the starter file KFKXN for charged particle induced (x,n) cross sections that contains 1025 different reactions and 24 600 data points. A complete set of differential ranges for light charged particles was generated for all elements from hydrogen to uranium and is stored in the KFKSTOP file which has 11 040 data points.

Contents

1. INTRODUCTION

This report contains progress achieved in the development of the nuclear data base needed for the treatment of sequential (x,n) reactions in activation calculations, x being the charged particle created by primary neutron interactions. Such calculations are of importance in the development of low activation materials (LAM) for fusion reactor applications [1]. It has been shown on several selected examples that sequential (x,n) reactions can contribute substantially to the total radioactive inventory [2], [3], [4] and [5]. Due to that a major task is being undertaken to develop necessary nuclear data libraries that allow for a kinematically complete treatment of these reactions.

Below we summarize the concept of sequential (x,n) reactions together with the corresponding formalism for inventory calculations, proceed by explaining the status of libraries implemented or being developed, provide sample results of activation calculations, and outline necessary further developments. Related developments for the preparatory code PCROSS to operate the inventory code FISPACT [6], [7] are described in an adjacent report [8].

2. SEQUENTIAL (x,n) REACTIONS

A so-called sequential (x,n) reaction is a two-step process in which charged particles x are created in first-step neutron induced reactions A(n,yx) which is followed by the second-step reaction $\bar{A}(x,n)C$ with the target isotope $\bar{A}$ (note that $\bar{A}$ is not necessarily identical with A) producing the residual nucleus C. This situation is demonstrated in Fig.1 where we considered $x = p, d, t, {}^3He, \alpha$, and included all dominant reaction channels with neutron emission.

We are interested in the number of atoms of the nuclide C that are created after irradiation time t via sequential reactions (x,n). Such time-dependent inventory, $N_C(t)$ (cm^{-3}), can be determined by the master equation

$$\begin{aligned} N_C(t) &= t_{eff} \sum_A \sum_{i=1}^{175} \Phi_n(E_{n_i}) \sigma_{n,x}(E_{n_i}) N_A \Delta E_{n_i} \\ &\quad \times \sum_{j=1}^{24} f_{n,x}(E_{n_i}, E_{x_j}) \Delta E_{x_j} \sum_{k=j}^{1} \sigma_{x,C}(E_{x_k}) N_{\bar{A}} \Delta R_x(E_{x_k}), \end{aligned} \tag{1}$$

where the effective irradiation time is defined as

$$t_{eff} = \frac{(1 - e^{-\lambda t})}{\lambda}, \tag{2}$$

λ being the decay constant. Eq.(1) contains four summations. The first two deal with the production of charged particles, and consider the incident neutron flux in its most detailed internationally accepted VITAMIN-J 175-group structure. The next two summations yield the probability to produce the nucleus C via charged particles x taking into account their energy distribution as well as their slowing down in the surrounding material. Thus, $\Phi_n(E_{n_i})$ $(cm^{-2}s^{-1}MeV^{-1})$ is the neutron flux in the i-th energy interval of the fusion spectrum, ΔE_{n_i} (u) refers to the neutron lethargy energy bin (VITAMIN-J)[1], $\sigma_{n,x}(E_{n_i})$ (cm^2) is the production cross sections of charged particle x in the neutron energy group E_{n_i}, and N_A (cm^{-3}) is the number of atoms of the target nuclide A . Next, $f_{n,x}(E_{n_i}, E_{x_j})$ (MeV^{-1}) represents the normalized charged particle spectrum given in uniform energy steps of $\Delta E_{x_j} = 1MeV$ and referring to the i-th incident neutron energy group, the charged particle energy being $E_{x_j} = 0.5, 1.5, \ldots, 23.5$ MeV. Finally, $\sigma_{x,C}(E_{x_k})$ (cm^2) stands for the production cross section of the nucleus C via the sequential reaction $\bar{A}(x,n)C$, $N_{\bar{A}}$ (cm^{-3}) is the number of the target nuclide $\bar{A}$, and $\Delta R_x(E_{x_k})$ (cm) is the differential thickness of the surrounding material corresponding to 1 MeV steps of energy losses of charged particles with the starting energy E_{x_k}.

Numerical calculation of the inventory using the above master equation is performed in two steps. One first calculates the core of Eq.(1) and represents it in terms of the so-called "pseudo" cross sections. These are then used as input for the global inventory code [6], [7]. Here all pathways are traced that can contribute to the production of the nucleus C and these contributions are summed up so that the complete inventory is obtained. Below we present our innovative formalism that have much similarities with the one originally used by Cierjacks and Hino [2]- [4], but it differs in several important aspects allowing to handle sequential (x,n) reactions already on a fairly general level.

Neutron flux together with the initial inventory of stable nuclides A can be considered as a source of the charged particle flux. We shall assume that this latter flux does not change considerably during the irradiation time what seems to be a very reasonable

[1] The The neutron flux is treated here in the most general definition in neutrons per cm^2, per second and energy unit. This does not apply for standard fluxes distributed by the UK Group given in units of $(cm^{-2}s^{-1}u^{-1})$ where u means unity. In this case ΔE_{n_i} also reduces to unity, and can be omitted.

