LA-UR- 11-02644

Approved for public release; distribution is unlimited.

Title: MCNPX270 LLNL Fission Model

Author(s): Gregg W. McKinney
John S. Hendricks
Jerome M. Verbeke
Chris Hagmann
Doug Wright

Intended for: WWW

Los Alamos NATIONAL LABORATORY EST. 1943

MCNPX270 LLNL Fission Model

Gregg W. McKinney
John S. Hendricks
Los Alamos National Laboratory

Jerome M. Verbeke
Chris Hagmann
Doug Wright
Lawrence Livermore National Laboratory

April 18, 2011

Executive Summary

The LLNL fission model is an available option in MCNPX version 2.7.0. It was developed at Lawrence Livermore National Laboratory and we have collaborated to implement it in MCNPX. We report here our observations and assessments of the LLNL fission model in MCNPX relative to alternative treatments in MCNPX.

The LLNL fission model is the only way for MCNPX to produce correlated prompt gammas from prompt fission, delayed fission, spontaneous fission, and photofission. The LLNL fission model also produces fission neutrons and gammas with the correct multiplicities for induced fission, spontaneous fission, and photofission. The exact modeling of the neutron- and photon-induced fission process enables coincidence counting of fission neutrons and gammas.

Comparisons were made to the MCNPX default fission capability which uses ACE table physics and the default *fmult* fission multiplicity capability. Also, several corrections were made in MCNPX27E and these are described.

Introduction

The LLNL fission model was put into MCNPX27C as an undocumented feature and it became an advertised feature in MCNPX27D (v27D). The v27D LLNL fission model (dated March 15, 2010) has been replaced in MCNPX27E (v27E) with LLNL fission model version v1.8, (dated 5/11/2010) provided by Douglas Wright and Jerome Verbeke, LLNL, received October 18, 2010. The C++ code is significantly larger but there are no tracking changes.

The LLNL fission model is documented in UCRL-AR-228518 [1]. It is a C++ general-purpose and extensible software library to accurately simulate neutron and gamma-ray

[1] Jerome M. Verbeke, Chris Hagmann, Doug Wright, "Simulation of Neutron and Gamma Ray Emission from Fission and Photofission," *Lawrence Livermore National Laboratory report* UCRL-AR-228518 (May 11, 2010) http://nuclear.llnl.gov/simulation/

distributions from fission reactions (spontaneous, neutron induced and photon induced). This library provides an event-by-event list of neutrons and gamma rays for a specific fission reaction and can be used in conjunction with a Monte Carlo transport code. The parent code provides the reaction cross-section information, whereas the LLNL library samples the neutron and gamma multiplicity and energy distributions. This library is data-driven and incorporates all available multiplicity measurements found in the literature. Empirical models are employed whenever multiplicity data are not available. Essentially no data are available for the correlations between the neutrons and gammas, so the LLNL model samples these distributions independently. By default, the LLNL model effectively scales the multiplicity data to match the average multiplicity value (ν) found in external evaluated data libraries. At present the gammas and neutrons are emitted isotropically. The LLNL model has been incorporated into Geant4 and is now in MCNPX. The standalone version of the software library can be downloaded from http://nuclear.llnl.gov/simulation .

Induced Fission

The LLNL fission model treats induced fission of the following nuclides: 225Ac, 226Ac, 227Ac, 227Th, 228Th, 229Th, 230Th, 231Th, 232Th, 233Th, 234Th, 229Pa, 230Pa, 231Pa, 232Pa, 233Pa, 230U, 231U, 232U, 233U, 234U, 235U, 236U, 237U, 238U, 240U, 241U, 234Np, 235Np, 236Np, 237Np, 238Np, 239Np, 238Pu, 239Pu, 240Pu, 241Pu, 242Pu, 243Pu, 244Pu, 246Pu, 240Am, 241Am, 242Am, 243Am, 244Am, 240Cm, 241Cm, 242Cm, 243Cm, 244Cm, 245Cm, 246Cm, 247Cm, 248Cm, 249Cm, 250Cm, 245Bk, 246Bk, 247Bk, 248Bk, 249Bk, 250Bk, 246Cf, 248Cf, 249Cf, 250Cf, 251Cf, 252Cf, and 253Cf.

