BS

STATE RESEARCH CENTER OF RUSSIA
INSTITUTE FOR HIGH ENERGY PHYSICS

IHEP 95-22

D.V.Gorbatkov, V.P.Kryuchkov

**SADCO-2: A MODULAR CODE SYSTEM
FOR GENERATING COUPLED NUCLEAR
DATA LIBRARIES TO PROVIDE
HIGH-ENERGY PARTICLE TRANSPORT CALCULATION
BY MULTIGROUP METHODS**

114836

Submitted to *Math. Phys.*

Protvino 1995

Abstract

Gorbatkov D.V., Kryuchkov V.P. SADC0-2: A Modular Code System for Generating Coupled Nuclear Data Libraries to Provide High-Energy Particle Transport Calculation by Multigroup Methods: IHEP Preprint 95-22. – Protvino, 1995. – p. 9, figs. 8, refs.: 24.

A system to produce coupled multigroup cross sections for providing calculations by multigroup methods over a wide range of energy for neutron, proton, pion, kaon, photon transport through matter has been developed. The main modules of the system as well as the SADC0-2 structure are described. The SADC0-2 nuclear data system is available from the Institute for High Energy Physics.

Аннотация

Горбатов Д.В., Крючков В.П. Система адронных констант SADC0-2 для обеспечения расчетов переноса высокоэнергетических частиц многогрупповыми методами: Препринт ИФВЭ 95-22. – Протвино, 1995. – 9 с., 8 рис., библиогр.: 24.

Разработана система адронных констант SADC0-2 для обеспечения расчетов переноса нейтронов, протонов, пионов, каонов, фотонов в широком диапазоне энергий многогрупповыми методами. Приводится описание структуры SADC0-2 и основных программных модулей системы. Представлены результаты расчетов с использованием разработанной системы.

Introduction

High requirements to the accuracy of computational results, particularly to the problems of deep penetration, electronuclear energetics, transmutation of radioactive waste, detector background resulted in a great interest to the extension of traditional, for the reactor energy region, multigroup methods of radiation transport calculation in a high energy region.

The main characteristic features of such methods are the multigroup approximation for energy and the discrete ordinates one for the angular dependence of particle fluxes and cross sections (for example, [1-4]).

These approaches allow one to separate mathematical and physical aspects of particle transport calculation problem. In this case the transport codes become independent of particles type and their energies. Nuclear data for the considered energy range and types of particles as the main input physical information are contained in multigroup libraries, prepared beforehand.

Presently such multigroup high-energy nuclear data libraries as BND-400 [5], HILO [1], SADCO-1 [6] are known. However, BND-400 and HILO contain the data only for neutrons with the energy lower than 400 MeV and SADCO-1 provides transport calculations for neutrons and protons with the energy up to 600 MeV.

The base for a new version of the SADCO system is a new fast code for the double differential cross sections of inelastic hA-interaction calculation [7]. This code allows one to sufficiently improve the accuracy of nuclear data and to extend the energy region and the number of particle types for providing neutrons (with the energy $0.01 \text{ eV} < E < 10 \text{ TeV}$), protons, pions, kaons ($20 \text{ MeV} < E < 10 \text{ TeV}$) and photons ($0.01 < E < 20 \text{ MeV}$) transport calculations by multigroup methods.

SADCO-produced cross sections can be used directly with a variety of discrete ordinates and Monte-Carlo radiation transport computer codes.

The description of the structure, peculiarities and capabilities of the SADCO-2 system are given below.

1. SADC0-2 structure

The SADC0-2 system scheme is presented in Fig.1.

Fig. 1. The SADC0-2 code system scheme

Each constituent of the system is an independent collection of codes and algorithms combined to solve the problem of multigroup cross sections processing.

The stages of this problem solution define the SADC0-2 structure and are the following:

- integral and differential cross sections of hA-interaction for a given atomic number and energy region calculation;
- a choice both of the optimal number of energy groups and sound methods for averaging cross sections;
- group microscopic cross sections and transfer matrices for n, p, π , K with the energy $E > 20$ MeV calculation ;
- cross sections and transfer matrices for low-energy ($E < 20$ MeV) neutrons and photons for a particular problem computation;
- creation of a coupled problem-dependent library with data for various particle types and the whole energy region.