approximation, except possibly of a few specific cases. The flux I of charged particles proceeds by producing nuclear reactions $\bar{A}(x,n)C$ creating thereby nuclei C. To illuminate this concept we rearrange the master equation (1) and get

$$N_C(t) = t_{eff} N_{\bar{A}} \sum_{k=1}^{24} \sigma_{x,C}(E_{x_k}) \times \sum_{A} \sum_{i=1}^{175} \Phi_n(E_{n_i}) \sigma_{n,x}(E_{n_i}) N_A \Delta E_{n_i} \sum_{j=k}^{24} f_{n,x}(E_{n_i}, E_{x_j}) \Delta E_{x_j} \Delta R_x(E_{x_k}), \quad (3)$$

where the summation over A, i and j represents the charged particle flux ($cm^{-2}s^{-1}$)

$$\Phi_x(E_{x_k}) = \sum_{A} \sum_{i=1}^{175} \Phi_n(E_{n_i}) \sigma_{n,x}(E_{n_i}) N_A \Delta E_{n_i} \sum_{j=k}^{24} f_{n,x}(E_{n_i}, E_{x_j}) \Delta E_{x_j} \Delta R_x(E_{x_k}). \quad (4)$$

One can thus write

$$N_C(t) = t_{eff} N_{\bar{A}} \sum_{k=1}^{24} \Phi_x(E_{x_k}) \sigma_{x,C}(E_{x_k}) \quad (5)$$

showing that indeed the master equation can be viewed as the inventory due to the flux of charged particles interacting on nuclei $\bar{A}$.

To make this latter expression fully understandable to the inventory code FISPACT we write it as

$$N_C(t) = t_{eff} \Phi_n^{int} N_{\bar{A}} \frac{1}{\Phi_n^{int}} \sum_{k=1}^{24} \Phi_x(E_{x_k}) \sigma_{x,C}(E_{x_k}), \quad (6)$$

where

$$\Phi_n^{int} = \sum_{i=1}^{175} \Phi_n(E_{n_i}) \Delta E_{n_i} \quad (7)$$

is the energy-integrated neutron flux ($cm^{-2}s^{-1}$). Eq. (6) can be finally presented as

$$N_C(t) = t_{eff} \Phi_n^{int} N_{\bar{A}} \sigma_{x,C}^{pseudo} \quad (8)$$

with the "pseudo" cross section given in units of (cm^2) and defined as

$$\sigma_{x,C}^{pseudo} = \frac{1}{\Phi_n^{int}} \sum_{k=1}^{24} \sigma_{x,C}(E_{x_k}) \times \sum_{A} \sum_{i=1}^{175} \Phi_n(E_{n_i}) \sigma_{n,x}(E_{n_i}) N_A \Delta E_{n_i} \sum_{j=k}^{24} f_{n,x}(E_{n_i}, E_{x_j}) \Delta E_{x_j} \Delta R_x(E_{x_k}). \quad (9)$$

This can be again rearranged to get back the order of summation as used in Eq. (1) so that

$$\sigma_{x,C}^{pseudo} = \frac{1}{\Phi_n^{int}} \sum_{A} \sum_{i=1}^{175} \Phi_n(E_{n_i}) \sigma_{n,x}(E_{n_i}) N_A \Delta E_{n_i} \times \sum_{j=1}^{24} f_{n,x}(E_{n_i}, E_{x_j}) \Delta E_{x_j} \sum_{k=j}^{1} \sigma_{x,C}(E_{x_k}) \Delta R_x(E_{x_k}). \quad (10)$$

Thus, it is clear that the solution of the master equation reduces essentially to the derivation of "pseudo" cross sections. These cross sections should , of course, be evaluated for all isotopes $\bar{A}$ and for a given initial composition of nuclei A.

An important feature of Eq.(8) is that charged particles x act on isotope $\bar{A}$ and the density $N_{\bar{A}}$ is automatically updated by the FISPACT. This also means that with the present formalism one can handle long chains of (n,x) and sequential (x,n) reactions without any change in the structure of the inventory code. The "pseudo" cross section as defined by Eq. (9) has a meaning of the cross section for the reaction $\bar{A}(x,n)C$ per one nucleus $\bar{A}$ and per one initial neutron. This latter point justifies the name "pseudo" since neutrons have to be first converted into charged particles and this is handled by the 'kernel' of expression (9). This 'kernel' also means that (x,n) "pseudo" cross sections are often a few orders of magnitude smaller than usual (x,n) cross sections.

For sequential (x,n) reactions our new "pseudo" cross section indeed plays the same role as the so-called "effective" cross section for one-step neutron induced inventory calculations. In this latter case the inventory of nuclei B in reactions A(n,x)B can be expressed as

$$N_B(t) = t_{eff}\Phi_n^{int} N_A \sigma_{n,B}^{eff}, \tag{11}$$

where the effective cross section (cm^2) is defined as

$$\sigma_{n,B}^{eff} = \frac{1}{\Phi_n^{int}} \sum_{i=1}^{175} \Phi_n(E_{n_i})\sigma_{n,B}(E_{n_i})\Delta E_{n_i}. \tag{12}$$

Full inventory calculation should include both the two-step sequential (x,n) reactions as well as one-step neutron induced reactions and requires the knowledge of "pseudo" as well as "effective" cross sections.

3. NUCLEAR DATA LIBRARIES

To perform the above inventory calculations one needs a set of basic data and 4 major nuclear data libraries. The basic data that include a list of isotopes under consideration, their half-lives, decay modes, natural isotopic abundancies as well as elemental densities, are provided by the inventory code itself [6], [7] and they are not discussed here. We just mention that the decay data library UKDECAY2 is employed [6] but it needs to be extended.

As regards nuclear data libraries, we are dealing with in the present report, they should provide the following information. First, particle production cross sections $\sigma_{n,x}$ as functions of the incident neutron energy E_{n_i}. Second, normalized charged particle spectra $f_{n,x}$ that correspond to these cross sections and are thus functions of both the incident neutron energy E_{n_i} and the outgoing charged particle energy E_{x_j}. Third, production cross sections $\sigma_{x,C}$ of isotopes C in charged particle induced reactions (x,n) as functions of the incident charged particle energy E_{x_j}. And fourth, differential ranges ΔR_x of these charged particles.

