APPENDIX IV

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OECD
Nuclear Energy Agency
Nuclear Science Committee

Specifications for an International Codes and Model Intercomparison for Intermediate Energy Activation Yields

Rolf Michel

Center for Radiation Protection and Radioecology
University Hannover, Germany
email: michel@mbox.zsr.uni-hannover.de

Pierre Nagel

NEA Data Bank, Issy-les-Moulineaux, France
email: Nagel@nea.fr

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I. Introduction

A number of applications (Accelerator based transmutation, medical therapy, ...) are beginning to require reliable nuclear data at energies above those needed for traditional fission reactors. These include - but are by no means limited to - data for nuclear reactions induced by neutrons and protons with energies of up to 1-2 GeV. Experiments to measure these data are costly and there are limited facilities available with which to make these measurements. It will therefore be important to rely upon nuclear modelling to provide these data.

A first exercise designed to assess the predictive power of current nuclear models consisted of an international code comparison in the intermediate energy regime for the calculation of thin target double differential cross sections, for which Zr-90 and Pb-208 were chosen. The results of this exercise were published in 1994 /1/. A follow-up specialists' meeting /2/, recommended that the next step, which is the present activity, should be a model and code intercomparison aimed at the calculation of isotope yields. The exercise should not be limited to isotopes near to the target, but should include a wide range of masses and atomic numbers so as to test also spallation, fragmentation and heavy cluster emission.

It is most fortunate that experiments of interest for this intercomparison are currently being undertaken at the SATURNE accelerator laboratory. These data will help in providing reference data for the comparison of the physical models.

The comparison would involve two complementary types of calculations: The basic modelling of nuclear reaction processes on one hand and the spallation processes on the other. In this exercise it is proposed to begin with calculations of basic microscopic nuclear reactions using thin targets for proton-induced reactions covering a large mass and energy range.

It is noticed that at high energies the models for neutron and proton reactions are quite similar. Thus there is no need to consider neutron-induced reactions in this exercise separately. The latter statement applies to the expectable quality of model calculations. It does, however, not imply that cross sections of proton- and neutron-induced reactions must necessarily be equal for a given target/product combination. Moreover, there is a practical aspect in not considering neutron-induced reactions, since there are no data at energies above 50 MeV which could be used for comparison. Though it is realised that pion-induced reactions are important at higher energies, it was decided not to consider pion-induced reactions. The experimental data base is by no means comparable with that for proton-induced reactions.

It is planned to analyze the results of this model and code intercomparison for intermediate energy activation yields towards the end of 1995.

II. Choice of reactions

This intercomparison will be made of calculations of thin target activation yields for incident protons with energies from thresholds up to 5 GeV. The choice of targets is restricted since a sufficiently large number of consistent experimental data has to be available. Targets were chosen in order to cover a large mass range and at the same time the different types of materials which are important for a technological application. The target elements oxygen, aluminum, iron, zirconium and gold have been selected for this purpose. Cobalt was further selected with some (p,xn) and (p,pxn) reactions in order to test the behaviour of models when calculating nuclide production near closed shells.

Oxygen is a main constituent of ambient air and shielding concrete, aluminum is a structural material, the most often used target element for monitoring purposes and one of the best investigated target nuclei. Iron and Zirconium are structural materials which, moreover, are well investigated experimentally. Gold was chosen instead of lead, to represent the heavy target elements which will be used in the spallation target since - in spite of ongoing activities - the experimental situation for lead is

still much worse than for gold. It also might be easier in this step of the exercise to use a non-magic target nuclide.

It was further decided that target elements of natural isotopic composition should be used, since the availability of experimental production cross sections is strongly dominated by data for targets of natural isotopic composition.

Participants in the intercomparison should provide results for all targets and the entire energy regime if this it practical. If data are given by a participant for a reduced energy range only, it will be assumed that the respective code is not applicable in the omitted energy ranges.

It is encouraged that for each target element as many product nuclides as possible, which can be calculated simultaneously by a given code, should be submitted. The target/product combinations given in table 1 just represent probably a maximum set of data required for estimating the capabilities of a particular code. This list was produced considering the availability of experimental data for comparison as well as the desired coverage of different reaction modes. In Table 1 there are nuclides not enclosed in parentheses and nuclides enclosed in parentheses. **The intercomparison will be performed on the nuclides not enclosed in parentheses**. For these nuclides, reliable experimental data are available. Since many experimental data contain contributions from radioactive precursors, a maximum set of precursor nuclides is listed in table 1 (nuclides in parentheses). Calculational results on as many as possible of these precursors are requested. The theoretical cross sections for the comparison with experimental results will be computed from the submitted calculated cross sections either at the NEA Data Bank or at the University Hannover.

