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Information

Memo CP-B/23

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I. Coding of Reaction-SF3

We appreciate the efforts of NDS (CP-D/60) to clarify the coding of spallation, and agree completely with it. If the explanations given in items 5. and 6. together with some of our earlier comments are entered in the respective manual and LEXFOR entries, we agree to the introduction of the code SPL.

We also appreciate the comments given in CP-D/60 about the discrepancies and differing interpretations for coding of variable endproducts. We feel, however, that there remain several misunderstandings, which are probably due to an unclear procedure how to code REACTION SF3 (also in cases of single reactions). We will try, therefore, to summarize our internal discussion on the entire topic as our contribution for further discussions at the Paris meeting.

One of the problems, which arose in the discussion of the variable product nucleus (VPN) formalism, was not to loose any information by combining any reaction type in one reaction string and reexpanding it into individual reactions via balancing of the emitted neutrons and protons. However, prior to this question, one should investigate, how single reactions are treated in cases where the emission of composite particles might be possible. One must distinguish two cases:

a) The outgoing particles (especially the composite ones like α, H-3, He-3 etc.) were identified directly. In this case the reaction path can be given unambiguously in SF3.

b) Only the residual nucleus has been identified in the experiment. In this case, in principle the sum of all possible reaction paths ought to be given (corresponding to the process code X in SF3), except when

(i) the Q-value excludes all but one path (e.g. for a (p,α) reaction at sufficiently low energies)

(ii) composite particles are impossible (e.g. for (p,xn) reactions)

(iii) the author has stated a specific path (which may be, however, incorrect as can be seen from many papers).

In all other cases (and - correctly - case (iii) ought to be included here!) SF3 should be coded with X or (a possibility which we propose for discussion) by the explicit number of outgoing neutrons and protons (xn+yp) which must then be declared explicitly "to include all energetically possible competing reactions".

Obviously, such a clear distinction (especially for case (iii)) has not been performed for the Kachapag file (thus, corrections will become necessary after final clarification of this topic).

Consequently,

- a process code X or
- giving explicitly xn+yp or
- quoting of a special reaction path by the author without experimental or at least theoretical justification

are all of the same relevance.

On the other hand, we are reluctant to code a reaction string other than the author has stated, at least, if it is not completely evident that the author is wrong.

In order to avoid these ambiguities, we propose the introduction of the code DEF (= defined) for the branch - SF5 in such cases, where composite particles might be involved. This code states that - similar to the code SEQ, which designates a given particle sequence in SF3 - the particles given in SF3 were definitely present in the reaction, justified either from

- experimental identification or from
- energy considerations or by
- theoretical reasoning.

Accordingly, reactions like (p,xn) or (p,yp) with only one kind of outgoing particles need no code DEF in SF5, since no competing reaction paths are possible. This use of the code DEF would allow to combine this kind of reactions with "undefined" reactions in case of variable product nucleus formalism (see below).

The following example should demonstrate that also more complex cases can be treated unambiguously. Regard a reaction (p,2α). For energies well above the threshold for (p,4n+4p) three cases are possible:

(i) both α-particles have been measured: It is coded:
(Z-S-A(p,2α) Z'-S'-A', DEF, ...) and the detected α-particles are, in addition, specified under PART-DET

(ii) only one α-particle was detected, the author assumes (but does not justify) a (p,2α)-reaction. Coding:
(Z-S-A(p,2α) Z'-S'-A',,...) and the one detected α-particle specified under PART-DET

(iii) only residual nucleus was identified, and the author specifies a (p,2α)-reaction (but without any justification as often occurs). Coding:
(Z-S-A(p,2α) Z'-S'-A',,...), no entry under PART-DET.

Case (iii) is clearly equivalent with the two forms:
(Z-S-A(p,X) Z'-S'-A',,...) and
(Z-S-A(p,4n+4p) Z'-S'-A',,...)
if the latter is interpreted as proposed above.

Due to the above mentioned ambiguities in the present coding practice there exist the same ambiguities with respect to retrievals. If our proposal were accepted

a) specific reactions, where composite particles were really present, can be retrieved unambiguosly via the code DEF, and

b) any general retrieval can only be performed on xn+yp due to the differing practices of different authors.

II. Variable Product Nucleus Formalism

The discussion of item I. above seemed necessary to us in order to explain, while we yet see more discrepancies for the VPN formalism as was assumed in CP-D/60. We will try, therefore, again to clarify our point of view and compare it to that of NNDC and NDS as we understand their proposals.

