A New MCNPX PTRAC Coincidence Capture File Capability: A Tool for Neutron Detector Design - 11432

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Abstract

The existing Monte Carlo N-Particle (MCNPX) particle tracking (PTRAC) coincidence capture file allows a full list of neutron capture events to be recorded in any simulated detection medium. The originating event history number (e.g. spontaneous fission events), capture time, location and source particle number are tracked and output to file for post-processing. We have developed a new MCNPX PTRAC coincidence capture file capability to aid detector design studies. New features include the ability to track the nuclides that emitted the detected neutrons as well as induced fission chains in mixed samples before detection (both generation number and nuclide that underwent induced fission). Here, the power of this tool is demonstrated using a detector design developed for the non-destructive assay (NDA) of spent nuclear fuel. Individual capture time distributions have been generated for neutrons originating from Curium-244 source spontaneous fission events and induced fission events in fissile nuclides of interest: namely Plutonium-239, Plutonium-241, and Uranium-235. Through this capability, a full picture for the attribution of neutron capture events in the detector can be simulated.

Introduction

Some features of the multi-particle transport code MCNPX [1] that can be used for neutron coincidence and multiplicity detector simulation are described by Swinhoe, *et al*. [2]. One feature, discussed here, is the ability to tally neutron capture events and create a PTRAC file which lists the time of a given neutron capture event relative to the start of the history (e.g. source spontaneous fission event). These files can be post-processed by an auxiliary code, for example, to generate a pulse train file by overlaying the real event rate (e.g. source spontaneous fission rate).

The rationale of this paper is to both inform the non-destructive assay (NDA) instrument design community about the latest status of the MCNPX PTRAC coincidence capture file capability, and demonstrate the power of this capability using one example of safeguards neutron instrumentation design. The previous PTRAC coincidence capture file capability in MCNPX has been extended to include fission nuclide identification (by ZAID i.e. a nuclear data table identifier generally containing the atomic number Z, mass number A, and library specifier ID) which is now available in MCNPX 2.7D [3]. The extended capability to distinguish the nuclides from which captured neutrons originated is a contribution to the field of modeling neutron coincidence and multiplicity detectors and enables a detailed analysis of the isotopic contributions to a detected signal. This paper will describe how to use this new feature and interpret the extended PTRAC file format.

Tallying Neutron Capture Events in MCNPX

A neutron capture tally must be specified in order to use the PTRAC capability. Neutron capture in any detection medium may be simulated by specifying the `FT8` capture tally in the MCNPX input deck. The `FT8 CAP` option converts the pulse-height `F8` tally to a neutron capture tally. The `FT8` capture tally scores the number of captured neutrons in specified combinations of nuclides at the end of each history. The following two lines in the MCNPX input deck can be used to specify the cell and nuclide in which capture events are tallied. In this example, ^{3}He (ZAID = 2003) neutron captures and moments are tallied in cell #4 of the MCNPX geometry which may represent, for example, a ^{3}He gas-filled proportional counter:

```
F8:N 4

FT8 CAP 2003
```

The use of time gating in the `FT8 CAP` tally, to set the duration of the pre-delay and coincidence gate width, is an optional feature useful for the simulation of neutron coincidence and multiplicity detectors. This allows the simulation of a “shift register” tally. The output of this tally can be used to calculate all of the multiplicity counting rates in neutron detectors up to any moment of the multiplicity distribution (e.g. singles, doubles, triples, quads etc.) [2]. This feature is described in the MCNPX Version 2.5.0. Extensions document [1]. Note that coincidence counting of capture multiplicities and moments requires analog capture (with no variance reduction) in the MCNPX input deck: `CUT:N 2J 0 0`. Fission multiplicity is also required: `PHYS:N J 100 3J -1`.

MCNPX PTRAC Capture File for Coincidence Counting

A PTRAC file may be generated which lists the time of a given neutron capture event relative to the start of the history (e.g. source spontaneous fission event). A PTRAC file is generated by specifying the following line in the MCNPX input deck:

```
PTRAC EVENT = CAP FILE = ASC
```

Either an ASCII (text) file (`FILE = ASC`) or binary file (`FILE = BIN`) may be created. The default is a binary file.