Careful searches through the nuclear data libraries virtually over the whole network of international nuclear data centers revealed that a great deal of the above nuclear data is only partly available, or even altogether not available. As the most extreme example of this situation we mention charged particle spectra where some authors even resorted to a purely classical kinematical approach to get some, whatever questionable, estimates of the data needed [9].

In order to meet an important requirement of completeness, we so far considered all isotopes over the mass table with Z = 1 through 42 ($A \leq 100$) having half lifes $T_{1/2} \geq 1\,day$. The list is identical with that of the up-to-date REAC-ECN-5 library (see below), and it has 211 items including 5 isotopes in their metastable states. In the next stage we shall add also isotopes with $A > 100$. However, they are expected to play a less important role, because of the relatively high Coulomb barrier that reduces considerably cross sections for charged-particle induced reactions and vice versa, charged particle emission.

The nuclear data libraries adopted or developed for the present application include

- REAC-ECN-5 for (n,x) cross sections,
- KFKSPEC for normalized (n,x) spectra ,
- KFKXN for (x,n) cross sections,
- KFKSTOP for stopping powers,

and their current status is discussed in some detail below.

3.1. (n,x) Cross Sections

We use the library of evaluated neutron-induced cross sections REAC-ECN-5 that was designed for applications in fusion reactor LAM development [10]. Cross sections

are given in the 175-group VITAMIN-J structure of neutron energies that span from $E_n = 19.6 MeV$ down to $E_n = 1.0 \times 10^{-5} eV$.

The REAC-ECN-5 library has been completed at ECN Petten in 1988 and represents an essential revision of the 1985 REAC data file [11] containing cross sections for neutron activation and transmutation reactions. The revisions were made by means of renormalizations of the cross sections to experimental data at 14.5-MeV systematics. A number of reactions has been added so that the file essentially contains cross sections for all stable and radioactive nuclides with half lifes exceeding 1 day. If a reaction can produce one or more isomers, the cross sections for producing the ground and isomeric states are given separately. From our point of view it is important that the file contains all reaction channels with emission of $x = p, d, t, ^3He, \alpha$ in whatever combination of accompanying exit particles. A sample view of the file is shown in Tab. I.

The cross sections given in the REAC-ECN-5 library refer to production cross sections of final nuclei. For the present application, however, we rather need production cross sections of charged particles. These are obtained by summing up contributions from all reaction channels for a given target nucleus that contain the charged particle of interest, including summation of cross sections for the ground and isomeric states. This summation is done in the special calculation of "pseudo" cross sections so that any possible updating of the REAC-ECN-5 can be readily taken into account.

3.2. Charged Particle Spectra

The library is called KFKSPEC and it has been developed from scratch since no basis, even in its starter form, are available. In certain instances though, there are experimental data for (n,p) and (n, α) spectra, but even those few are limited to 14 MeV neutron incident energy. We have, therefore, undertaken development of this library using appropriate nuclear reaction models.

It is well known that in the energy range of interest the dominant nuclear reaction mechanism is that of the compound nucleus. This should be superimposed with the contribution from preequilibrium stages of the reaction that preceed creation of the fully equilibrated compound nucleus. A notable advantage of these models is that, although they have a sound quantum-mechanical basis, they still can be formulated in a fairly transparent manner [12]. Furthermore, their applicability for nuclear data evaluation has

been widely tested and they are presently used almost as standard tools in predicting unknown cross sections by nuclear data evaluators. Another important advantage is that there is continuing international effort to improve the underlying physics [13] as well as to establish well tested sets of parameters, such as those needed for optical potential [14] and nuclear level densities [15].

The code used here is ALICE as developed at the Lawrence Livermore National Laboratory by M. Blann et al. [16]- [18] over more than two decades. It is based on the preequilibrium hybrid model and the evaporation statistical model. We used the latest version due to December 1990 [19]. It can handle whatever incident particle, but it is limited to n,p,d, α and γ in exit channels.

All parameters that we employed are provided as optional by ALICE. We used global sets of optical potential parameters and the corresponding parabolic approximation to calculate inverse cross sections. For level densities we used the standard set of parameters. The calculations were performed for 205 target isotopes from ^{10}B to ^{100}Mo, and for outgoing charged particles x = p, d, α. Incident neutron energies were set to the middle of the respective VITAMIN-J bins so that the whole energy range is reasonably covered by 20 steps; we used E_n = 18.5, 17.1, 16.1, 14.7, 14.0, 13.2, 12.4, 11.3, 10.2, 9.3, 8.4, 7.6, 6.9, 5.9, 5.1, 4.3, 3.3, 2.4, 1.5 and 0.6 MeV. Contributions from appropriate reaction channels are summed up so that full production spectra of particle x are obtained. The spectra are given in 1 MeV steps of charged particle energies E_x = 0.5, 1.5, ..., 23.5 MeV; they are normalized to unity and stored together with the energy-integrated absolute cross sections.

Included in the starter file are 12 300 different spectra. A sample case of the file is shown in Tab. II.

3.3. (x,n) Cross Sections

The name of the library is KFKXN and it is presently available in its starter form. The approach adopted was the same as described above. We used again the code ALICE with the same set of parameters as above. The calculations were performed for (x,n) reactions on all isotopes from ^{10}B to ^{100}Mo, and for x = p,d,t, ^3He and α. The file contains 1025 different reactions, each at E_x = 0.5, 1.5, ..., 23.5 MeV, and it has thus 24 600 data points. A sample view of the file can be found in Tab. III.

Two comments should be made. First, calculated (t,n) cross sections should be considered with caution, since they may contain appreciable contributions from the break-up mechanism [20]. On the other hand, the preequilibrium hybrid model treats the first reaction stage as decay of the 3-particle doorway state to the 2-particle final state which is close to the break-up picture. Second, deuterons as well as tritons are loosely bound so that they provide considerable excitation energy for emission of two neutrons. Often, cross sections of (d,2n) and (t,2n) exceed considerably cross sections of (d,n) and (t,n), respectively, and this should be taken into account in future considerations.