Again it will be assumed that a model or code is not able to calculate a given target/product combination if no data are submitted for it. If this is not the case it should be clearly stated in a letter accompanying the results.

For the target elements from iron to gold it is desirable to have results for as many products as possible in order to compare isobaric, isotopic and isotonic yields for different parts of the mass yield curves among the different codes, even if it is not possible from the available experimental data to make a systematic survey. A comparison among systematic calculated data alone already allows to distinguish differences in the treatment of particular reaction modes.

Proton induced reaction have been chosen for the intercomparison, since just a few experimental data exist for neutron induced activation yields at medium energies. The existing neutron data do not allow a systematic and comprehensive intercomparison.

The results will in any case be representative for the understanding of neutron induced reactions which are due to the same reaction mechanisms for endoenergetic reactions.

Table 1

Target/product combinations for which production cross sections shall be calculated for proton-induced reactions from thresholds up to 5 GeV. For the nuclides not in parentheses detailed experimental data are available for comparison. Intercomparison between experimental and calculated data will be made for these nuclides only. Cross sections for the production of nuclides in parentheses are needed to calculate the contributions from radioactive progenitors which are contained in the experimental data.

target	product nuclides
O-16	Be-7, Be-10, C-11, C-14
Al-27	H-3, He-3, He-4, Be-7, Be-10, Na-22 (Mg-22), Na-24 (Ne-26), (Si-26)
Fe(nat)	H-3, He-3, He-4, Be-7, Be-10, Ne-20 (all mass 20 nuclides), Ne-21 (all mass 21 nuclides), Ne-22 (F-22), Na-22 (Mg-22), Na-24 (Ne-24), Mg-28 (Na-28), Al-26 (Si-26), Cl-36, Ar-36 (K-36, Ca-36), Ar-38 (all mass 38 nuclides), Sc-46, V-48 (Cr-48), Cr-51 (Mn-51, Fe-51), Mn-52m+g (Fe-52), Mn-53 (Fe-53, Co-53), Mn-54, Fe-55 (Co-55, Ni-55), Co-56
Co-59	Co-56, Co-57, Co-58, Ni-56, Ni-57
Zr(nat)	Be-7, Na-22 (Mg-22), Sc-46, V-48, (Cr-48)), Cr-51 (Mn-51, Fe-51), Mn-54, Co-56 (Ni-56), Co-58, Co-60, Zn-65 (Ga-65, Ge-65), Ga-67 (Ge-67, As-67), Ge-69 (As-69, Se-69), As-71 (Se-71, Br-71, Kr-71) As-74, Se-75 (Br-75, Kr-75, Rb-75), Br-77 (Kr-77, Rb-77, Sr-77), Kr-78 (Br-78, Rb-78), Kr-79 (Rb-79, Sr-79), Kr-80 (Br-80, Rb-80, Sr-80, Y-80), Kr-81 (Rb-81, Sr-81, Y-81, Zr-81), Kr-82 (Br-82, Rb-82, Sr-82, Y-82, Zr-82), Kr-83 (all mass 83 nuclides), Kr-84 (Br-84, Se-84, Rb-84), Kr-85 (Se-85, Br-85), Kr-86 (Se-86, Br-86, Rb-86), Rb-83 (Sr-83, Y-83, Zr-83), Rb-84, Rb-86, Sr-82 (Y-82, Zr-82), Sr-83 (Y-83, Zr-83), Sr-85 (Y-85, Zr-85, Nb-85), Y-86 (Zr-86, Nb-86), Y-86m, Y-87 (Zr-87, Nb-87), Y-87m, Y-88 (Zr-88, Nb-88), Zr-86 (Nb-86), Zr-88 (Nb-88), Zr-89 (Nb-89), Zr-95 (Y-95), Nb-90, Nb-92m, Nb-95, Nb-95m, Nb-96
