BLIND INTERCOMPARISON OF NUCLEAR MODELS FOR PREDICTING CHARGED PARTICLE EMISSION

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Abstract

An international comparison of nuclear-model calculations has been performed. The excitation functions of the reactions $^{60}\text{Co}(n,p)$ and $^{60}\text{Co}(n,\alpha)$ were calculated together with proton- and $\alpha$-particle emission spectra in the incident-energy range from 1 to 20 MeV. The final results are graphically presented.

**Dr. Siegfried Cierjacks made a great effort in organising this work. He died before he could accomplish it. We would like to dedicate this publication to his memory.**
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1. Introduction

Neutron activation data are important for dosimetry, radiation-damage and production of long-lived activities. For fusion energy applications, it is required to develop "low-activation materials" from the viewpoints of safety, maintenance and waste disposal. Existing evaluated activation cross-section libraries are to a large extent based on nuclear-model calculations. The former Nuclear Energy Agency Nuclear Data Committee, NEANDC, (presently replaced by the NEA Nuclear Science Committee) organized the working group on activation cross sections. The first meeting of the group was held in 1989, and it was then agreed that a blind intercomparison of nuclear-model calculations should be undertaken in order to test the predictive power of the theoretical calculations.

As a first stage the working group selected the reactions $^{60}$Co(n,p)$^{60}$Fe and $^{60m}$Co(n,p)$^{60}$Fe, for which no experimental data were available, in the energy range from 1 to 20 MeV. The calculated quantities are:

1. excitation functions
2. angle-integrated proton emission spectra for the two reactions.

No specification was made concerning the parameters required as input to nuclear model codes. Thus, participants selected their own "best parameters", reflecting their preferences.

The preliminary results compiled at the NEA Data Bank were sent to each participant and a meeting was held during the International Conference on Nuclear Data for Science and Technology in Jülich 1991 to discuss the results. Following the outcome of the discussion in Jülich, it was decided to extend this intercomparison:

1. to perform additional calculation of $^{60m}$Co(n,α) reactions with "best parameters"
2. to repeat the exercise with fixed model parameters (referred to as "default parameters" hereafter) as the second stage.

In the second-stage calculation, the same optical-model parameters were employed for neutrons, protons and α-particles, i.e., V = 50 MeV, W = 10 MeV, r = 1.25 fm and a = 0.6 fm with the Woods-Saxon volume-type form factors. No spin-orbit interaction was considered. Concerning the level density, the Fermi gas model with $a = A/8$ MeV$^{-1}$ was assumed without pairing corrections. Moreover, gamma-ray competition was neglected to simplify the calculation.

This report describes the final results of the blind comparison. Section 2 deals with a survey of the received contributions. The final results are graphically presented in section 3.
2. Received Contributions

- Hauser-Feshbach code
  — CINDY [1], E. Sheldon (LOWELL, U.S.A.)

- Modified Hauser-Feshbach codes
  — GNASH [2], P.G. Young (LANL, U.S.A.)
  — GNASH, S.B. Garg (BARC, India)
  — GNASH, S. Iwasaki and N. Odano (TOH, Japan)
  — GNASH, N. Yamamuro (DE, Japan)
  — GNASH, V. Konshin (IAEA, Austria)
  — PCROSS [3], R. Capote, V. Osorio, R. Lopez, E. Herrera and M. Piris (INST, Cuba)
  — PRIMA-2, O.T. Grudzevich and A.V. Zelenetskij (IAE, Russia)
  — MAURINA [4], M. Uhl (IRK, Austria)
  — STAPRE [5], S. Sudár (KOS, Hungary)
  — STAPRE-H [6], M. Avrigeanu and V. Avrigeanu (INPE, Romania)
  — UNIFY-2 [7], Zhang Jingshang (CNDC, China)

- Hybrid-model code
  — ALICE-85 [8], M. Blann (LLNL, U.S.A.)

- Statistical multistep reaction code
  — EXIFON [9], H. Kalka and D. Seeliger (TUD, Germany)

- Systematics
  — THRESH-ECN [10], J. Kopecky (ECN, The Netherlands)

Fifteen groups from eleven countries (five OECD countries and six non-OECD countries) participated in the present work. Many participants employed modified Hauser-Feshbach codes, widely used to create evaluated neutron cross-section libraries. M. Blann provided two sets of calculations using different level-density options.