3.4. Differential Ranges

The name of the file is KFKSTOP, it is considered to be complete for all elements with atomic number from 1 to 92 and no future updating is foreseen.

The stopping powers and the ranges of protons, deuterons, tritons, ^3He as well as α particles in solids were calculated by the program PRAL. This code was created by Ziegler et al. [21] and it was extended very recently by Möslang [22] so that it can be used for elements from Z 1 through 92. For each of these elements we have calculated ranges in energy steps of 1 MeV for $E_x = 0$ to 24 MeV. By subtracting these ranges by pairs we got the values for the energy-dependent differential ranges that correspond to 1 MeV loss in charged particle energy. These values are then attached to charged particle energies $E_x = 0.5, 1.5, ..., 23.5\, MeV$. The advantage of the above method is that the interpolation takes place in small intervals. Thus, the accuracy is much higher compared with the possibility to calculate differential ranges by interpolating the full range of charged particles. A sample view of the file is shown in Tab. IV.

4. SAMPLE OF ACTIVATION CALCULATIONS

The calculations were done using the code FISPACT together with the preparatory code PCROSS [8] for the case of Na. The sequential (x,n) reaction of interest is $^{23}Na(\alpha, n)^{26}Al$, the half-life of ^{26}Al being 7.2×10^5 y.

The calculated inventory can be seen in Fig.2 as a function of time both for one-step neutron induced reactions and for sequential (x,n) reactions.

5. FURTHER IMPROVEMENTS

We intend to proceed by using the above data sets for extensive inventory calculations. The aim is to identify those sequential (x,n) reactions that make important total inventory contributions, find out the sensitivity of related nuclear data on inventory, and improve the quality of the important data. However, already at the present stage one can make some more general statements about further developments and these are outlined below.

Out of the four libraries discussed above, the REAC-ECN-5 as well as KFKSTOP are considered to be in good shape for the present application and no improvements from our side are foreseen. Note that REAC-ECN-5 has already a rather long history and any updating (version 6) will be readily accepted by us. The situation with the libraries KFKSPEC and KFKXN is different, we have to stress their current starter status and underline that most likely several major improvements and/or developments must be done until a satisfactory stage is reached. These steps are as follows: (1) improved calculations with ALICE, (2) full completness of the libraries, (3) their validation by comparison with experimental and/or evaluated data, and (4) inclusion of several special reactions that are not of the (x,n) type (see Sec. 5.4).

5.1. Improved Calculations

As a natural way of how to improve our two starter libraries, we would like to mention better parametrization of the calculations performed so far and up-dating of the ALICE code itself. This latter point concerns the full introduction of the γ competition into the code being solved now by M. Blann [23]. In this way one should remove some low energy spikes in charged particle spectra that may occasionally occur when secondary neutron emission is energetically not possible. Following the suggestion of the originator we presently cured this problem by cutting charged particle transmission coefficients to zero as soon as they are smaller than 0.01.

5.2. Completeness

As regards full completeness, KFKSPEC has to be extended to include (n,t) and $(n, {}^3He)$ reactions. To do so one has to deal with another reaction mechanisms, such as

pick-up [23] and this can be probably handled by the approach developed by Harada et al. [24]-[26]. Next, the file should be extended to cover also the $A > 100$ isotope range. Furthermore, one has to add a few very light isotopes which cannot be reasonable handled by statistical/preequilibrium model calculations.

KFKXN is also not yet fully complete. It should be extended to cover the $A > 100$ isotope range. Furthermore, one has to add a few very light isotopes; in this respect a useful source of information should be provided by the charged particle libraries for very light elements such as ECPL-86 [27, 28] and GRAZ-87 [29]. As already mentioned, one should furthermore include (d,2n) and (t,2n) cross sections that, because of their high Q-values, may often surpass (d,n) and (t,n) cross sections, respectively.

5.3. Validation

As regards validation, for KFKSPEC this would at least include comparison of the (n,x) production cross sections with those provided by the REAC-ECN-5 file (note that KFKSPEC keeps information also on the absolute energy-integrated production cross sections). A reasonable agreement of the respective cross sections should indicate that also the corresponding spectra as calculated by ALICE are acceptable. This comparison is technically feasible since all information is computerized. Another possibility, which is much more laborious and less systematic, consists in comparing the KFKSPEC spectra with experimental data whenever available.

KFKXN should also be validated and one should benefit from an older systematics developed for x = p, d and α by Münzel et al. [30, 31]. This systematics is based on experimental data and statistical model considerations. Although its latest computerized version got lost [32], there is still a somewhat earlier computerized version available as worked out by Pearlstein in 1975 and re-issued by IAEA in 1985 [33]. We note, however, that Pearlstein's version keeps no information on t and ^3He, and it is limited to x = p, d and α on stable isotopes from Z 21 through 83. As another possibility we mention thick target yields for charged-particle induced reactions as collected in USSR [34], and available on a tape from the Kurchatow laboratory [35]. However, the overlap of these data is also limited.

Another interesting procedure of validation can be done by comparing important individual radioactivities from calculations with those measured at the Karlsruhe (KIZ)

cyclotron. The expected flux is high enough to study also certain reaction chains, thereby avoiding measurements on special radioactive samples.

5.4. Special Reactions

Finally, we would like to mention that one, in principle, should consider also some special reactions not included above. As an example of possible considerable interest we mention $^{7}Li(t,\gamma)$ leading to ^{10}Be with $T_{1/2} = 1.6 \times 10^{6}$ y. Such cross sections may be very difficult to measure, their theoretical estimates are also not trivial, and each of these cases should be treated individually.