Note that the LLNL fission model is the only MCNPX setting for which gamma-rays are sampled in analog mode for fission reactions. Thus to get fission gammas, one must set *fism = 5* on the PHYS:N card as follows:

PHYS:N 3J -1 J 5

Note that the 4th entry, *dnb = -1,* is the default of analog delayed neutrons so the following also works:

PHYS:N 5J 5

Photons produced from the LLNL induced-fission model are emitted at the time of the fission interaction (whether neutron or photon induced.) Delayed gammas from fission are unaccounted by the LLNL fission model but can be provided via the CINDER code and its database (ACT card or 6th PHYS:P entry.)

Most significantly, gamma production from fission is now correlated with fission reactions.

Spontaneous Fission

MCNPX has had spontaneous fission sources with multiplicity for years. This is referred to the *fmult* default treatment. The new LLNL fission model now adds and is the only way to get prompt photons from the spontaneous fission source:

```
MODE  N P              $ run neutrons and photons
PHYS:N  5J  5          $ use LLNL fission model
SDEF  par = sf         or        SDEF  par = -sf
```

As with the default treatment, all spontaneous fission source neutrons and photons are emitted isotropically and at *time = 0* or whatever time is specified on the SDEF source definition.

The LLNL fission model treats spontaneous fission for 232Th, 232U, 233U, 234U, 235U, 236U, 238U, 237Np, 238Pu, 239Pu, 240Pu, 241Pu, 242Pu, 241Am, 242Cm, 244Cm, 249Bk, and 252Cf. For other nuclides the default *fmult* spontaneous fission model is used. Prompt fission gammas will only be emitted from the nuclides using the LLNL fission model. Both LLNL and *fmult* use the same *fmult* spontaneous fission yields.

Photofission

To enable the analog production of photons and neutrons from photofission reactions, the 7th entry of the PHYS:P card should be set to 1:

```
phys:p 3j ±1 2j 1
```

Note that the 4th entry, *ispn = ±1,* is not the default and must be also be set to turn on photonuclear events: *ispn = -1* for analog photonuclear and *ispn = 1* for biased photonuclear which produces one photonuclear event per photon collision. The LLNL photofission has three advantages over the default ACE treatment: (1) prompt photofission gammas are produced; (2) photofission neutrons and gammas are correlated; and (3) the correct multiplicity of photofission neutrons and gammas is used rather than being the number just above or below the average multiplicity value.

When the 7th entry, *illnlphfis = 1,* is set, photofission secondaries are sampled only when a photofission event occurs; the remaining photonuclear reactions continue to use the default ACE table photon physics. The LLNL photofission model requires the ENDF/B-VII photonuclear data library, ENDF7U. Photofission is only available for the following 39 isotopes 232Th, 233Th, 234Th, 234Pa, 233U, 234U, 235U, 236U, 237U, 238U, 239U, 240U, 236Np, 237Np, 238Np, 239Np, 237Pu, 238Pu, 239Pu, 240Pu, 241Pu, 242Pu, 243Pu, 244Pu, 242Am, 243Am, 244Am, 243Cm, 244Cm, 245Cm, 246Cm, 247Cm, 248Cm, 249Cm, 250Bk, 250Cf, 251Cf, 252Cf, and 253Cf.

MCNPX27E Corrections

Notification of LLNL fission model use

MCNPX27D gave no indication in the OUTP file whether or not the LLNL fission model is used.

- The OUTP file now indicates if LLNL fission multiplicity is used:
  Using LLNL fission multiplicity model

- The OUTP file now indicates if LLNL photonuclear is used:
  Using LLNL Photofission Model

This notification is particularly useful when the LLNL photofission model is disabled by not turning on photonuclear physics.

New fatal error for improper fission multiplicity use

- It is a FATAL error if LLNL fission multiplicity is used with delayed neutron biasing which gives wrong answers and sometimes loses particles:

```
fatal error.  LLNL fission multiplicity requires analog delayed neutrons.
```

Figures 1 and 2 illustrate the erroneous answers with delayed neutron biasing. DNB indicates delayed neutron biasing is on (*dnb > 0* on PHYS:N card 4th entry.) Comparisons are between the default ACE library treatment of fission and the LLNL fission model (*fsim = 1 or 5* on PHYS:N 6th entry.) Figure 1 shows that DNB has no effect for the prompt spectra (*time < 1e-4 sec)* and both ACE and LLNL give similar results. Figure 2 shows that analog ACE and LLNL give similar results, but delayed neutron bias changes the LLNL spectra but not the ACE spectra. Thus LLNL fails with DNB. The input for this problem is *Input 1* in the Appendix.