Au-197	Be-7, Na-22 (Mg-22), Na-24 (Ne-24), Sc-46, V-48 (Cr-48), Mn-54, Fe-59 (Mn-59), Co-56 (Ni-56), Co-58, Co-60, Zn-65 (Ga-65, Ge-65), As-74, Se-75 (Br-75, Kr-75, Rb-75), Rb-83 (Sr-83, Y-83, Zr-83), Rb-84, Rb-86, Sr-85 (Y-85, Zr-85, Nb-85), Y-87 (Zr-87, Nb-87), Y-88 (Zr-88, Nb-88), Zr-88 (Nb-88), Zr-89 (Nb-89), Zr-95 (Y-95), Nb-95 (Rb-95, Sr-95, Y-95, Zr-95), Tc-96, Ru-103 (Nb-103, Mo-103, Tc-103), Rh-102, Ag-105 (Cd-105, In-105), Ag-110m, Ag-110, Sn-113 (Sb-113, Te-113, I-113, Xe-113), Te-121 (I-121, Xe-121, Cs-121, Ba-121), Te-121m, Te-121m+g, Xe-127 (Cs-127, Ba-127, La-127), Ba-131 (La-131, Ce-131), Ce-139 (Pr-139, Nd-139, Pm-139, Sm-139), Eu-145 (Gd-145), Eu-147 (Gd-147, Tb-147), Eu-148, Eu-149 (Gd-149, Tb-149, Dy-149, Ho-149), Gd-146 (Tb-146), Gd-147 (Tb-147, Dy-147), Gd-149 (Tb-149, Dy-149, Ho-149), Gd-151 (Tb-151, Dy-151, Ho-151), Gd-153 (Tb-153, Dy-153, Ho-153), Tb-149 (Dy-149, Ho-149), Tb-151 (Dy-151, Ho-151), Tb-153 (Dy-153, Ho-153), Tm-165 (Y-165, Lu-165, Hf-165), Tm-166 (Y-166, Lu-166, Hf-166, Ta-166, W-166), Tm-167 (Y-167, Hf-167, Ta-167), Tm-168, Yb-166 (lu-166, Hf-166, Ta-166), Yb-169 (Lu-169, Hf-169, Ta-169) , Lu-169 (Hf-169, Ta-169), Lu-170 (Hf-170, Ta-170), Lu-171 (Hf-171, Ta-171), Lu-172 (Hf-172, Ta-172), Lu-173 (Hf-173, Ta-173), Hf-172 (Ta-172, W-172, Re-172), Hf-173 (Ta-173, W-173), Hf-175 (Ta-175, Re-175, Os-175), Re-181 (Os-181, Ir-181), Re-182 (Os-182, Ir-182, Pt-182), Re-183 (Os-183, Ir-183, Pt-183, Au-183), Os-182 (Ir-182, Pt-182, Au-182, Hg-182), Os-185 (Ir-185, Pt-185, Au-185, Hg-185), Os-191 (Re-191), Ir-185 (Pt-185, Au-185, Hg-185), Ir-186 (Pt-186, Au-186, Hg-186), Ir-187 (Pt-187, Au-187, Hg-187), Ir-188 (Pt-188, Au-188, Hg-188), Ir-189 (Pt-189, Au-189, Hg-189), Ir-190, Ir-192, Pt-188 (Au-188, Hg-188), Pt-191 (Au-191, Hg-191), Au-193 (Hg-193), Au-194 (Hg-194), Au-195 (Hg-195), Au-196, Hg-193, Hg-194, Hg-195, Hg-195m, Hg-197, Hg-197m

III. Contributions

Participants must provide information which will allow the identification of the physics and methods used in codes of this exercise. A list of requested information is included in this document and additional comments are invited on special features of codes used, which are not covered in the questionnaire.

On reception of the contributions, they will be first checked to ensure that there has been no misunderstanding on what was requested. If there is a question, the participant will be contacted. If not, a draft summary report will be prepared and sent to participants for comments. When these have been considered (if received within the deadlines set), the OECD/NEA NSC will issue a report summarizing this intercomparison of codes. It is hoped that this will aid in identifying codes which are adequate in various energy regimes, and in giving an estimate of their reliability and range of applicability.

Participants who use codes which cover only part of the requested data may also contribute to that subset of the exercise. Both code users and authors of codes are encouraged to participate in the intercomparison. Authors are additionally invited to provide their code and documentation to the NEA Data Bank's Computer Program Services.