ACKNOWLEDGMENTS

This work has been performed within the framework of the Nuclear Fusion Project of the Kernforschungszentrum Karlsruhe and is supported by the European Communities within the Fusion Technology Program.

The authors would like to thank Dr. K. Anderko and Prof. K. Ehrlich for stimulating discussions and their ongoing support of this work. They are most grateful to M. Blann for many useful suggestions and his ongoing advice on the use of the code ALICE. They appreciate also useful suggestions by J. Kopecký and H. Gruppelaar concerning the REAC-ECN-5 file and preequilibrium emission of clusters. Helpful information was obtained from M.B. Chadwick, F.E. Chukreev, P.P. Dmitriev, M. Drosg, H. Münzel, A. Paschenko as well as R. White.

References

[1] K. Anderko, *unveröffentlichter Bericht* (KfK, Karlsruhe, 1990).

[2] S. Cierjacks and Y. Hino: *The role of sequential (x,n) reactions on element activation of fusion reactor materials and related nuclear data needs*, Proc. Specialists' Meeting on Neutron Activation Cross Sections for Fission and Fusion Energy Applications, Argonne, 13^{th} - 15^{th} September 1989, see Report NEANDC-259 'U', eds. M. Wagner and H. Vonach (OECD, Paris, 1989) pp. 19-28.

[3] S. Cierjacks and Y. Hino: *The importance of sequential (x,n) reactions on element activation of fusion reactor materials*, J. Nucl. Mat. **170** (1990) 134-139.

[4] S. Cierjacks and Y. Hino: *Study of element activities in fusion reactor materials*, Report KfK-4523 (KfK, Karlsruhe) in preparation.

[5] S. Cierjacks : *Nuclear data needs for "low-activation" fusion materials development*, Fusion Eng. and Design **13** (1990) 229-238.

[6] R. A. Forrest, D. A. J. Endacott and A. Khursheed: *FISPACT - Program Manual*, Report AERE-M3655 (AERE, Harwell, 1988).

[7] R. A. Forrest and D. A. J. Endacott: *FISPACT - User Manual*, Report AERE-M3654 (AERE, Harwell, 1988).

[8] S. Ravndal et al.: *PCROSS - User Manual*, Report KfK-4873 (KfK, Karlsruhe, 1991).

[9] T. D. Beynon and B. S. Sim: *^{10}Be and ^{14}C production rates in NET-type blankets*, Ann. Nucl. Energy, **5** (1990) 271-278.

[10] H. Gruppelaar, H. A. J. Van der Kamp, J. Kopecký and D. Nierop: *The REAC-ECN-3 data library with neutron activation and transmutation cross-sections for use in fusion reactor technology*, Report ECN-207 (ECN, Petten, 1988). We use version No.5, due to December 1990.

[11] F. M. Mann, D. E. Lessor and J. S. Pintler: *REAC nuclear data libraries*, Int. Conf. on Nuclear Data for Basic and Applied Science, May 1985, Santa Fe, New Mexico (Gordon and Breach, 1986), p. 207.

[12] H. Feshbach, A. Kerman and S. Koonin: *Statistical multistep compound and statistical multistep direct models of nuclear reactions*, Ann. Phys. (NY) **125** (1980) 429.

[13] NEANDC Specialists' Meeting on Preequilibrium Nuclear Reactions, February 1988, Semmering, Austria.

[14] NEANDC Specialists' Meeting on Optical Potential, 1986, Paris, France.

[15] NEANDC Specialists' Meeting on Nuclear Level Densities, November 1989, Bologna, Italy.

[16] M. Blann and J. Bisplinghoff: *Code ALICE/Livermore 82*, Report UCID-19614 (LLNL, Livermore, 1982).

[17] M. Blann and H. K. Vonach: *Global test of modified precompound decay models*, Phys. Rev. C **28** (1983) 1475-1492.

[18] M. Blann: *Code ALICE/85/300*, Report UCID-20169 (LLNL, Livermore, 1984).

[19] M. Blann (LLNL Livermore): *Code ALICE, version 1990*, private communication, January 1991.

[20] M. Drosg (Universität Wien), private communication, December 1990.

[21] J.F.Ziegler, J.P. Biersack and U. Littmark: *The stopping and range of ions in solids* (Pergamon Press, New York,1985).

[22] A. Möslang, *unveröffentlichter Bericht* (KfK, Karlsruhe, 1990).

[23] M. Blann (LLNL Livermore), private communication, January 1991.

[24] A. Iwamoto and K. Harada, Phys. Rev. C **26** (1982) 1821.

[25] K. Sato, A. Iwamoto and K. Harada: *Pre-equilibrium emission of light composite particles in the framework of the exciton model*, Phys. Rev. C **28** (1983) 1527-1537.

[26] H. Gruppelaar (ECN Petten), private communication, January 1991.

[27] R. White (LLNL Livermore): *ECPL-86, evaluated charged particle library*, private communication, December 1990.

[28] *ECPL-86, The LLNL evaluated charged-particle data library, summary of contentens by O. Schwerer*, Report IAEA-NDS-56, Rev. 1 (IAEA, Vienna, 1987).

[29] R. Feldbacher: *The AEP Barnbook DATLIB. Nuclear reaction cross sections and reactivity parameter, library and files*, Report INDC(AUS)-12/G (IAEA, Vienna, 1987).

[30] J. Lange and H. Münzel: *Abschätzung unbekannter Anregungsfunktionen für* $(\alpha, xn)-$, $(\alpha, pxn)-$, $(d, xn)-$ *und* $(p, xn)-$ *Reaktionen*, Report KfK-767 (KfK, Karlsruhe, 1968).