Six groups participated in the second stage of the comparison. The code CINDY calculated only (n,p) cross sections to discrete levels, whereas other codes gave a sum of the cross sections to discrete and continuum levels. Therefore, the data calculated by CINDY could not be compared with any others.

3. Results and Discussion

3.1 Calculations with "best parameters"

Figures 1 and 2 show the final results of the (n,p) cross sections calculated with "best parameters". It is found from Fig. 1 that the code THRESH-ECN produced cross sections completely different from other calculations. The cross sections were calculated at the Data
Bank by using the NX-1 code [11] which is a code based on systematics, and the calculated result was found to be similar to that of the THRESH-ECN code. Therefore, nuclear-data evaluators should be careful in applying systematics in calculating reactions where measurements are not available. For the $^{60}_{\text{Co}}$(n,p) reaction, three sets of the GNASH calculations are consistent, although the input-parameters are different. A bump is seen around 4 MeV in this reaction. It might have some physical meaning.

The (n,$\alpha$) cross-section results shown in Figs. 3 and 4 are discrepant. An NX-1 calculation was also performed for this reaction, and the result was found to differ considerably from the calculations shown in Fig. 3.

Proton and $\alpha$-particle emission spectra are shown in Figs. 5-18 and Figs. 19-32, respectively. The spectra were so normalized that the energy-integration should give unity. In the high energy region of the proton spectra, the MAURINA and STAPRE-H codes yielded smaller cross sections than other codes as the incident energy increased. At an incident energy of 20 MeV, several codes produced an enhanced peak in the lower energy end of proton spectra. The difference in the gradient of $\alpha$-particle spectra on the high outgoing-energy side becomes pronounced with incident energy, whereas that on the low outgoing-energy side is small.

### 3.2 Calculations with "default parameters"

Figures 33-64 show the results obtained with "default parameters". These results show a larger spread than those calculated with "best parameters". This fact is surprising since we would rather expect the contrary. Nothing was however specified to calculate pre-equilibrium effects. Hence, in order to clarify what occurred, simple calculations using the modified Hauser-Feshbach codes TNG and GNASH were performed at the Data Bank. Width-fluctuation and pre-equilibrium were turned off in the calculation. It is found from Table 1 that the compound-nucleus formation cross sections calculated by the two codes are consistent with each other within one percent at every incident energy. Figures 65-67 show one-step pure Hauser-Feshbach calculations. The compound elastic scattering cross section is included in the (n,n') reaction, but the shape elastic one is excluded. The difference in the (n,n') cross section is 1-4% in the energy range from 1 to 20 MeV. However, the differences are magnified in the (n,p) and (n,$\alpha$) reactions, because these two cross sections are small as compared with the (n,n') cross section and there is a constraint that a sum of the cross sections for the three reactions should be equal to the compound-nucleus formation cross section. At 14 MeV, the differences between the cross sections calculated by the two codes are 15% for the (n,p) reaction and 50% for the (n,$\alpha$) reaction. A similar tendency was seen in the previous intercomparison work [12]. These differences might be due to the intrinsic characteristics of each code such as energy-binning and interpolation of transmission coefficients.
4. Conclusions

A blind intercomparison of nuclear-model calculations was performed by fifteen groups from eleven countries. The cross sections for the $^{60}$Co(n,p) and $^{60}$Co(n,$\alpha$) reactions together were calculated with proton and $\alpha$-particle emission spectra. In the first phase of the exercise, no input parameters were specified, so that the calculated results would reflect the "best estimate" of each participant. The code based on the experimental systematics produced results much different from those given by other nuclear-model codes.

The exercise was repeated with specified optical-model and level density parameters. The results were in this case more scattered than in the first phase. Simple analyses showed that this could be understood by differences in numerical algorithms used in each code. It is confirmed that predictions of cross sections and spectra for charged particle emission have a rather large sensitivity to the numerical algorithms used and relatively large discrepancies between results from different computer codes can thus be expected.