Time schedule

Draft specification for comments	17th December 1994
Deadline for comments	15th February 1995
Final specifications distribution	30 May 1995
Deadline for contributions	1st November 1995
Draft analysis completed	1st May 1996
Final report	1st September 1996

IV Exercises for Code Intercomparison

We request the cross sections for the production of residual nuclides by proton-induced reactions in units of mb for energies from 0 MeV to 5 GeV for target element/product nuclide combinations given in table 1. In addition we request for each target element the total reaction cross section from 0 MeV to 5 GeV.

Energies should be chosen in sufficiently small steps to represent any structure in the cross sections, i.e. 1 MeV steps below 25 MeV and progressively larger steps at higher energies. Please indicate also whether the data are given as points or as histograms.

The following list of energies in MeV can be taken as an example:
1 MeV steps below 25 MeV, 2 MeV steps up to 50 MeV, then: 60, 70, 80, 90, 100, 120, 140, 160, 180, 200 , 250, 300, 350, 400, 450, 500, 600, 700, 800, 900., 1000, 1200, 1400, 1600, 1800, 2000, 2600, 3000, 4000, 5000 MeV.

For energies up to 200 MeV mostly experimental excitation functions are available which are equally dense in energies. For energies above 200 MeV most experimental data exist at 300, 400, 600, 800, 1200, 1600 and 2600 MeV. Therefore, these latter energies should be explicitly included in the medium energy exercise.

If it is not possible to cover the entire exercise or to choose a coarser energy grid, acontributor should do as much as he/she can. Energies should be chosen, then, in a way that also the limitations (at low or high energies) become clear by the intercomparison. If targets and/or products are not covered in a particular exercise, the reasons should be made clear in the accompanying letter in order that the analyses does not blame the model or code.

If random number generated results are submitted, please indicate the statistical sampling uncertainties at each cross section or for each cross section type for a representative energy.

If the entire energy region cannot be covered by the particular code or model, we request the coverage of all possible energies. If not all target element/product nuclide combinations can be covered by the calculations, as many as possible combinations should be given.

V Preferred format for contributions

In order to avoid unnecessary retyping of the calculations, participants should send their results on MS-DOS diskettes or preferably electronic mail, if possible, in the order indicated by the above table 1 by increasing energy.

The cross sections should be given separately for each target element/product nuclide combination, and for the reaction cross section. A one line header should precede the data for each of the data sets. If possible, a simple three column format should be chosen giving in each line: energy in MeV, cross section in mb, uncertainty of the cross section in mb, e.g. from statistical considerations in Monte Carlo codes. . A format of 3(E10.3,1x) would be preferred. A zero for the energy shall be the last entry for one item.

An example is given below:

<reaction>
0.100E+01 0.xxxE+xx 0.xxxE+xx
0.500E+04 0.xxxE+xx 0.xxxE+xx
0.0

<reaction>:

"Fe-000(xxp,xxn)Co-056" if natural isotopic composition is used
"Au-195(xxp,xxn)Co-056" else
"Fe-000(RCS)" reaction cross section of protons on iron

The yields of an isomeric state should be indicated by an "m" behind the mass number of the product nuclide.

If no free choice of the output format is possible submit the standard ASCII output with a short description. The required data will be extracted by the NEA Data Bank or by the university Hannover.

VI. Code Information Questionnaire

Please supply the following information only if not already done for the previous exercise or indicate new features if the code is different version.

VI.1. General Questions:

1. Name of the code
2. First name of the participant
3. Responsible author of the code
4. Reference for the code
5. Is a manual available? Yes No (may be needed for the analysis)
6. What nuclear reaction models are contained?
   - intranuclear cascade
   - Precompound decay
     - exiton closed form
     - exiton master equation
     - hybrid
     - Quantum mechanical multi-step
     - angular distributions from N-N scattering
     - angular distributions from systematics
   - evaporation
     - Weisskopf-Ewing
     - Hauser Feshbach
   - Fermi statistics
   - Fission model:
     - .....
7. Range of targets allowed
8. Range of projectiles allowed
9. Incident energy regime permitted

VI.2. Specific Questions:

1. How are reaction cross-sections generated in the entrance channel?
2. What nuclear density distribution is used and how do these enter the calculation?
3. Is the Fermi energy calculated in a local density approximation?
4. What nuclear radius parameterization is used'?
5. For INC models:

5.a. What nucleon nucleon cross-sections are used? Are energy and isospin dependent?

5.b. How is Pauli exclusion handled in the INC?

5.c. How are nuclear density effects treated?

5.d. How are ejectile binding energies handled?

5.e. Is any nucleon-cluster scattering considered?