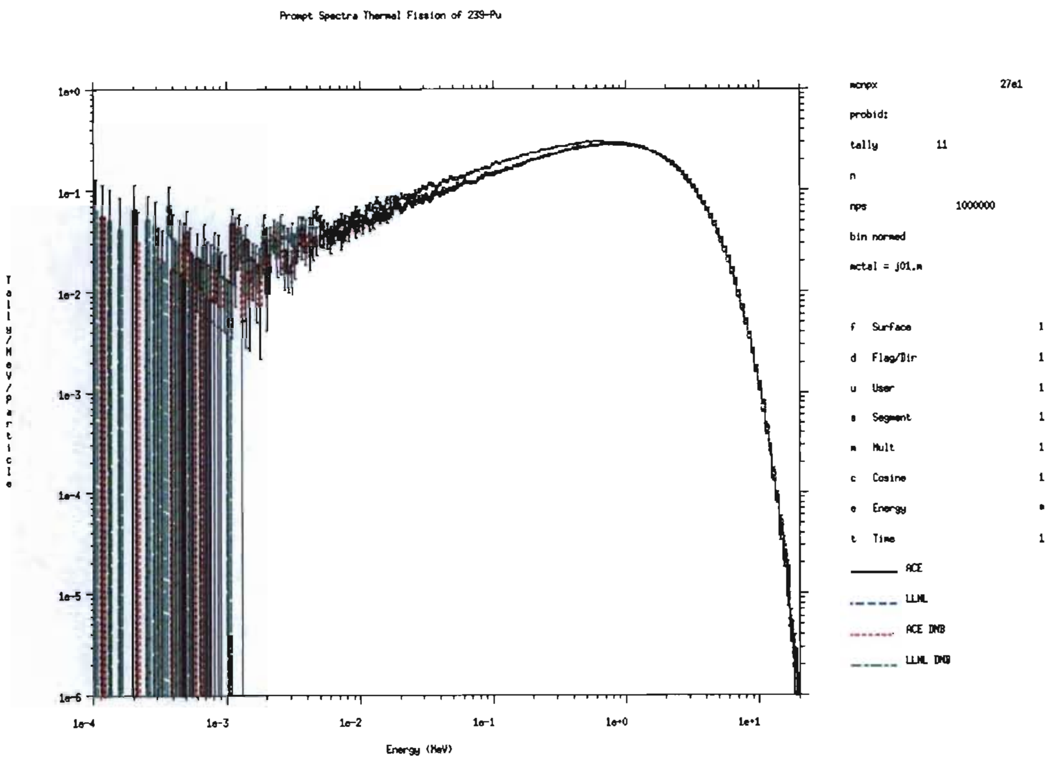

Figure 1. Prompt spectra thermal fission, ACE vs LLNL, with and without DNB

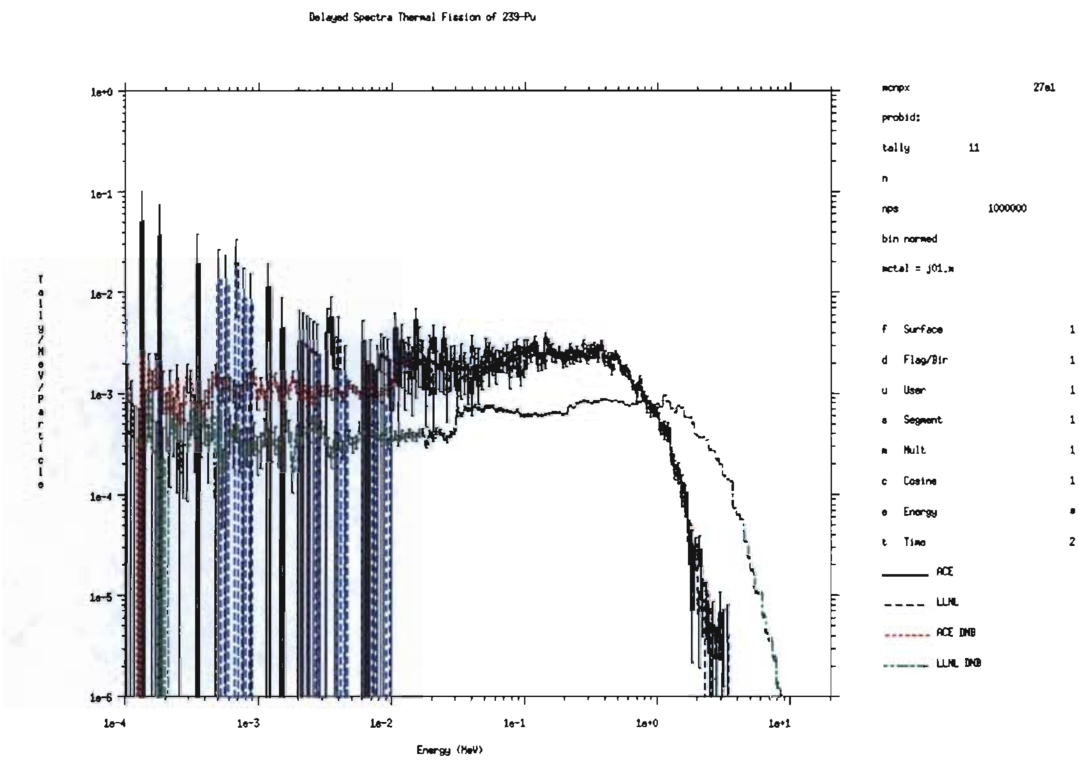

Figure 2. Delayed spectra thermal fission, ACE vs LLNL, with and without DNB

Treatment of non-LLNL spontaneous fission nuclides

When spontaneous fission sources are requested for nuclides not in the LLNL spontaneous fission model, MCNPX27D does not crash, but it stops, leaves the OUTP file incomplete, the RUNTPE not updated, the MCTAL file unwritten, etc. The failure mode is the error message

"Fission Error in Function SmpSpWatt, Severity=6 :"

MCNPX27E has been upgraded so that when the LLNL fission model is requested (PHYS:N 3J -1 J 5) for a nuclide not in the LLNL spontaneous fission library, then the default *fmult* treatment is used with the following run-time warning at the first occurance:

```
warning.  "using fmult, not LLNL, for spontaneous fission of ZA."
 nps =        993      nrn =             102      ZA =94236
```

Note that the spontaneous fission gammas are not produced for the non-LLNL spontaneous fission nuclides.

Note that the *fmult* treatment is substituted for the LLNL model for nuclides disallowed by LLNL, subroutine FISSNU would get called with the LLNL flag set, *ifisnu = 5*, and cause errors. Subroutine FISSNU has been corrected.

Removal of warning error for improper photonuclear use

The following MCNPX27D warning message has been removed:

```
warning.    LLNL photofission inactive when ispn!=-1 on PHYS:P card.
```

<u>*Comparison of LLNL to ACE / fmult*</u>

Fission multiplicity

The neutron energy and time spectra for neutron induced fission are close for both ACE and LLNL. Calculations for both incident thermal (2.53e-8 MeV) neutrons on 239-Pu and incident 2-MeV neutrons on 235-U were examined. (See *Input 2* in the Appendix.) The total fission multiplicity (number of fission neutrons per fission) is nearly the same:

	ACE	LLNL
Thermal 239-Pu nubar	2.87741	2.87972
2-Mev 235-U nubar	2.65136	2.64906

The differences are .08% with a .05% - .1% error. The spectra of neutrons looks the same although the average energy of fission neutrons produced is 5% lower for LLNL.

Although the total number of fission neutrons produced is about the same for ACE and LLNL, the production of 0,1, 2, 3, … neutrons from fission – that is, the individual multiplicities - are about 5% different. ACE had twice as many fissions with no fission neutrons compared to LLNL for 239-Pu and 50% more for 235-U. These differences were to be expected, because the LLNL fission library samples measured multiplicity distributions directly, rather than ones fitted by Gaussians. Gaussian distributions often poorly approximate the tails of measured multiplicity distributions. The factorial moments are also up to 5% different between ACE and LLNL, which is outside the 0.5% statistical errors.