[31] K. A. Keller, J. Lange and H. Münzel: *Q-values and excitation functions of nuclear reactions. Part c: Estimation of unknown excitation functions and thick target yields from p,d,* ^3He *and* α *reactions.* In Landolt - Börnstein New Series in Physics (Springer-Verlag, Berlin, 1974) vol. I5c.

[32] H. Münzel (TU Darmstadt), private communication, December 1990.

[33] S. Pearlstein: *NNDC evaluated charged particle reaction data library*, Report IAEA-NDS-59, Rev. 1 (IAEA, Vienna, 1985).

[34] P. P. Dmitriev: *Radionuclide yield in reactions with protons, deuterons, alpha particles and helium-3 (Handbook)*, Report INDC(CCP)-263/G (IAEA, Vienna, 1986).

[35] F. E. Chukreev (Kurchatow Institute of Atomic Energy, Moscow, private communication, March 1991.

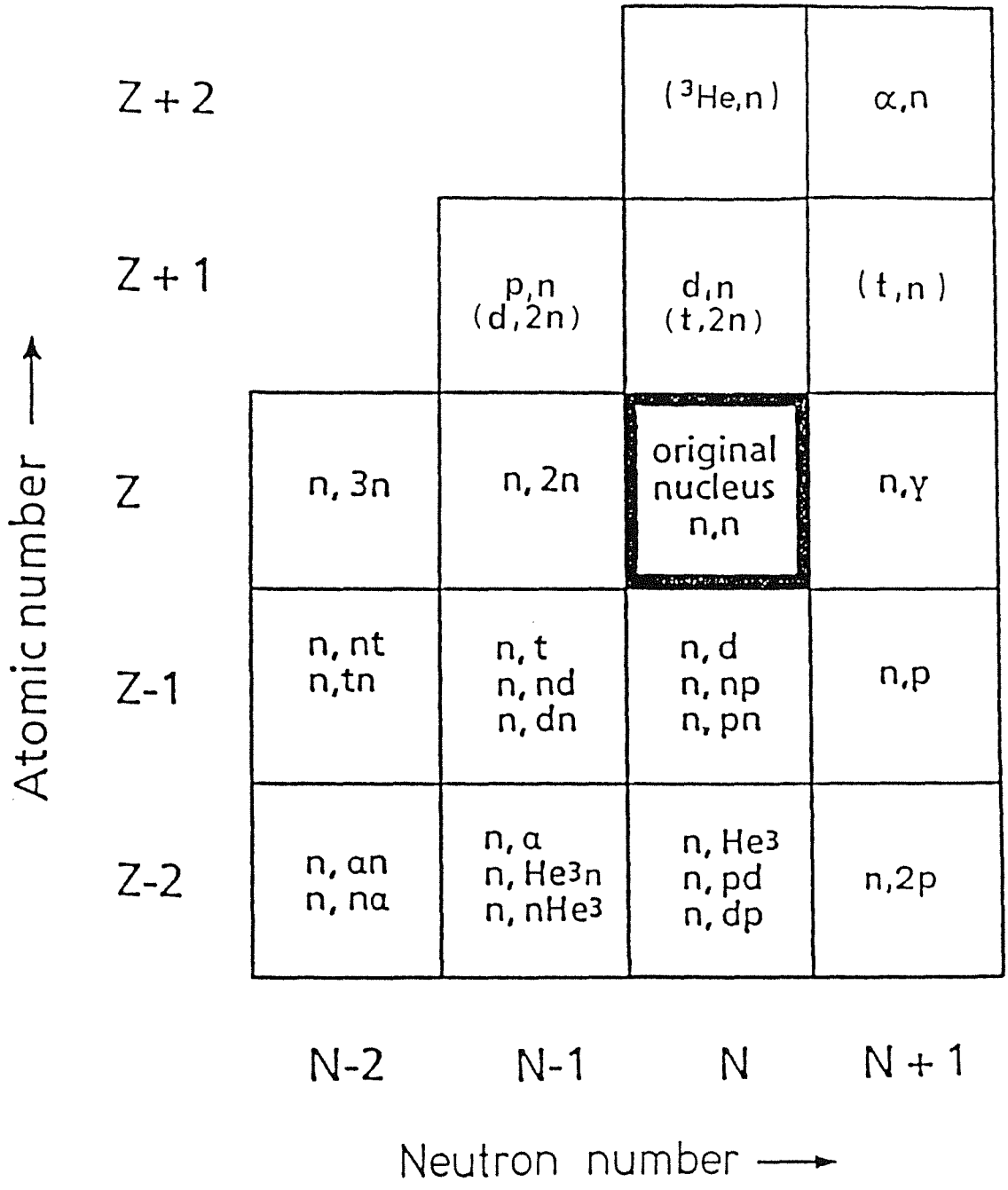

Fig. 1. Kinematically allowed neutron-induced and sequential (x,n) reactions for neutron energies $E_n \leq 15\,MeV$. Given in brackets are also sequential reactions to be considered in future work.

