

A Proposed Format Structure for Storing Prompt $p_n(\nu, E_i)$ and Prompt $\chi_{i=1,\nu}(\nu, E_i)$ Spectra in an Evaluated File
Skip Kahler, Patrick Talou, Ionel Stetcu

We propose using MF=6/MT=18 to store prompt $p_n(\nu, E_i)$ and prompt $\chi_{i=1,\nu}(\nu, E_i)$ data. For each of $\nu = 0, 1, 2, \dots, \nu_{\max}$, $p_n(\nu, E_i)$ is an incident neutron energy-dependent distribution function that defines the probability of a fission event accompanied by ν prompt neutrons. $\chi_{i=1,\nu}(\nu, E_i)$ are the corresponding prompt neutron spectra.

The ENDF format currently allocates MF=1/MT=456 for the definition of prompt nu, or $\overline{\nu_p(E_i)}$. This is a single, energy-dependent function that defines the average number of prompt neutrons emitted during the fission process. When defining $p_n(\nu, E_i)$ the evaluator can include additional information by providing the probability of fission accompanied by each of $\nu = 0, 1, 2, \dots, \nu_{\max}$ neutrons. ν_{\max} is an evaluator determined integer that will likely vary from nuclide to nuclide. In order to assure consistency between $\overline{\nu_p(E_i)}$ and the various $p_n(\nu, E_i)$ distribution functions, the following constraints exist:

- (i) The sum of $p_n(\nu, E_i)$ over all ν values at each energy should be normalized to unity, i.e.,

$$\sum_{j=0}^{\nu_{\max}} p_n(j, E_i) = 1.000000,$$

to within 6 significant digits, and

- (ii) At each energy, E_i , the individual $\overline{\nu_p(E_i)}$ values that appear in the MF=1/MT=456 TAB1 function may be calculated from the various $p_n(\nu, E_i)$ distribution functions as:

$$\overline{\nu_p(E_i)} = \sum_{j=0}^{\nu_{\max}} j * p_n(j, E_i).$$

The ENDF format currently allocates MF=5 (or =6)/MT=18 for the definition of the prompt fission neutron spectrum (pfns), or $\overline{\chi_p(E_i)}$. In reality this spectrum represents the average of many spectra, since for any given incident neutron energy, E_i , there is one spectra associated with $p_n(1, E_i)$, two spectra associated with $p_n(2, E_i)$, etc. When multiple spectra are possible, i.e., for $\nu \geq 2$, we assume that they each occur with equal probability. Since $p_n(\nu, E_i)$ functions are defined for $\nu=0, 1, 2, \dots, \nu_{\max}$ there could be as many as $NK = 0.5 * (\nu_{\max}) * (\nu_{\max} + 1)$ $\chi_{i=1,\nu}(\nu, E_i)$ spectra defined that, when combined, yield the current MF=5 (or =6)/MT=18 $\overline{\chi_p(E_i)}$. In order to assure consistency between $\overline{\chi_p(E_i)}$ and the individual $\chi_{i=1,\nu}(\nu, E_i)$, the following constraints exist:

- (i) The integral of any individual $\chi_{i=1,\nu}(\nu, E_i)$ over all energies is unity, and

- (ii) At each energy, E_i , the individual $\overline{\chi_p(E_i)}$ values that appear in MF=5 (or 6)/MT=18 may be calculated from the various $\chi_{i=1,\nu}(\nu, E_i)$, as:

$$\overline{\chi_p(E_i)} = \sum_{j=1}^{\nu_{\max}} \sum_{k=1}^j \frac{p_n(j, E_i)}{j} \chi_k(j, E_i).$$

The current structure for data stored in MF=6 is:

```
[MAT, 6, MT/ ZA, AWR, 0, LCT, NK, 0] HEAD
[MAT, 6, MT/ ZAP, AWP, LIP, LAW, NR, NP/Eint/Yi(E)] TAB1
    <LAW-dependent structure for product 1>
    -----
    <repeat TAB1 and LAW-dependent structures ...
    ... for the rest of the NK subsections.>
[MAT, 6, MT/ 0.0, 0.0, 0, 0, 0, 0] SEND
```

The “repeat TAB1 and LAW-dependent structures ...” records are given in decreasing ZAP and AWP order. Definitions for the variables given above are:

ZA, AWR	Standard target material charge and mass parameters;
LCT	Reference frame flag for secondary energy-angle data;
NK	Number of subsections in this section (MT). Each subsection describes one reaction product.
ZAP	Product identifier, 1000*Z+A, with Z=0 for photons and A=0 for electrons and positrons. A section with A=0 can also be used to represent the average recoil energy or spectrum of an elemental target.
AWP	Product mass in neutron units;
LIP	Product modifier flag, or flag pointing to one of multiple, identical, outgoing particles in a sequential reaction (with comments in File 1);
LAW	Flag to distinguish among differing secondary distribution function options;
NR, NP, E _{int}	Standard TAB1 parameters.