The LLNL documentation cites all the same sources of fission multiplicity data that were used in the MCNPX ACE fission multiplicity treatment and a number of additional references as well. Thus the reasonable agreement is expected.

Neutron-induced photons

The LLNL fission multiplicity model (PHYS:N 3J -1 J 5 as above and MODE N P) produces neutron-induced photons correlated with fission events. Gamma production from neutron-induced fission is significantly different between ACE and LLNL as shown in Figures 3 and 4. From the summary table:

	------- 239-Pu ---------		-------- 235-U ---------	
	ACE	LLNL	ACE	LLNL
Photon tracks from neutrons	2000000	5465251	1000000	2239147
Photon weight from neutrons	6.6648	6.1619	2.0732	3.3124
Photon energy from neutrons	6.6315	6.3619	1.7437	2.8552

LLNL ran 30% slower than ACE. The ACE calculations tracked exactly between MCNPX27C and MCNPX27E. For the ACE fission treatment the 239-Pu had exactly two photons produced per fission at thermal energy and the 235-U had exactly one photon produced per fission at 2-MeV as seen in the above table (2000000 and 1000000 photon tracks from 1000000 source neutrons.

Use of the LLNL fission model to produce neutron-induced photons does not appear to affect anything other than fission. The same input (*Input 2* in the Appendix) was used with gold and MCNPX27E with the LLNL fission tracked MCNPX27C demonstrating that results are unchanged for non-fissionable nuclides such as gold.

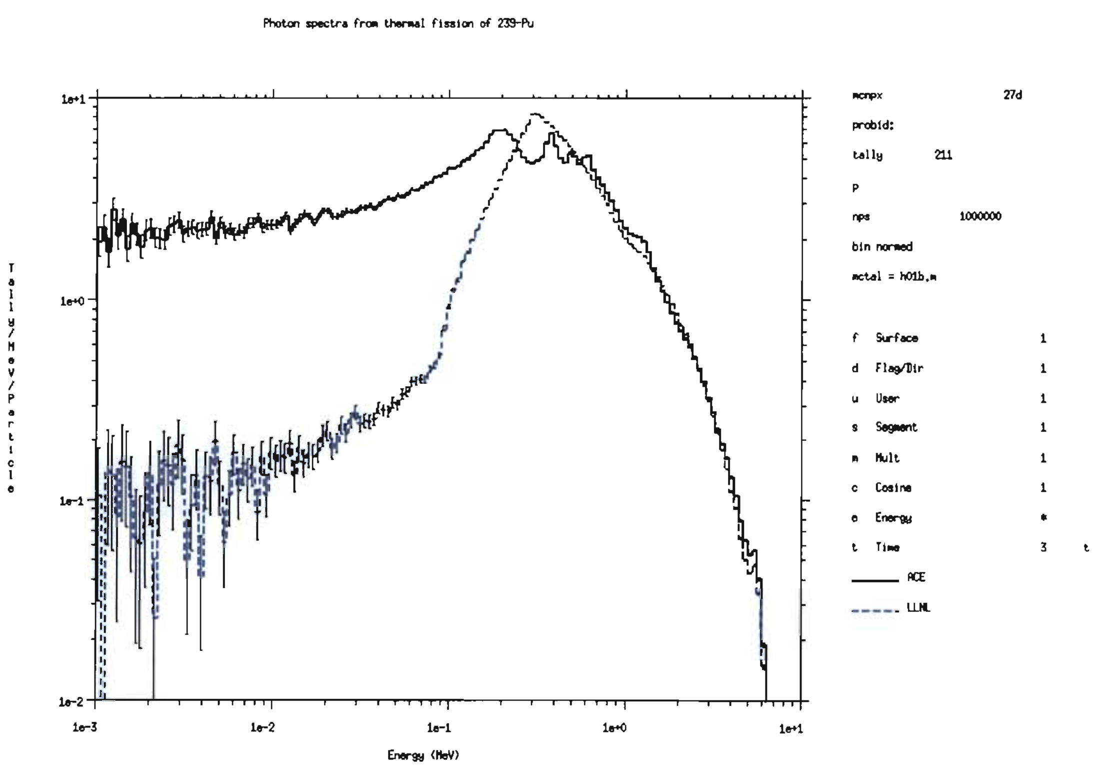

Figure 3. Photon energy spectra of induced gammas from 239-Pu thermal induced fission.