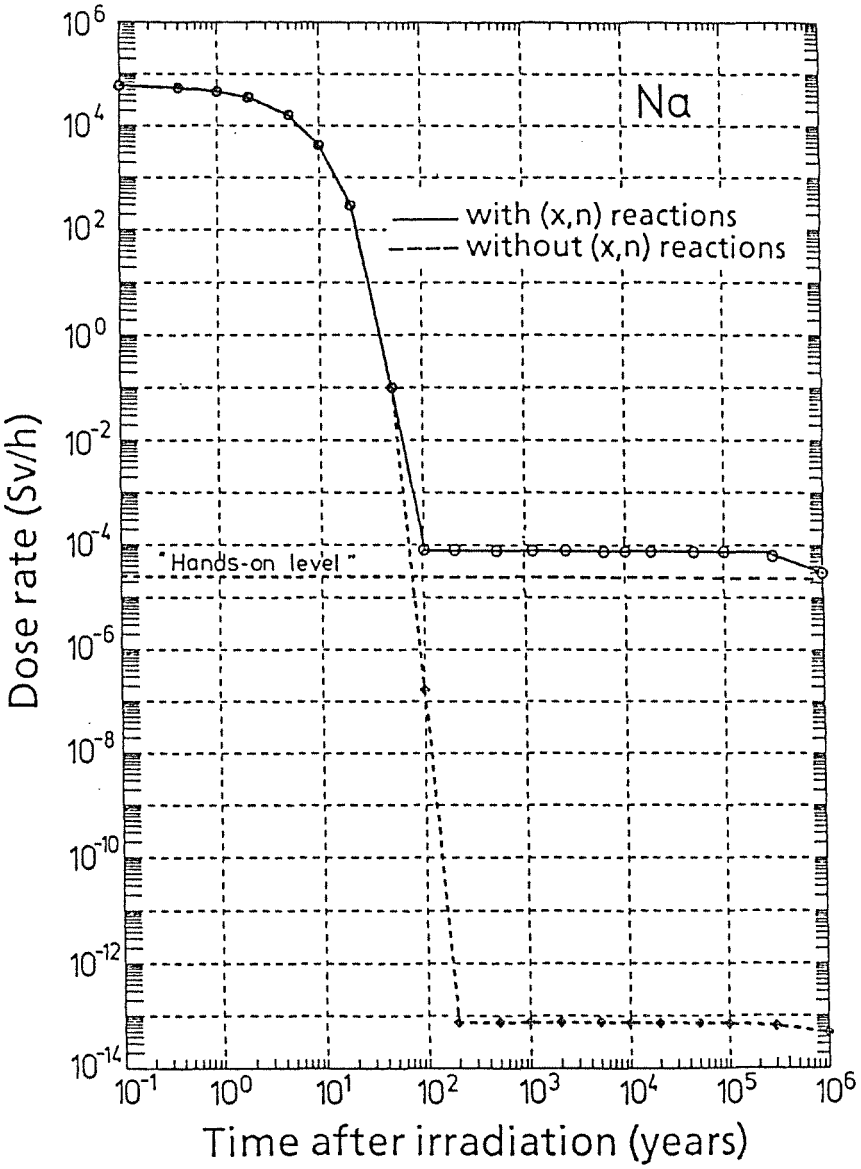

Fig. 2. Sample of inventory calculations using nuclear data libraries discussed in the text which shows the calculated dose rates versus time after irradiation. The results refer to neutron irradiation in the first wall of a DEMO fusion reactor. A 14-MeV neutron wall loading of 12.5 MWa/m^2 was assumed. The difference between the two curves is a measure of the contribution of the ^{26}Al activity ($T_{1/2} = 7.2 \times 10^5\, y$) produced by the sequential reaction $^{23}Na(\alpha, n)^{26}Al$.

Tab.I. Sample printout from the library REAC-ECN-5 in its 175-group structure. Shown are 3 reaction channels on ^{7}Li. A heading line and two comment lines are followed by cross sections in barns starting from the highest neutron energy down to the threshold energy.

```
 30070  220   41   LI  7  (N,NA ) H  3                9.1811-01*
 THRESH OUTPUT  .  ENDF CORRECTED
COMMENT.  LI-7 N,NT IS SAME REACTION| RN - EVL-YO81(P.YOUNG LASL)
2.56863E-01 2.67631E-01 2.71021E-01 2.75944E-01 2.84453E-01 2.91677E-01
2.99409E-01 3.06884E-01 3.13055E-01 3.19530E-01 3.31613E-01 3.39250E-01
3.50479E-01 3.61642E-01 3.71222E-01 3.78199E-01 3.81227E-01 3.83402E-01
3.85657E-01 3.87240E-01 3.89592E-01 3.88664E-01 3.86833E-01 3.81972E-01
3.75958E-01 3.71324E-01 3.59782E-01 3.42583E-01 3.15960E-01 2.67621E-01
2.00234E-01 1.34356E-01 8.62989E-02 4.09028E-02 1.54655E-02 8.09595E-03
3.45318E-03 2.20974E-03 1.19174E-03 6.89832E-05 0.00000E+00
 30070  240   17   LI  7  (N,2NA) H  2                1.0000+00*
                     ENDF EVALUATION

3.88066E-02 4.04334E-02 4.09456E-02 4.16893E-02 4.27120E-02 3.98175E-02
3.64389E-02 3.31066E-02 2.95135E-02 2.56543E-02 1.97022E-02 1.61452E-02
1.21160E-02 7.26964E-03 3.48144E-03 1.01733E-03 0.00000E+00
 30070 1040   20   LI  7  (N,D  )HE  6                1.0000+00*
                     ENDF EVALUATION
COMMENT.  AGREEMENT QA81= 9.8+-1.1 (DOES NOT INCLUDE N,2NAD)
1.08296E-02 1.12836E-02 1.14266E-02 1.16342E-02 1.19360E-02 1.13670E-02
1.06917E-02 1.00337E-02 9.38522E-03 8.68305E-03 7.39609E-03 6.25654E-03
4.75070E-03 3.40840E-03 2.53055E-03 1.45667E-03 7.43013E-04 2.68517E-04
2.31104E-06 0.00000E+00
```