In our opinion there are three topics which should be discussed separately:

1. Applicability of the VPN-formalism

The main purposes of such a formalism are in our opinion the following:

- combination of data of a mass/product distribution since a distribution gives more information than single cross sections (in analogy to an excitation function)
- reduction of the length of the file and omission of repeated information
- reduction of the effort of the compiler.

The most important requirements to the formalism are

- no information is to be lost by combining several reactions into one subentry
- no information, however, is to be added during the reexpansion e.g. for the index (possible misinterpretations of processes or reaction paths which are not at all clear or present must be avoided)
- the rules for application must be unambiguous and as general as possible with as few as possible restrictions.

In this context we try to compare the two proposals (by NNDC and by us). Both have in common that distributions of product nuclei (with respect to variable Z and/or A) shall be coded by this formalism. We see, however, in the NNDC proposal a further restriction by emphasizing the processes (F,SPL,X) as primary preconditions for the applicability. This is supported by the proposal of NNDC to code (p,2n), (p,3n), (p,4n),... reactions rather in the multiple reaction formalism.

We have the following arguments, why we prefer the measured physical variable (energy-distribution=excitation function or product-distribution = Z and/or A-distribution) as the only precondition:

a) A process is in our opinion more likely to become ambiguous than the independent variable. The kind of distribution is mostly obvious from the purpose of the experiment as described in the paper. Admittedly, there remain borderline cases. In no case, however, information is lost, if outgoing-particle-balance is performed (see item 2. below), as might be possible in case of an incorrect interpreted process. The indexing (and editing) program, as announced by NDS, will always retain the complete reaction string (including outgoing particles). This is, in our opinion, especially valid in the context of item I. above.

b) We see a clear analogy of mass/product-distributions and other kinds of distributions, like angular distributions, which are always coded in one subentry, independent from the kind of process to which they belong. Therefore, the VPN formalism should also be applicable for all kinds of product distributions independent from the process involved. Therefore, we would not recommend to have different coding practices (variable product nucleus formalism for fission / spallation product-distributions and multiple reaction formalism for product distributions from other types of reactions)

c) The restriction to one incident particle energy (as proposed in CP-B/14 p.5) was not meant to be an a priori condition, but came out rather as a consequence of the concept to have the independent variable as an indication of applicability of the formalism. We are very willing to discuss possibilities like multidimensional tables (as proposed in CP-D/60) or others to cover borderline cases as far as possible.

d) Our proposal to have the primary independent variable as an indicator for the formalism is certainly not the only one possibility. We are open to discuss every other proposal, which allows the formalism to be used for all kind of product distributions and puts no restrictions on the reaction type.

Summarizing we would propose to have only the following rules or restrictions for the VPN-formalism:

(i) The formalism is applicable for all mass-, charge-, or product distributions where A and/or Z act as independent variable

(ii) It cannot be used, if any subfield of the reaction string differs for the individual reactions besides of SF4 and X in SF3 (we interpret X as a varying number, since it represents a well defined number of neutrons and protons). This restriction applies also for the code DEF in SF5 (as proposed in item L).

(iii) We would recommend - for clarity only - to have only one energy value for a data table with Z/A as independent variable. We are, however, open to discuss the inclusion of every other possibility.

2. Process code X; Balancing of outgoing particles

In our opinion a lot of the discrepancies is correlated with the uncertainties explained in item I. above. If the proposed code DEF and the given interpretation of SF3 were accepted, the problems arising from coding of SF3 in case of VPN formalism and of balancing of the outgoing particles seem to be easy to solve.

The following cases seem possible:

(i) Unambiguous reaction paths with code DEF in SF5, if necessary. All identified composite particles must be given explicitly in SF3. The residual outgoing particles are then only unbound neutrons and protons which are calculated unambiguously via balancing. E.g. reactions like (p,n+α), (p,2n+α),... would then be coded in the VPN-formalism as (Z-S-A(P,A+X)Z'-S'-MASS, DEF,...).

(ii) No individual reaction path identified. Balancing gives xn+yp, which is defined (according to the proposal in item I.) to imply all competing reactions due to missing of the code DEF in SF5.

In every case, the complete information is guaranteed, since the code DEF ensures the correct outgoing particles to be calculated and printed by the indexing and editing programs.

This proposed formalism is in our opinion unambiguous and applicable to all kinds of reaction processes. We see, therefore, no reason to restrict it to fission and spallation and use e.g. the multiple reaction formalism for compound nuclear reactions, as proposed by NNDC.