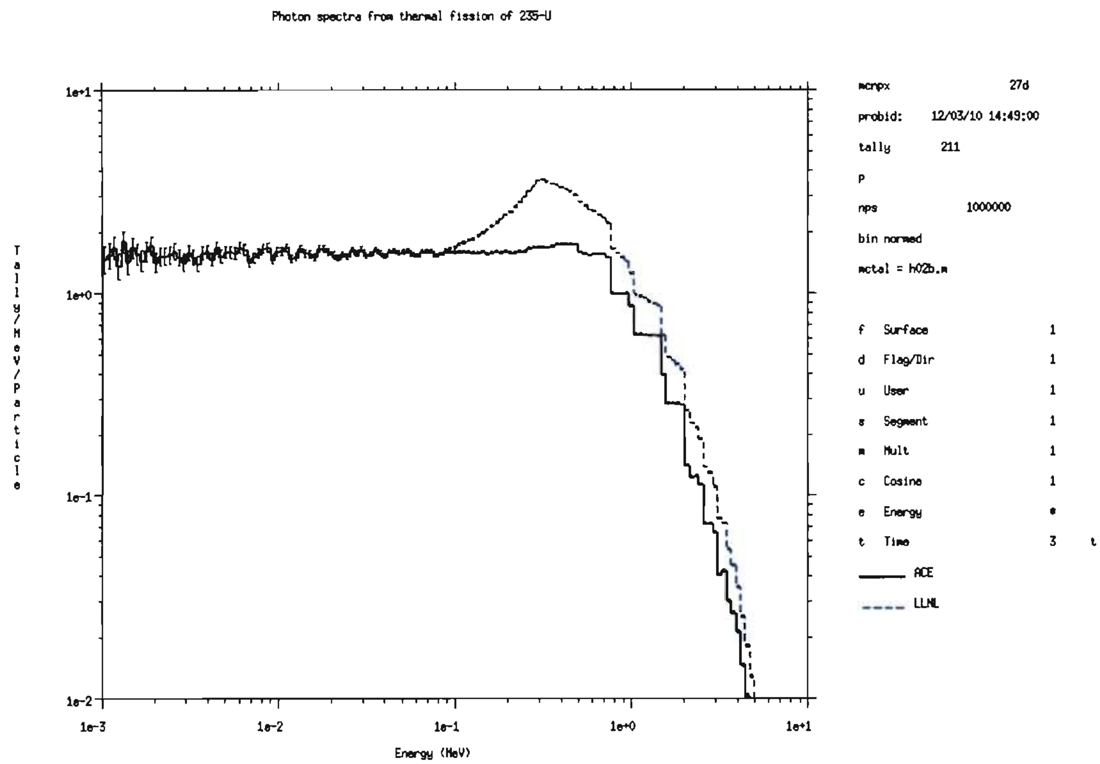

Figure 4. Photon energy spectra of induced gammas from 235-U 2-MeV induced fission.

Spontaneous Fission Source

Spontaneous fission nuclides

The LLNL fission model treats spontaneous fission for 232Th, 232U, 233U, 234U, 235U, 236U, 238U, 237Np, 238Pu, 239Pu, 240Pu, 241Pu, 242Pu, 241Am, 242Cm, 244Cm, 249Bk, and 252Cf. Both spontaneous fission neutrons and prompt photons are produced for these nuclides.

The LLNL fission model fails for 246Cm, 248Cm, 246Cf, 250Cf, 254Cf, 257Fm, and 252No because the Watt parameters are unavailable. Even though the number of spontaneous fission neutrons could be sampled, no energy could be attributed to them, and the LLNL fission library module fails for these 7 nuclides. MCNPX27E has been modified to use the default *fmult* treatment when the LLNL fission module would otherwise fail. In these cases a warning is issued at the first instance that the *fmult treatment* is used for any nuclide.

Yields: The default *fmult* treatment spontaneous fission yield is used for all spontaneous fission events so that the sampling of nuclides in a mixed material is the same regardless of LLNL or *fmult* model.