5. Acknowledgments

The authors would like to thank all participants in the present comparison. They are indebted to the Nuclear Data Section of IAEA for providing the data from non-OECD countries.
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12. H. Gruppelaar and P. Nagel: "International Nuclear Model and Code Comparison on Pre-
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a) Incident neutron energy.
b) Cross sections calculated by GNASH.
c) Cross sections calculated by TNG.
d) $\Delta\sigma = (\sigma_G - \sigma_T) \times 100 / \sigma_T$. 

- 12 -
$^{60}\text{Co}(n,p)^{60}\text{Fe}$

(Best Parameters)

Legend
- Avrigeanu (STAPRE)
- Blann-1 (ALICE)
- Blann-2 (ALICE)
- Copote (PCROSS)
- Fu (TNG)
- Gorg (GNASH)
- Grudzhevich (PRIMA-2)
- Iwaski (GNASH)
- Kalka (EXIFON)
- Konshin (GNASH)
- Kopelczyk (THRESH)
- Sudar (STAPRE)
- Uhl (MAURINA)
- Yamamuro (GNASH)
- Young (GNASH)
- Zhang (UNIFY-2)
Fig. 2 $^{60m}$Co(n,p)$^{60}$Fe reaction cross sections calculated with "best parameters"
Fig. 3 $^{60}$Co(n,α)$^{57}$Mn reaction cross sections calculated with "best parameters"
Fig. 4 $^{60m}\text{Co}(n,\alpha)^{57}\text{Mn}$ reaction cross sections calculated with "best parameters"
Fig. 5 Proton emission spectra from the $^{60}$Co(n,xp) reaction at 8 MeV.

The spectra were calculated with "best parameters".
Fig. 6 Proton emission spectra from the $^{60}\text{Co}(n,\text{xp})$ reaction at 10 MeV. The spectra were calculated with "best parameters".

![Graph showing proton emission spectra from $^{60}\text{Co}(n,\text{xp})$ reaction at 10 MeV.]
Fig. 7 Proton emission spectra from the $^{60}$Co(n,xp) reaction at 12 MeV. The spectra were calculated with "best parameters".
Fig. 8  Proton emission spectra from the $^{60}$Co(n,xp) reaction at 14 MeV.
The spectra were calculated with "best parameters".
Fig. 9  Proton emission spectra from the $^{60}$Co(n, xp) reaction at 16 MeV.
The spectra were calculated with "best parameters".
Fig. 10 Proton emission spectra from the $^{60}$Co(n, xp) reaction at 18 MeV. The spectra were calculated with "best parameters."
Fig. 11  Proton emission spectra from the $^{60}$Co(n,xp) reaction at 20 MeV.
The spectra were calculated with "best parameters".
Fig. 12 Proton emission spectra from the $^{60m}$Co(n,xp) reaction at 8 MeV. The spectra were calculated with "best parameters".
Fig. 13  Proton emission spectra from the $^{60m}$Co(n,xp) reaction at 10 MeV.
The spectra were calculated with "best parameters".
Fig. 14  Proton emission spectra from the $^{60}$Co(n,xp) reaction at 12 MeV.
The spectra were calculated with "best parameters".
Fig. 15 Proton emission spectra from the $^{60m}$Co(n,xp) reaction at 14 MeV.
The spectra were calculated with "best parameters".
Fig. 16  Proton emission spectra from the $^{60m}$Co(n,xp) reaction at 16 MeV.
The spectra were calculated with "best parameters".
Fig. 17  Proton emission spectra from the $^{60m}$Co(n,xp) reaction at 18 MeV. The spectra were calculated with "best parameters".
Fig. 18  Proton emission spectra from the $^{60}\text{Co}(n,\alpha)$ reaction at 20 MeV. The spectra were calculated with "best parameters".
Fig. 19  α-particle emission spectra from the $^{60}$Co(n,x$\alpha$) reaction at 8 MeV.
The spectra were calculated with "best parameters".

Legend:
- Arranz-Navarro (STAPP)
- Blenn---1 (ALICE)
- Blenn---2 (ALICE)
- Koeha (EXFON)
- Konshin (GAMSH)
- Young (GNASH)
Fig. 20  $\alpha$-particle emission spectra from the $^{60}$Co(n,x$\alpha$) reaction at 10 MeV. The spectra were calculated with "best parameters".
Fig. 21  $\alpha$-particle emission spectra from the $^{60}$Co($n,x\alpha$) reaction at 12 MeV. The spectra were calculated with "best parameters".
Fig. 22  $\alpha$-particle emission spectra from the $^{60}\text{Co}(n,\alpha)$ reaction at 14 MeV. The spectra were calculated with "best parameters".
Fig. 23  $\alpha$-particle emission spectra from the $^{60}\text{Co(n,x}\alpha\text{)}$ reaction at 16 MeV.