2. Multigroup cross sections processing

The central and main constituents of the SADC0-2 system are the algorithm and fast code [7] for the integral and double differential cross sections of hA-interaction calculation.

The algorithm is based on an approximation of the available experimental and calculated data, accumulated in RD [8] and SADC0 nuclear data bases.

The procedure of the functional χ^2 minimization was used to generate the evaluated point cross section:

$$\chi^2 = \frac{1}{N} \sum_i^N \left(\frac{\sigma_m^i - \sigma_e^i}{\Delta \sigma_m^i} \right)^2, \quad (1)$$

where σ_m is the available measured point cross section (or, where necessary, nuclear model calculation), N is the number of σ_m , $\Delta \sigma_m$ is the measured cross section error, σ_e is the evaluated cross section.

The integral cross sections are obtained by approximating the measured and calculated evaluated data from compilations [9, 10]. The inelastic cross sections used in compiling the SADC0-2 multigroup nuclear data libraries are presented in Fig.2 in comparison with the experimental data. References to the various experimental data are given in [9, 10].

Numerical estimations and comparisons with experimental data show that the SADC0-2 system allows one to obtain the total cross sections with the error less than 10% for the energy region 20 MeV ÷ 10 TeV. The exception is the energy region 10 ÷ 50 MeV for pions, where a set of experimental data is quite poor.

The uncertainty of the double differential cross sections calculated using method [7] can come up to 50% at most. Calculated data are in a good agreement with the experiment (Figs.3-5).

The total group microscopic cross sections (σ_{ti}^q) are produced using the evaluated cross sections (σ_{ti}):

$$\sigma_{ti}^q = \frac{\int_{E^q}^{E^{q+1}} \sigma_{ti}(E) \varphi_i(E) dE}{\int_{E^q}^{E^{q+1}} \varphi_i(E) dE}, \quad (2)$$

where $\varphi_i(E)$ is the weighting spectrum for the particle of the i^{th} type, E^q, E^{q+1} are the lower and upper boundaries of an energy group q , respectively.

The total microscopic cross section describes attenuation of the "narrow" beam of hadrons with energy within the group number q and determines particles distribution in matter completely. Production of various secondary particles in hA-interactions is accounted with transfer matrices $\hat{\sigma}_s^{p \rightarrow q}$. The $\sigma_s^{p \rightarrow q}$ is the multigroup cross section representing the scattering between energy groups (i. e. it is the combination of all upscatter, within-group, and downscatter terms):

$$\sigma_s^{p \rightarrow q}(\mu_s) = \frac{\int_{E^q}^{E^{q+1}} dE \int_{E^p}^{E^{p+1}} dE' \sigma_s(E' \rightarrow E, \mu_s) \varphi(E')}{\int_{E^p}^{E^{p+1}} \varphi(E) dE}, \quad (3)$$

where $\mu_s = \vec{\Omega}' \cdot \vec{\Omega}$ is the scattering angle cosine.

Fig. 2. Inelastic cross section for uranium, iron and carbon versus incident proton or neutron energy. Here, $\square$, — (nA)-reaction; $\square$, - - - (pA)-reaction. Lines are the SADC0-2 data, symbols are the experimental data.

Fig. 3. Double differential proton emission spectra at 20°, 40° and 60° calculated for the 60.7-MeV $n + O^{16}$ reaction as compared with the data from [11].

Fig. 4. Double differential neutron emission spectra at 30° calculated for the 585-MeV $p + Pb^{207}$ and $p + Al^{27}$ reactions as compared with the data from [12].

To calculate the charged particles transport in the approximation of continuous slowing down, the stopping power values β ($\beta = -dE/dx$) are calculated as well. The group analog of β (β^g) is calculated for each energy boundary according to algorithm [15]. The values of mean square deflection per a unit path length, needed to solve the problem with highly anisotropic scattering by Fokker-Planck approximation [4], are calculated both for elastic and inelastic processes using the formulas from [16].