Previous Capability (MCNPX 2.7C): PTRAC Capture File for Coincidence Counting

Previous Format

The previous PTRAC capability is described in the MCNPX Version 2.5.0 Extensions document [1]. The PTRAC capture file for coincidence counting lists neutron events captured in a given cell of the MCNPX geometry and provides the capability of identifying whether these neutrons originated from an induced fission (via negative flags in the cell column). The previous PTRAC capture file for coincidence counting may be written to an ASCII file with entries on each line in the following format:

```
NPS   Time  Cell  Source
```

Where `NPS` = the particle history number

`Time` = the time (in shakes, 10^{-8} s) from source event to analog capture in any FT8 capture tally

`Cell` = the cell in which analog capture occurred, and

`Source` = the source particle number of a given history. If a source can have multiple source particles, as in the case of spontaneous fission, then this would be the multiple source number e.g. source particle number listed as 4, for a spontaneous fission event of multiplicity 4.

Captured neutrons originating from induced fission events are flagged with a negative cell number.

Example 1: Previous PTRAC File

```
NPS   Time    Cell  Source

 1     4.5e01  22     4
 1     0.0e00   0     3
 1     2.6e02 –22     2
 1     3.5e02 –22     2
 1     1.5e00  23     2
 1     0.0e00   0     1
```

The above extract is taken from an example of the previous ASCII PTRAC file [1]. Example 1 shows that source history 1 (NPS = 1) produced four spontaneous fission neutrons (4, 3, 2, 1 in the Source column). Source neutron 4 was captured in Cell 22 at Time = 45 shakes after the source spontaneous fission. Source neutron 3 was not captured, as indicated by zeros in the Time and Cell columns. Source neutron 2 first caused induced fission, as indicated by the negative flag in the Cell column. Two neutrons from induced fission due to source neutron 2 were captured in Cell 22 at Time = 260 shakes and Time = 350 shakes. Source neutron 2 also led to a capture in Cell 23 at Time = 15 shakes; this neutron must have been a branch (e.g. after an (n, 2n) reaction) that did not undergo fission. Source neutron 1 was not captured.

New (Extended) Capability (MCNPX 2.7D): PTRAC Capture File for Coincidence Counting with Fission Nuclide Identification by ZAID

New Format

A new capability has been developed for MCNPX to distinguish the nuclide from which both spontaneous and induced fission events originated by ZAID. This new capability greatly benefits neutron detector design applications such as the NDA of nuclear material by allowing greater access to the physics. Five additional columns have been added to the PTRAC capture file for coincidence counting with entries on each line in the following format:

```
NPS   Time  Cell  Source ZAIDs ZAID1 ZAID2 ZAID3 ZAIDf
```

Where `NPS` = the particle history number

`Time` = the time (in shakes, 10^{-8} s) from source event to analog capture in any FT8 capture tally

`Cell` = the cell in which analog capture occurred,

`Source` = the source particle number of a given history. If a source can have multiple source particles, as in the case of spontaneous fission, then this would be the multiple source number e.g. source particle number listed as 4, for a spontaneous fission event of multiplicity 4.

`ZAIDs` = Lists the ZAID of the source spontaneous fission nuclide, if there is one, from which source neutron events were launched (e.g. ZAID = 94240 for ^{240}Pu). For radioactive decay sources (e.g. Pu-Be) or neutron generator, etc., “0” is given in the column.

`ZAID1` = Lists the ZAID of the first induced fission nuclide (if any) in the reaction chain i.e. first, induced fission generation; which eventually led to neutron capture.

`ZAID2` = Lists the ZAID of the second induced fission nuclide (if any) in the reaction chain i.e. second induced fission generation; which eventually led to neutron capture.

`ZAID3` = Lists the ZAID of the third induced fission nuclide (if any) in the reaction chain i.e. third induced fission generation; which eventually led to neutron capture.

[Note: columns `ZAID1`, `ZAID2`, and `ZAID3` list neutron production from induced fission events only. “0” is given for other neutron production mechanisms, or if no induced fission reaction occurred.]

`ZAIDf` = Lists the ZAID of the last (spontaneous or induced) fission nuclide prior to neutron capture i.e. the spontaneous or induced fission nuclide that directly produced the captured neutron.

The cell number is flagged negative if an (n, xn) event follows the last source or induced fission event before the neutron capture. This indicates that the captured neutron was from an (n, xn) reaction rather than from (n, f). This is a different meaning than the negative cell flag for MCNPX 2.7C i.e. neutrons from induced fission are no longer be flagged as a negative cell number, since the fission ZAID allows the user to identify neutrons originating from spontaneous fission and replaces the need for this function.