5.f. Are ejectiles subject to surface refraction/reflection angular distributions?

5.g. What channels other than neutron and proton are treated e.g. alpha, deuterons, tritons, pi, K, p, etc.?

5.h. How is the transition made to the next phase of the calculation?

5.i. What criteria for p-h excitation? is the next phase precompound or compound'?

6. If there is a precompound phase, describe the PE model used, parameters, i.e. partial! state densities, transition rates? Are clusters treated multiple PE decay, relativistic kinematics used? How are angular distributions computed? Source of inverse cross-sections?
7. What physics are used for the final de-excitation stage: evaporation model, Fermi breakup? Describe parameters used: level densities inverse cross-sections or transmission coefficient, choice of optical model parameters if relevant (or reference to source),range of excitations allowed, inclusive or exclusive results?
8. Is there any limit as to the number of nucleons from target for which yields may be calculated?
9. Any other comments on aspects not covered in the above questions?
10. References to the literature or reports discussing these codes as implemented'?

VII References

1 M. Blann, H. Gruppelaar, P. Nagel, J. Rodens, International Code Comparison for Intermediate Energy Nuclear Data, NEA/OECD, 1994

2 Intermediate Energy Nuclear Data: Models and Codes, Proceedings of a Specialists' meeting, Issy-les-Moulineaux (France), 30 May - 1 June 1994, OECD, Paris, 1994.

VIII Summary of comments received on the draft specifications

Response to comments by Rolf Michel are in italics.

There were some major and often made comments :

1.the terms “cummulative” and “independent” gave rise to misunderstanding of the tasks to be performed.

In the revision I try to make clear this point. What we want is simple (t=0) cross sections. However, since we need for comparison with existing experimental data also the cross sections for radioactive precursors, I included a maximum set of precursors in table 1. I do not think that all of them will be important and do not suppose that we shall get data for all of them. For Monte Carlo Codes it should be possible to extract all the information.

2.It was proposed that the calculation of cummulative production cross sections should be made by one person and program.

I think that this is a good proposal. We could make the calculations at Hannover, since we have such programs available.

3.It was feared that there are too many energy points and consequently too much computer time would be needed.

I agree that this is a problem. However, it is a general problem when dealing with activation and nuclide production at medium energies for applications. We have found that the quality of a code cannot be judged from calculations at single energy points. It is of fundamental importance to see agreements or disagreements as functions of energy. Usually, we have experimental data for comparison from threshold to 2.6 or 3 GeV for the energies indicated in the specifications, i.e.

> ”1 MeV steps below 25 MeV, 2 MeV steps up to 50 MeV, 60, 70, 80, 90, 100, 120, 140, 160, 180, 200 , 250, 300, 350, 400, 450, 500, 600, 700, 800, 900., 1000, 1200, 1400, 1600, 1800, 2000, 2600, 3000, 4000, 5000 MeV. For energies above 200 MeV most experimental data exist at 300, 400, 600, 800, 1200, 1600 and 2600 MeV. Therefore, these energies should be explicitly included in the exercise.”

Therefore, I would like to have as many of these energies as possible. I made a remark in the specifications on priorities. Since not all codes are applicable to all energies, this will anyway reduce the number of calculations for the individual contributor to this exercise.

Further comments were

1.To consider some reactions on Co-59 or Ni, since (p,xn) and (p,pxn) reactions near the closed shells Z=28 and N=28 can provide information on the quality of calculations of multiple cascade/precompound emission and of level densities calculation near closed shells.

I added the target nucleus Co-59 with only a few products to table 1.

2.It was pointed out that the time schedule might be too tight.

I made a proposal for a longer time schedule in the draft

3.There was a remark on metastable products, fearing that just a few models may be able to give results here. It was proposed that one should ask for cross sections for the m+g production also.

If there is asked for metastable products in table 1, then there are just data on the metastable nuclide available. Well knowing that we will just get spurious results of cross sections for metastable products, I added them to table 1 because I am really curious whether somebody can do it.

4.There was a remark stressing to include pion-induced reactions.

I do not think that the experimental data base for pion-induced reactions is so extensive that we can make an adequate intercomparison at present. I, therefore, made just a comment on this in the specifications

5.There was a comment that there are differences in the treatment of neutron- and proton-induced reactions on heavy target elements and that neutron-induced reactions would be desirable too.

In view of the fact that there are practically no medium energy neutron-induced activation yields available, I do not see any chance to do an intercomparison for them.