The upper limit of the number of emitted neutrons and protons, for which a balancing is meaningful, is rather arbitrary. Obviously, it makes no sense to specify the sum of outgoing neutrons and protons for fission products or for the residuals of light-particle producing reactions (where these light particles are coded in SF4 or in the data columns ELEMENT/MASS, respectively). One could think of a limit of 15 or 20 nucleons up to which a balancing should be performed. This value could easily be changed if any necessity arises. The alternative of stating individually for each publication by a special code (XNYP)

whether to balance the outgoing particles or not, as proposed earlier by us, has the advantage of more flexibility but the disadvantage of increasing possible inconsistencies of the compilations.

3. Coding Rules for SF4 in case of VPN-formalism

There exist certainly several possibilities which have advantages and disadvantages. In our opinion, such rules should fulfil the following conditions:

- no information is to be lost, also with respect to retrievals
- any index-register must contain all specific reactions (also from mass-distributions)
- the rules should be easy to handle for the compilers.

These conditions seem to be fulfilled by both proposals:

- NNDC: only ELEM and/or MASS in SF4,
- Kachapag: keeping the fixed Z and/or A value in SF4 additionally

Since many of our considerations regarding coding rules (as well as the problems treated above) were correlated with our planned printed version of the Kachapag file, we would prefer our proposal. However, if programming problems for other centers are too serious, we are willing to meet their wishes, especially, because NDS promised to provide the necessary programs, whatever agreement would be reached.

Summarizing, we would like to emphasize that there are a lot of charged particle induced reactions producing a distribution of final nuclei with not too many but explicitly specificable outgoing particles, which are very suitable for a variable product nucleus formalism (and probably more than in the case of - especially thermal - neutron induced reactions). Thus, we are strongly interested to find a good and practicable solution for the present problems. The main purpose of such a solution should be clarity and uniformity (no different formalisms for similar cases) and general applicability with as few as possible restrictions (the multiple reaction formalism as proposed by NNDC, becomes impracticable with increasing number of end products due to the increasing number of data-columns).

III. Decay-Flag; Heading Isomer

We had the opinion that we had stated our preference for the 'Decay-Flag' and apologize that it was obviously not sufficiently clear.

From the two proposals of CP-D/36 we prefer the Decay- Flag for the following reasons:

In our opinion, the 'Flag' as used until now has the character of a footnote related to single data lines and explained under the keyword FLAG*. In contrast, the new concept which links probably several BIB-keywords to a residual nucleus specified in one data line, has rather the character of a pointer and will in general not use the keyword FLAG at all. In view of this different meaning we would rather expect confusion if the two cases were not distinguished by different data-headings.

On the other hand, we would prefer to have this concept available for as much as possible BIB-keywords where it is relevant. Though we cannot see any difference between both proposed concepts except of the data-headings to be used (FLAG or DECAY-FLAG), which would necessitate a restriction of the number of BIB-keywords allowed with the DECAY-FLAG with respect to those allowed with the "generalized FLAG", we would also accept the latter one, if the DECAY-FLAG must - by what reasons ever - be restricted to DECAY-DATA and RAD-DET.

Regarding the heading ISOMER, we can accept it, though here may be only few cases (several DECAY-DATA with parent - and daughter activity for one residual nucleus) where it is necessary. We would like to propose, however, that it may be omitted in cases where the entries under DECAY-DATA identify the states of the residual nuclei unambiguously.

IV. Nuclides Dictionary 27

Supplementary to the comments of CP-C/31 and CP-D/58 we want to report on some experiences and deficiencies which we found when using the NDS check program implying checks from dict. 27.

1. In some cases there exist incomplete isomeric state codes e.g. Z-S-A-G or Z-S-A- leading to error messages since only Z-S-A and Z-S-A-M1 are entered in dict. 27.

   Since meanwhile the proposal of CP-C/31 and the corresponding action as described in CP-D/61 (to which we agree) seem to have solved these problems,

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*(In this sense, e.g. the information under the keyword FLAG is given as a footnote below the data table in the printed version of the Kachapag file).

there is no further alternative proposal necessary.

2. In some cases (e.g. ^{209}Po, ^{41}Ca) flag (3) in col. 26 is missing resulting in the error message that "these nuclides are invalid for REACTION SF3".

When indicating such a validity, one should take into account that longlived or even stable residual nuclei are possible in in-beam experiments as well as in cases where the outgoing particles have been measured.

V. FLAG

We had encountered a problem in the use of the data-column FLAG. The general definition in the manual and LEXFOR reads that "it supplies information to specific lines in a data table". We interpret this that the information is correlated to the whole line.

In manual sect. V. we find that "columns with additional information (including FLAG) may be placed next to one of several dependent variable-columns to which they refer". We would like to have such a possibility. However, we see serious difficulties, how a computer program shall distinguish between the two possibilities, if only one kind of FLAG is used.

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