It is very important to correctly choose energy group boundaries as well as the sound method of averaging cross section in each energy group. The uniform in lethargy scale ($u = \ln(E^{g-1}/E^g)$) for energy group structure at energies above 20 MeV is used. The increment of lethargy in each group is 0.72 both for high energy hadrons and for neutrons and photons with energy less than 20 MeV.

The usage of the finer group structure does not seem reasonable, because it does not increase the accuracy of multigroup cross sections. Their accuracy can be achieved by the refinement of the evaluated data only. Besides, it is known that cross sections slightly depend on energy in the energy range above 20 MeV. As an example the energy dependence of inelastic hA-interaction cross sections for various nucleus targets is presented in Fig.2. That is why the choice of the point-to-group weighting function in the region above 10 MeV is not so important as for low energy neutrons, where a resonance behavior of cross sections is much more marked. The error, depending upon the weighting spectrum $\varphi_i(E)$ (see equations (2, 3)), is less than 2%, that is much lower than the uncertainty of the evaluated data.

The most typical neutron spectra behind the concrete and iron accelerator shielding, accepted for multigroup cross sections processing, are presented in Figs. 6–7. For the energy range above 10 MeV these spectra can be well approximated by function $\varphi \sim E^{-\alpha}$, where α is 1 for $10 < E < 200$ MeV and 1.5 for $E > 200$ MeV.

The neutron and photon energy group boundaries below 20 MeV are the same as those used in USCONS [17] (49n + 15 γ groups) or VITAMIN-C [18] (171n + 36 γ groups) multigroup libraries (up to user's choice), included into the system.

The result of the SADCO-2 system operation is the coupled multigroup cross sections file in a given format prepared with account for the shielding composition, that includes the data both for high-energy hadrons and low-energy neutrons and photons.

The type of SADCO-2 output file format is determined by the transport code, used with SADCO. For instance, the SADCO-2 system can generate the multigroup data file in FMAC-M format for ROZ-6H code [19], MOSKIT format for MOSKIT code [20], ANISN format for ANISN [21] and DOT [22] codes, MORSE format for MORSE code [23].

As an example of the developed code system usage and as an illustration of its capabilities we calculated using the ROZ-6H/SADCO-2 package the spectra of neutrons, protons, pions and photons at 120 cm into the pure iron slab with a monodirectional and monoenergetic 40-GeV neutron source (see Fig.8).

The interested reader can find more detailed results of particle (n, p, π , γ) transport through iron and concrete shielding calculation obtained with the ROZ-6H/SADCO-2 package in [24].

Fig. 5. Double differential proton emission spectra at 0° and 5.7° calculated for the 22.2-GeV $p + Be^7$ and $p + Pb^{207}$ reactions are compared with the data from [13] and [14].

Fig. 6. Neutron spectra behind homogeneous concrete and heterogeneous iron+concrete shield for 10-GeV protons incident versus neutron energy.

Fig. 7. Neutron spectra calculated at various depths into the iron shield for 10-GeV protons incident versus neutron energy.

Fig. 8. Fluence spectra for neutrons, protons, pions and photons at 120 cm into the iron slab with a 40-GeV neutron source.

4. Conclusions

A new version of the SADC0 code system to provide transport calculations of protons, pions, kaons with the energy 20 MeV ÷ 10 TeV, neutrons (0.02 eV ÷ 10 TeV), photons (0.01 ÷ 20 MeV) by multigroup methods has been developed. The harnessing of the evaluated point cross sections of hA-interactions, prepared using method [7], allows one to generate multigroup data with high accuracy. A set of the service codes, incorporated in the system, is quite user-friendly and enables convenient work with the SADC0-2 system.

Acknowledgements

We would like to thank Dr V.V.Talanov and E.N.Gorina for assistance in the preparation of this manuscript.