This format structure, a loop consisting of a TAB1 function followed by a “LAW-dependent structure” is ideally suited for defining $p_n(v, E_i)$ and $\chi_{i=1,v}(v, E_i)$ data.

For MF=6/MT=18 the value for NK shall continue to be the number of subsections that follow. Although we are only discussing prompt neutron data at this time, the outline that follows is easily expanded to accommodate prompt photon spectra as well. For now, if there are $\nu_{\max}+1$ $p_n(v, E_i)$ functions this becomes the value for NK. For each of these NK subsections the initial TAB1 record shall contain one $p_n(v, E_i)$ function, beginning with $v = 0$. For this first TAB1 function, set LAW = 0 since there are no prompt neutron spectra. Use the standard values of 1.0 and 1.0 respectively for the values of ZAP and AWP to indicate that this is an outgoing neutron related data record. We do not need the product modifier flag and so set LIP = 0. With LAW = 0, there are no additional data and we proceed to define $v = 1$ data.

Start again with a TAB1 record that defines $p_n(1, E_i)$. As before, ZAP = AWP = 1.0. There is no need for LIP so once again it is set to zero. Following the TAB1 record we need a “LAW-dependent structure” to define $\chi_1(1, E)$. For all values of $v \geq 1$, we require that LAW = 1 or a negative integer. LAW = 1 is an already defined ENDF-6 structure and no change to the current definition is needed. Use of a negative integer for LAW requires an expansion of the existing MF=6 LAW definition. We propose that when a negative integer is used, its absolute value be interpreted to correspond to the LF value from File 5 for purposes of defining the spectrum, $\chi_1(1, E)$ in this instance.

Moving on to the format option(s) for $v = 2$ (or greater), we again start with a TAB1 record that allows for the definition of $p_n(2, E_i)$. Again, ZAP = AWP = 1.0. We now need to define the structure to specify $\chi_1(2, E_i)$ and $\chi_2(2, E_i)$, i.e., the spectra for the first neutron out when $v = 2$ and the spectra for the second neutron out when $v = 2$. In order to reduce redundant information this definition should allow evaluators the option to specify one set of spectra plus a flag to indicate it is applicable to both neutrons. As before, use LAW = 1 or = -LF, but also use LIP. In particular, if LIP = 0 there

will be a single LAW-dependent set of data and the resulting $\chi_{1}(v, E_i)$ is applied to 2 (or all v) neutrons. If LIP = 1 then there will be v sets of LAW-dependent (the same LAW for all v neutrons) data, one for each $\chi_{i=1,v}(v, E_i)$.

As noted previously, it is already possible to store $\overline{\chi_p(E_i)}$ in MF=6/MT=18, and so we also need to allow evaluators and users to understand whether the data in this section provide (i) $\overline{\chi_p(E_i)}$ only, (ii) both $\overline{\chi_p(E_i)}$ as well as prompt $p_n(v, E_i)$ and prompt $\chi_{i=1,v}(v, E_i)$, or (iii) prompt $p_n(v, E_i)$ and prompt $\chi_{i=1,v}(v, E_i)$ only. We propose to use the currently undefined L1 variable in the MF=6/MT=18 HEAD record as a flag to distinguish among these options. Define this variable "JP", and if L1=JP=0, then this section contains $\overline{\chi_p(E_i)}$ data only. This is the situation for several ENDF/B-VII.1 nuclides, including ^{231,233}Pa and ²³²Th, and this definition allows them to be grandfathered into the expanded MF=6/MT=18 definition proposed here. If L1=JP=1, then both $\overline{\chi_p(E_i)}$ as well as prompt $p_n(v, E_i)$ and prompt $\chi_{i=1,v}(v, E_i)$ are given (with $\overline{\chi_p(E_i)}$ appearing first) and if L1=JP=2 only prompt $p_n(v, E_i)$ and prompt $\chi_{i=1,v}(v, E_i)$ are given. NK's value depends upon JP and will be at least 1 (when JP=0), nu_{max}+2 (when JP=1) or nu_{max}+1 (when JP=2). If photon data, denoted by ZAP = 0.0, are present they follow the neutron data and NK is adjusted accordingly.