Example 2: New PTRAC File

NPS	Time	Cell	Source	ZAIDs	ZAID1	ZAID2	ZAID3	ZAIDf
477	5.27053E+03	-1005	2	96244	94239	0	0	94239
479	9.70570E+02	1005	2	96244	0	0	0	96244
486	8.56686E+03	1005	3	96244	94239	92238	0	92238
487	2.79425E+02	1005	2	96244	92238	0	0	92238
501	2.49817E+03	1005	1	96244	0	0	0	96244
505	1.18081E+03	1005	1	96244	0	0	0	96244
507	4.71189E+02	1005	4	96244	94239	0	0	94239
509	5.29588E+03	1005	1	96244	0	0	0	96244
517	3.98797E+02	1005	2	96244	0	0	0	96244
519	2.67331E+03	1005	1	96244	0	0	0	96244
525	1.84132E+03	1005	1	96244	0	0	0	96244
530	3.36479E+03	1005	2	96244	0	0	0	96244
546	4.08109E+02	1005	3	96244	0	0	0	96244
548	9.35168E+03	1005	5	96244	94239	92235	92235	94239
548	5.68849E+03	1005	5	96244	94239	92235	92235	94239
548	5.65753E+03	1005	5	96244	94239	92235	92235	94239

The above extract is taken from an example of the new ASCII PTRAC file for neutron captures in ^{3}He from the simulated measurement of a spent nuclear fuel assembly. The spent nuclear fuel assembly was initially enriched to 4 wt % ^{235}U, achieved a burnup of 45 GWd/tU over 3 cycles, and was cooled for 5 years following discharge from reactor before measurement in borated water. Example 2 shows the source history 477 (NPS = 477) was ^{244}Cm spontaneous fission (96244 in the ZAIDs column). Source neutron 2 (2 in the Source column) induced the fission of ^{239}Pu, as indicated by 94239 in the ZAID1 column. An (n, 2n) reaction occurred following this induced fission and prior to the neutron capture event, as indicated by the negative Cell number. One neutron from the (n, 2n) reaction was captured in Cell 1005 at Time = 5270.5 shakes. Note that this new PTRAC capture file gives no information regarding the multiplicity of the spontaneous fission event i.e. how many neutrons were produced. This information can be obtained from the MCNPX event log.

Source history 479 (NPS = 479) was ^{244}Cm spontaneous fission (96244 in the ZAIDs column). Source neutron 2 (2 in the Source column) did not induce further fission, as indicated by zeros in the ZAID1, ZAID2 and ZAID3 columns. Source neutron 2 was captured directly from the spontaneous fission event in ^{244}Cm, as indicated by 96244 in the ZAIDf column. Source neutron 2 was captured in Cell 1005 (in this case corresponding to the sum of the ^{3}He tubes in the detection system) at Time = 970.6 shakes.

Source history 486 (NPS = 486) was another ^{244}Cm spontaneous fission (96244 in the ZAIDs column). Source neutron 3 induced the fission of ^{239}Pu, as indicated by 94239 in the ZAID1 column. A ^{239}Pu neutron then induced the fission of ^{238}U, as indicated by 92238 in the ZAID2 column. A neutron was then captured directly from the induced fission of ^{238}U, as indicated by zero in the ZAID3 column and 92238 in the ZAIDf column. The ^{238}U fission neutron was captured in Cell 1005 at Time = 8566.8 shakes.

The same logic can be applied to the interpretation of the rest of the file. More histories than those discussed are provided to illustrate the variety of fission chains that may occur and thus the level of detail of the event histories that can be extracted using this new feature.

Improvements to File Size

Previously, if a neutron was not captured this was indicated by zeros in the Time and Cell columns, as shown in Example 1. In the new PTRAC file format, output is provided only for events resulting in capture in the `FT8 CAP` tally, thus null events are no longer recorded. This greatly reduces the size of the PTRAC file and thus reduces the run time in post-processing software. The multiplicity information that could be gained from the Source column is given as a histogram in the MCNPX output file.

Backwards Compatibility

The previous format from MCNPX 2.7C may be obtained (except for the negative fission flag) by setting the 21st `DBCN` card entry non-zero to cause MCNPX 2.7D to track MCNPX 2.7C. This is detailed in the MCNPX Extensions Version 2.7D document [3].

Application

We take for example the design of neutron instrumentation for the NDA of spent nuclear fuel. This is a departure from the traditional applications of neutron coincidence and multiplicity counting in the sense that the system is highly multiplying. The new PTRAC feature was initially developed with this application in mind but can benefit neutron detector design in general.