The spectra were calculated with "best parameters".
Fig. 24 $\alpha$-particle emission spectra from the $^{60}\text{Co}(n,x\alpha)$ reaction at 18 MeV. The spectra were calculated with "best parameters".
Fig. 25  $\alpha$-particle emission spectra from the $^{60}$Co(n,x$\alpha$) reaction at 20 MeV. The spectra were calculated with "best parameters".
Fig. 26  $\alpha$-particle emission spectra from the $^{60m}$Co($n,x\alpha$) reaction at 8 MeV. The spectra were calculated with "best parameters".
Fig. 27 $\alpha$-particle emission spectra from the $^{60m}\text{Co}(n,x\alpha)$ reaction at 10 MeV. The spectra were calculated with "best parameters".
Fig. 28  $\alpha$-particle emission spectra from the $^{60m}$Co($n,x\alpha$) reaction at 12 MeV. The spectra were calculated with "best parameters".
Fig. 29  α-particle emission spectra from the $^{60}$Co(n,xα) reaction at 14 MeV. The spectra were calculated with "best parameters".
Fig. 30  α-particle emission spectra from the $^{60m}$Co(n,xα) reaction at 16 MeV. The spectra were calculated with "best parameters".
Fig. 31 α-particle emission spectra from the $^{60}$Co(n,xα) reaction at 18 MeV. The spectra were calculated with "best parameters".
Fig. 32  α-particle emission spectra from the $^{60m}$Co(n,x$\alpha$) reaction at 20 MeV. The spectra were calculated with "best parameters".
Fig. 33 $^{60}\text{Co}(n,p)^{60}\text{Fe}$ reaction cross sections calculated with "default parameters".
Fig. 34  $^{60m}$Co(n,p)$^{60}$Fe reaction cross sections calculated with "default parameters".
Fig. 35 $^{60}\text{Co}(n,\alpha)^{57}\text{Mn}$ reaction cross sections calculated with "default parameters".
Fig. 36 $^{60m}\text{Co}(n,\alpha)^{57}\text{Mn}$ reaction cross sections calculated with "default parameters".
Fig. 37  Proton emission spectra from the $^{60}$Co(n,xp) reaction at 8 MeV.
The spectra were calculated with "default parameters".
Fig. 38 Proton emission spectra from the $^{60}$Co(n,xp) reaction at 10 MeV. The spectra were calculated with "default parameters".
Fig. 39 Proton emission spectra from the $^{60}$Co(n,xp) reaction at 12 MeV.
The spectra were calculated with "default parameters".
Fig. 40  Proton emission spectra from the $^{60}$Co(n,xp) reaction at 14 MeV. The spectra were calculated with "default parameters".
Fig. 41 Proton emission spectra from the $^{60}$Co(n,xp) reaction at 16 MeV.
The spectra were calculated with "default parameters".
Fig. 42  Proton emission spectra from the $^{60}$Co(n,xp) reaction at 18 MeV. The spectra were calculated with "default parameters".
Fig. 43  Proton emission spectra from the $^{60}$Co(n,xp) reaction at 20 MeV. The spectra were calculated with "default parameters".
Fig. 44 Proton emission spectra from the $^{60}$Co(n,xp) reaction at 8 MeV. The spectra were calculated with "default parameters".
Fig. 45  Proton emission spectra from the $^{60}\text{Co}(n,\text{xp})$ reaction at 10 MeV. The spectra were calculated with "default parameters".
Fig. 46 Proton emission spectra from the $^{60m}$Co(n,xp) reaction at 12 MeV.
The spectra were calculated with "default parameters".
Fig. 47  Proton emission spectra from the $^{60m}$Co(n,xp) reaction at 14 MeV. The spectra were calculated with "default parameters".