In summary, any combination of $\overline{\chi_p(E_i)}$ and/or $p_n(v, E_i)$ and $\chi_{i=1,v}(v, E_i)$ data can be defined in MF=6/MT=18 as follows:

```
[MAT, 6, 18/      ZA,      AWR, L1=JP,  LCT,  NK,  0]      HEAD
-----
[MAT, 6, 18/ ZAP=1.0, AWP=1.0,  LIP,  LAW,  NR0,  NP0/Eint/Yi(E)]  TAB1 (L1=0 or 1)
      <LAW-dependent structure for  $\overline{\chi_p(E_i)}$ > (L1=0 or 1)
-----
[MAT, 6, 18/ ZAP=1.0, AWP=1.0, LIP=0, LAW=0,  NR0,  NP0/Eint/p(v=0, Eint)] TAB1 (L1=1 or 2)
[MAT, 6, 18/ ZAP=1.0, AWP=1.0, LIP=0,  LAW,  NR1,  NP1/Eint/p(v=1, Eint)] TAB1 (L1=1 or 2)
      <LAW=1 or -LF structure to define the single neutron pfns, (L1=1 or 2)>
[MAT, 6, 18/ ZAP=1.0, AWP=1.0,  LIP,  LAW,  NR2,  NP2/Eint/p(v=2, Eint)] TAB1 (L1=1 or 2)
      <LIP=0/1 & LAW=1 or -LF structure(s) to define the two neutron pfns's, (L1=1 or 2)>
-----
      <repeat TAB1 and LAW structures for the remaining subsections>
-----
[MAT, 6, 18/      0.0,      0.0,      0,      0,      0,      0]      SEND
```

When LAW > 0, refer to the current MF=6 definition; when LAW < 0, refer to the appropriate MF=5 abs(LAW) = LF definition.

Changes needed to ENDF-102:

1. Add a new variable, JP, to the list in Section 6.2 whose definition shall read "a flag, whose value is 0, 1 or 2. When zero it indicates that the spectrum averaged over multiple outgoing particles is given, when unity indicates that both the average spectrum as well as probability functions for each of multiple particles and their individual spectra are given, and when set to two indicates that only the probability functions and individual spectra are given."
2. Expand the definition of LIP in Section 6.2. Add a new paragraph stating ...
"LIP may also be used in conjunction with LAW=-LF to identify whether a single (LIP=0) or multiple (LIP=1) secondary law records follow. See Section 6.3.9 for further discussion. "
3. Expand the definition of LAW in Section 6.2 to include ...
"LAW=-LF, where abs(LF) is the secondary distribution law defined in Section 5.1.1".
4. Add a new Section under "6.3 Procedures" ...
"6.3.9 Fission P(v) and Associated Prompt Fission Neutron Spectra (pfns)

Distribution functions describing $P(\nu)$ for $\nu=0,1,\dots,\nu_{\max}$ and the associated pfns are given in $mt=18$. ZAP and AWP parameters are set to unity, denoting neutron data. The evaluator defines an initial TAB1 record with $LAW=0$ to define $P(\nu=0)$. With no associated pfns, this is followed by another TAB1 record to define $P(\nu=1)$. The data structure that follows, for the associated pfns, depends upon the value of LAW . Specifically, LAW may be +1 if the pfns is given as a continuum energy-angle distribution, or LAW may be a negative integer (one of -1, -5, -7, -9, -11, or -12). In the latter case, $|LAW|$ is a flag that specifies the secondary distribution law, LF , defined in File 5, which is used to define the pfns. Next will be a TAB1 record for $P(\nu=2)$. The evaluator now has the choice of defining two spectra, each governed by their own LAW , or a single pfns. The LIP parameter is used to distinguish between these options. When $LIP=1$ there will be ν sets of energy-dependent spectra defined, when $LIP=0$ there is a single energy-dependent set of spectra defined that the evaluator judges to be appropriate for each of the ν neutrons. The sequence of a $P(\nu)$ TAB1 function followed by a LIP and LAW dependent pfns structure continues until $P(\nu=\nu_{\max})$, where ν_{\max} is an evaluator determined integer, and the associated spectra are defined.

The evaluator is still required to provide the average prompt ν in $MF=1/MT=456$ and the average prompt fission neutron spectrum in $MF=5/MT=18$ or $MF=6/MT=18$. In the latter case the $MF=6/MT=18$ HEAD record $L1=JP$ flag must also be set to one of 0, 1 or 2 per the JP definition given in Section 6.2.