Post-Processing the New PTRAC Capture File for Coincidence Counting

Example 3: Isotopic Capture Time Distributions

By implementation of the new PTRAC capability, it is our goal to be able to distinguish between neutron capture events that are produced by the following:

(1) The source (e.g. spontaneous fission, neutron generator, etc)

(2) Induced fission events immediately preceding the capture event

(3) Neutrons that are not directly produced from the source, but are produced via other reaction mechanisms e.g. (n, 2n) reactions, excluding induced fission

To ascertain the contribution from #1 to neutron capture events in the detector, events can be filtered that have non-zero entries in the ZAIDs column and zero entries in the ZAID1, ZAID2 and ZAID3 induced fission columns. To ascertain the contribution from #2, events can be filtered that have non-zero entries in the ZAIDf last fission column. To ascertain the contribution from #3, events can be filtered that have negative entries in the Cell column.

For spent nuclear fuel measurements for the quantification of fissile mass, we are also interested in the contribution of the separate fissile nuclides to the detected neutron signal. Figure 1 illustrates the isotopic capture time distributions derived from post-processing of the new PTRAC file. Results are presented for the simulated measurement of a spent nuclear fuel assembly, as in Example 2. The spent nuclear fuel assembly was initially enriched to 4 wt % ^{235}U, achieved a burnup of 45 GWd/tU over 3 cycles, and was cooled for 5 years following discharge from reactor before measurement in borated water.

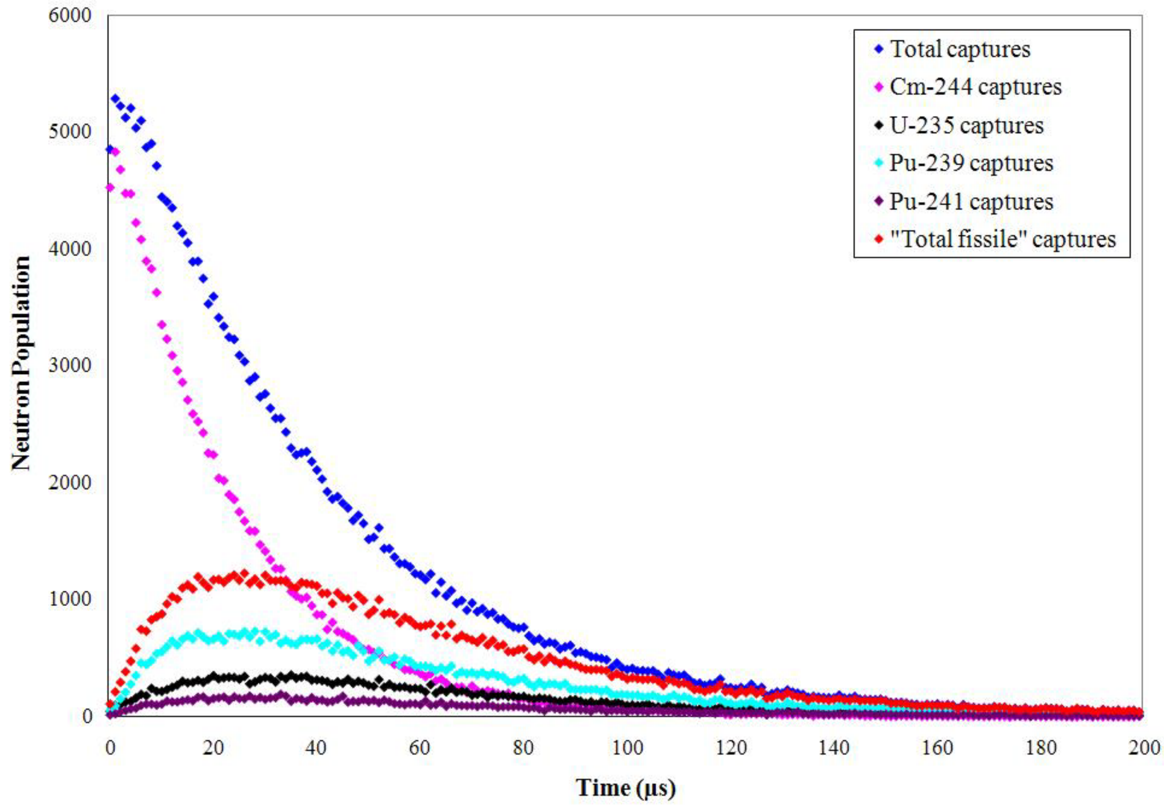

Figure 1. Neutron capture time histograms for events originated from ^{244}Cm spontaneous fission, ^{235}U induced fission, ^{239}Pu induced fission and ^{241}Pu induced fission. The total capture time histogram is presented for the sum of all neutron capture events in the ^{3}He detector, as could be obtained with the previous PTRAC file. The total fissile capture time histogram is presented for the sum of the fissile contributions.