Tab.II. Sample printout from the KFKSPEC library. Shown are normalized charged particle spectra from $^{23}Na(n,*x)$ reactions. Data are given for outgoing $x = p, d, \alpha$, cases $x = t$, ^{3}He are presently filled with zeros. Full specification of each reaction is given in its heading line, followed by the sequence number of the related VITAMIN-J group, incident neutron energy as well as the production cross section given in barns.

```
110230          ********* NA 23(N,*X) ***********                KFKSPEC
                  ALICE OUTPUT  EN=18.5MEV
110230 1030  1  1 18.5 0.382E+00 0.382E+00                        KFKSPEC
0.000000 0.228371 0.274213 0.185579 0.098549 0.061950 0.042209 0.029272
0.021716 0.017039 0.014078 0.011388 0.008960 0.006679 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
110230 1040  1  1 18.5 0.163E-01 0.163E-01                        KFKSPEC
0.000000 0.037683 0.148466 0.190795 0.172632 0.143579 0.109656 0.078796
0.054698 0.038109 0.025588 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
110230 1050  1  1 18.5 0.000E+00 0.000E+00                        KFKSPEC
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
110230 1060  1  1 18.5 0.000E+00 0.000E+00                        KFKSPEC
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
110230 1070  1  1 18.5 0.126E+00 0.126E+00                        KFKSPEC
0.000000 0.000000 0.023083 0.127107 0.166862 0.155137 0.128963 0.108408
0.092009 0.071835 0.050581 0.035397 0.024140 0.016478 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
```

Tab.III. Sample printout from the library KFKXN. Shown are (p,n) cross sections on $^{44m,45,46}Sc$. A heading line and a comment line are followed by cross sections in barns for incident energies $E_x = 0.5, 1.5, ..., 23.5\, MeV$. Identification of reactions follows the ECPL-86 style (2=incident proton, 11=outgoing neutron).

```
210441 2 11        SC 44M(P,N)                                          KFKXN
                   ALICE OUTPUT
0.0000E+00  0.0000E+00  0.9964E-01  0.1117E+00  0.1867E+00  0.2177E+00
0.2504E+00  0.2540E+00  0.2649E+00  0.2644E+00  0.2700E+00  0.2673E+00
0.2323E+00  0.1872E+00  0.1474E+00  0.1141E+00  0.8743E-01  0.7113E-01
0.5852E-01  0.4959E-01  0.4316E-01  0.3673E-01  0.3361E-01  0.3050E-01
210450 2 11        SC 45(P,N)                                           KFKXN
                   ALICE OUTPUT
0.0000E+00  0.0000E+00  0.0000E+00  0.1329E+00  0.2243E+00  0.2926E+00
0.3678E+00  0.3884E+00  0.4099E+00  0.4063E+00  0.4117E+00  0.4406E+00
0.4538E+00  0.4732E+00  0.4023E+00  0.3139E+00  0.2382E+00  0.1728E+00
0.1247E+00  0.9410E-01  0.7742E-01  0.6073E-01  0.5301E-01  0.4529E-01
210460 2 11        SC 46(P,N)                                           KFKXN
                   ALICE OUTPUT
0.0000E+00  0.0000E+00  0.1116E+00  0.1583E+00  0.3109E+00  0.4234E+00
0.5235E+00  0.5755E+00  0.5938E+00  0.5896E+00  0.5894E+00  0.5236E+00
0.4054E+00  0.2985E+00  0.2209E+00  0.1654E+00  0.1286E+00  0.1007E+00
0.8054E-01  0.6649E-01  0.5814E-01  0.4980E-01  0.4566E-01  0.4152E-01
```

Tab.IV. Sample printout from the library KFKSTOP. Given are differential ranges of α particles for Ge (Z=32) through Br (Z=35). Data are given in cm and refer to 1 MeV energy steps from 0 to 24 MeV.

```
320740  20040  ALPHA      0-24MeV ;    1MeV-steps                KFKSTOP
 0.3633E-03  0.2907E-03  0.3402E-03  0.3920E-03  0.4418E-03  0.4897E-03
 0.5357E-03  0.5804E-03  0.6238E-03  0.6663E-03  0.7078E-03  0.7486E-03
 0.7887E-03  0.8281E-03  0.8670E-03  0.9053E-03  0.9431E-03  0.9805E-03
 0.1018E-02  0.1054E-02  0.1090E-02  0.1126E-02  0.1162E-02  0.1209E-02
330750  20040  ALPHA      0-24MeV ;    1MeV-steps                KFKSTOP
 0.3069E-03  0.2713E-03  0.3286E-03  0.3839E-03  0.4356E-03  0.4842E-03
 0.5307E-03  0.5753E-03  0.6186E-03  0.6606E-03  0.7017E-03  0.7419E-03
 0.7812E-03  0.8199E-03  0.8580E-03  0.8955E-03  0.9325E-03  0.9690E-03
 0.1005E-02  0.1041E-02  0.1076E-02  0.1111E-02  0.1145E-02  0.1191E-02
340800  20040  ALPHA      0-24MeV ;    1MeV-steps                KFKSTOP
 0.4218E-03  0.3433E-03  0.4089E-03  0.4731E-03  0.5344E-03  0.5929E-03
 0.6492E-03  0.7036E-03  0.7564E-03  0.8078E-03  0.8580E-03  0.9071E-03
 0.9554E-03  0.1003E-02  0.1049E-02  0.1095E-02  0.1140E-02  0.1185E-02
 0.1229E-02  0.1272E-02  0.1315E-02  0.1358E-02  0.1400E-02  0.1456E-02
350790  20040  ALPHA      0-24MeV ;    1MeV-steps                KFKSTOP
 0.6058E-03  0.4595E-03  0.5549E-03  0.6383E-03  0.7165E-03  0.7916E-03
 0.8644E-03  0.9353E-03  0.1005E-02  0.1073E-02  0.1140E-02  0.1205E-02
 0.1270E-02  0.1334E-02  0.1397E-02  0.1460E-02  0.1521E-02  0.1582E-02
 0.1643E-02  0.1703E-02  0.1762E-02  0.1821E-02  0.1879E-02  0.1956E-02
```