References

- [1] Alsmiller R.G., Jr., Barish J.//Nucl. Sci. Eng. 80 (1982) 448;
Alsmiller R.G., Jr., Barnes J.M., Drischler J.D. – ORNL/TM-9801 (1986).
- [2] Kotegawa H. et. al. JAERI-M93-020 (1993).
- [3] Lorence L.J., Jr., Morel J.E., Valdez G.D. SAND 89-2211 (1990).
- [4] Gorbalkov D.V., Kryuchkov V.P. – IHEP Preprint 92-171, Protvino, 1992.
- [5] Kryuchkov V.P. – IHEP Preprint 80-35, Serpukhov, 1980.

- [6] Gorbalkov D.V., Kryuchkov V.P., Semenova G.I. In Journal: **Questions of atomic science and technique** (series "Nuclear constants") (1990) vol.1.
- [7] Gorbalkov D.V., Kryuchkov V.P., Striganov S.I. – IHEP Preprint 92-172, Protvino, 1992.
- [8] Alekhin S.I. et al. – IHEP Preprint 87-125, Protvino, 1987.
- [9] Barashenkov V.S. Cross sections of particles and nuclei interactions with nuclei, Dubna, JINR, 1993.
- [10] Sychev B.S., Kalmykov A.R., Otroschenko E.A. – MRTI 834, Moscow (1983).
- [11] Subramian T.S., Romero J.L., Brady F.D. et al.//Phys. Rev. C 34 (1986) 1580.
- [12] Cierjacks S., Hino Y., Raupp F. et al.//Phys. Rev. C 36 (1987).
- [13] Dekkers D. et al.//Phys. Rev. 137 (1965) 504.
- [14] Landy R.A. et al.//Phys. Rev. Lett., vol.14 (1965) 504.
- [15] Voloschenko A.M., Gorbalkov D.V., Kryuchkov V.P. et al. Numerical Solution of the Boltzmann-Fokker-Planck Equation for Charged-Particle Transport. – In the book: International Symposium "Numerical Transport Theory" (abstracts) – Moscow, 1992.
- [16] Remizovich V.S. et al. Fluctuations of charged particles runs. – Moscow, Energoatomizdat, 1988.
- [17] Voronkov A.V., Juravlev V.I. et al. USCONS: A Code System to Compute Group Cross Sections Using GNDL Data Library. – Keldysh Institute of Applied Mathematics, Moscow, 1983.
- [18] Roussin R.W. et al. VITAMIN-C: The CTR Processed Multigroup Cross-Section Data. RSIC Library DLC-23 (1973).
- [19] Averin A.V., Voloschenko A.M., Kondratenko E.P. et al. – Proc. Top. Mtg. Adv. in Mathem., Comput. and Reactor Physics, Pittsburgh, USA (1991) vol.5.
- [20] Kryuchkov V.P., Sumaneev O.V. – IHEP Preprint 92-132, Protvino, 1992.
- [21] Engle W.W., Jr., A User's Manual for ANISN, a One Dimensional Discrete Ordinates Transport Code, Union Carbide Report K-1693 (1967).
- [22] Rhoades W.A., Munatt F.R. The DOT-III Two-Dimensional Discrete Ordinates Transport Code. – ORNL-TM-4280 (1973).
- [23] Emmett M.B., The MORSE Monte-Carlo Radiation Transport Code System. – ORNL Report ORNL-4972 (1975).

- [24] Gorbatkov D.V., Kryuchkov V.P. Space-Energy Characteristics of Radiation Components Behind High-Energy Accelerator Shielding. – Proc. of the Fourth European Particle Accelerator Conference, London, vol.3 (1994) 2591.

Received February 10, 1995

Д.В.Горбатков, В.П.Крючков

Система адронных констант SADCO-2 для обеспечения расчетов переноса высокоэнергетических частиц многогрупповыми методами.

Оригинал-макет подготовлен с помощью системы $\text{\LaTeX}$.

Редактор Е.Н.Горина.

Технический редактор Н.В.Орлова.

Подписано к печати 13.02.1995 г. Формат 60 × 84/8. Офсетная печать.
Печ.л. 1,12. Уч.-изд.л. 0,86. Тираж 120. Заказ 272. Индекс 3649.
ЛР №020498 06.04.1992 г.

ГНЦ РФ Институт физики высоких энергий
142284, Протвино Московской обл.

ПРЕПРИНТ 95-22, И Ф В Э, 1995