Legend

- $^*$ Ferrer (GNASH)
- $^*$ Fu (TNG)
- $^*$ Young (GNASH)

$^{60m}$Co(n,xp) at 14 MeV
(Default Parameters)

Normalized Distribution (1/MeV)

Outgoing Energy (MeV)
Fig. 48 Proton emission spectra from the $^{60m}$Co(n,xp) reaction at 16 MeV. The spectra were calculated with "default parameters".
Fig. 49  Proton emission spectra from the $^{60m}$Co(n,xp) reaction at 18 MeV. The spectra were calculated with "default parameters".

Legend:
- Pu (CNG)
-注视于 (GNSH)
- Young (GNSH)

$^{60m}$Co(n,xp) at 18 MeV
(Defaut Parameters)

Normalized Distribution (1/MeV)

Outgoing Energy (MeV)
Fig. 50  Proton emission spectra from the $^{60}$Co(n,xp) reaction at 20 MeV.
The spectra were calculated with "default parameters".
$^{60}\text{Co}(n,x\alpha)$ at 8 MeV
(Default Parameters)

Normalized Distribution (1/MeV)

Outgoing Energy (MeV)

Legend

- Fu (TNG)
- Iwasaki (GNASH)
- Koike (EXIFON)
- Young (GNASH)

Fig. 51: $\alpha$-particle emission spectra from the $^{60}\text{Co}(n,x\alpha)$ reaction at 8 MeV. The spectra were calculated with "default parameters".
Fig. 52 $\alpha$-particle emission spectra from the $^{60}$Co(n,$\alpha\alpha$) reaction at 10 MeV. The spectra were calculated with "default parameters".
Fig. 53  $\alpha$-particle emission spectra from the $^{60}$Co(n,x$\alpha$) reaction at 12 MeV. The spectra were calculated with "default parameters".
Fig. 54 $\alpha$-particle emission spectra from the $^{60}\text{Co}(n,x\alpha)$ reaction at 14 MeV. The spectra were calculated with "default parameters".
Fig. 55  $\alpha$-particle emission spectra from the $^{60}\text{Co}(n,x\alpha)$ reaction at 16 MeV. The spectra were calculated with "default parameters".
Fig. 56 α-particle emission spectra from the $^{60}$Co(n,xα) reaction at 18 MeV. The spectra were calculated with "default parameters".
Fig. 57 $\alpha$-particle emission spectra from the $^{60}$Co(n,$\alpha\alpha$) reaction at 20 MeV.

The spectra were calculated with "default parameters".
Fig. 58  α-particle emission spectra from the $^{60m}$Co(n,xα) reaction at 8 MeV.
The spectra were calculated with "default parameters".
Fig. 59  $\alpha$-particle emission spectra from the $^{60m}\text{Co}(n,x\alpha)$ reaction at 10 MeV. The spectra were calculated with "default parameters".

Legend

- $\Delta$ Young (GNASH)
- $\triangledown$ Fu (GNASH)
- $\vartriangle$ - (GNASH)
Fig. 60  $\alpha$-particle emission spectra from the $^{60m}\text{Co}(\text{n},\alpha\gamma)$ reaction at 12 MeV. The spectra were calculated with "default parameters".
Fig. 61 $\alpha$-particle emission spectra from the $^{60m}\text{Co}(n,x\alpha)$ reaction at 14 MeV. The spectra were calculated with "default parameters".
Fig. 62  $\alpha$-particle emission spectra from the $^{60m}\text{Co}(n,x\alpha)$ reaction at 16 MeV.
The spectra were calculated with "default parameters".
Fig. 63  α-particle emission spectra from the $^{60m}$Co(n,xα) reaction at 18 MeV. The spectra were calculated with "default parameters".
Fig. 64 $\alpha$-particle emission spectra from the $^{60m}\text{Co}(n,x\alpha)$ reaction at 20 MeV.

The spectra were calculated with "default parameters".
Fig. 65 One-step Hauser-Feshbach calculations for neutron emission.
$^{60}\text{Co}(n,p)^{60}\text{Fe}$ without preequilibrium effects
(1st Step with Default Parameters)

Legend

\(\nabla\) Fu (TNG) ---
\(\Delta\) Young (GNASH)

Cross Section (mb)

Incident Energy (MeV)
Fig. 67  One-step Hauser-Feshbach calculations for α-particle emission.