Example 4: Quantitative Information as an Indicator of Detector Performance

Post-processing the PTRAC file enables a full attribution history of neutron capture events in a detection medium to be obtained (including fission chains). Table 1 is an extract from the new PTRAC output file. This example shows the ^{3}He neutron capture attribution histories obtained from the measurement of a spent nuclear fuel assembly initially enriched to 4 wt % ^{235}U, with 45 GWd/tU burnup (high burnup) and 5 years cooling since discharge from reactor. The assembly was measured in borated water. A measurement was performed with a Cadmium (Cd) liner surrounding the fuel assembly to absorb thermal neutrons, and repeated with the Cd liner removed. Table 1 presents results for these two measurements of the fuel assembly with and without a Cd liner surrounding the fuel assembly. The removal of the Cd liner allows the reflected thermal component of the neutron flux to return to the assembly and interrogate the assembly. A greater number of captures are observed in the detector in the case without the Cd liner since the returning thermal flux leads to greater induced fission in the fuel assembly and therefore a greater number of counts in the detector. The left hand side of the table corresponds to the measurement with Cd, and the right hand side corresponds to the measurement without Cd. The first six lines of data correspond to the total neutrons that were captured in the detector directly from spontaneous fission events i.e. neutron source events in the spent fuel assembly. Neutrons were captured mainly due to ^{244}Cm and ^{240}Pu spontaneous fission events from the source generation. The next six lines of data correspond to the total neutrons that were captured following an induced fission event during the first generation of fission in the chain. The final six lines of data in Table 1 correspond to the total neutrons that were captured in the detector following an induced fission event in the last generation of fission directly before neutron capture. Neutron capture events that originated from induced fission in the fissile nuclides of interest (^{235}U, ^{239}Pu, and ^{241}Pu) are highlighted. It can be seen that the first and last generation are equivalent within statistical uncertainty.

With Cadmium			**Without Cadmium**		
Source Generation	Total Neutron Captures (N)	±	Source Generation	Total Neutron Captures	±
^{244}Cm	218280	467	^{244}Cm	242586	493
^{238}U	1	1	^{238}U	4	2
^{235}U	0	0	^{235}U	0	0
^{239}Pu	1	1	^{239}Pu	0	0
^{241}Pu	0	0	^{241}Pu	0	0
^{240}Pu	559	24	^{240}Pu	574	24
First Generation	Total Neutron Captures	±	First Generation	Total Neutron Captures	±
^{244}Cm	6	2	^{244}Cm	8	3
^{238}U	9938	100	^{238}U	11153	106
^{235}U	24386	156	^{235}U	33158	182
^{239}Pu	39639	199	^{239}Pu	52378	229
^{241}Pu	10191	101	^{241}Pu	13489	116
^{240}Pu	158	13	^{240}Pu	202	14
Last Generation	Total Neutron Captures	±	Last Generation	Total Neutron Captures	±
^{244}Cm	133933	366	^{244}Cm	132145	364
^{238}U	9722	99	^{238}U	10495	102
^{235}U	24402	156	^{235}U	33949	184
^{239}Pu	39790	199	^{239}Pu	52360	229
^{241}Pu	10246	101	^{241}Pu	13375	116
^{240}Pu	480	22	^{240}Pu	535	23

Table 1. Attribution histories of neutron capture events in the ^{3}He detectors. Data is shown for the spent nuclear fuel assembly with 4 wt % initial ^{235}U enrichment, burnup of 45 GWd/tU and 5 years cooling time.

Identification of the initiating event and associated tracking allows sensitivity to various nuclear species to be assessed in-situ with perturbation, since the species compete and interfere which is important. In defining effective fissile mass, for instance, this approach has proven important.

Summary

In summary, we have extended the previous PTRAC coincidence capture file capability to include fission nuclide identification by ZAID. Through this new capability, a full picture for the attribution of neutron capture events in the detector can be simulated. It is a powerful tool for neutron detector design since the isotopic contributions to the detected signal can be studied and quantified. In formatting interpretational and inversion models this is invaluable. In the safeguards context it also allows a new view of diversion and substitution strategies. This new feature is a contribution to the field of simulation of neutron coincidence and multiplicity detectors.

Recommendations for Future Work

Future extensions to the PTRAC capture file for coincidence counting may include writing to the file the number of the cell in which the fission events occurred. This extension would enable a full geometry-based description of the attribution of neutron capture events in the detector.

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References

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