Spontaneous fission photons

The LLNL fission model is the only MCNP/X method emitting spontaneous fission prompt photons. These are neglected in the MCNPX default *fmult* spontaneous fission source. Figure 5 shows the spontaneous fission photons produced for various nuclides.

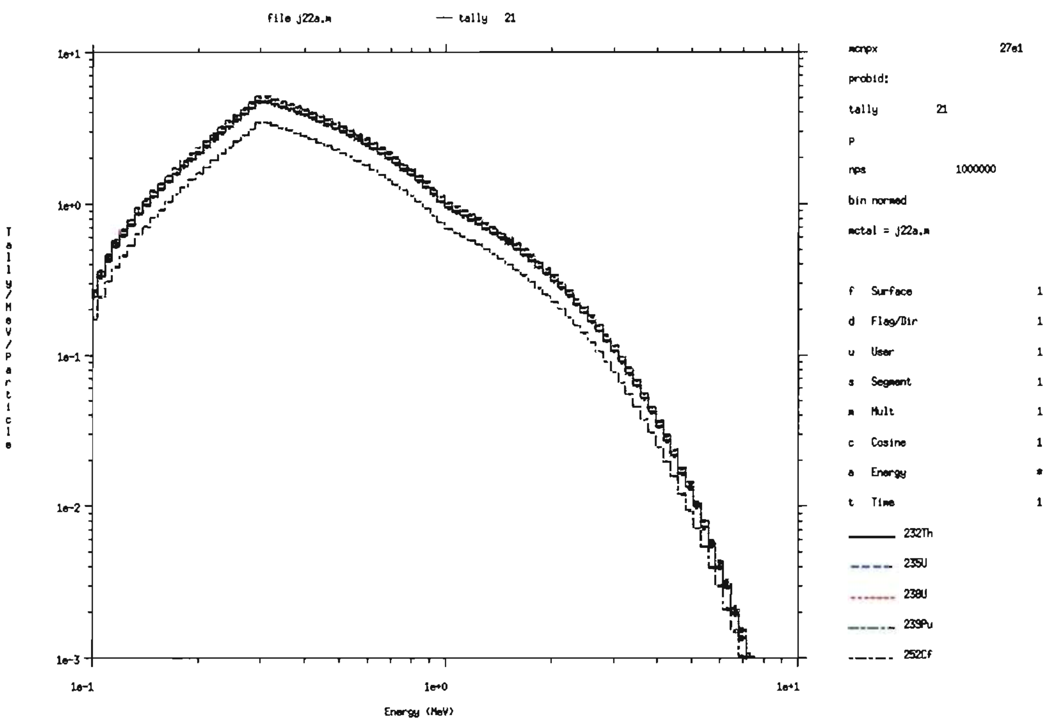

Figure 5. Spontaneous fission photons produced with LLNL spontaneous fission model.

The emission spectra have the same distribution for all nuclides, as shown in Figure 5. The total spontaneous fission prompt photon emission differs by 54% as follows:

Nuclide	Photons
232Th	3.0449E+00
232U	3.4011E+00
233U	3.3648E+00
234U	3.3316E+00
235U	3.3006E+00
236U	3.2717E+00
238U	3.2440E+00

237Np	3.0908E+00
238Pu	2.9331E+00
239Pu	2.9807E+00
240Pu	3.0150E+00
241Pu	2.9547E+00
242Pu	3.0739E+00
241Am	2.3212E+00
242Cm	2.6429E+00
244Cm	2.5748E+00
249Bk	2.2903E+00
252Cf	2.2041E+00

These spontaneous fission photon results were all obtained with *Input 3* in the Appendix with the mode, f21:p. and e21 inputs at the end.

Spontaneous fission neutrons

The spontaneous fission neutron spectra are statistically the same between LLNL and *fmult*. Consequently the heating is the same. The average number of spontaneous fission neutrons, *nu*, is statistically the same for all but 252-Cf where it is 3.77248E+00 0.0003 for 3.75657E+00 0.0003, a 0.42% difference with .03% relative error. The multiplicity distributions and moments are nearly identical for 233U, 238U, 238Pu, 240Pu, 242Pu, 242Cm, and 244Cm. They are statistically different, but similar (within 1%) for 252Cf. But they are quite different for 232Th, 232U, 234U, 235U, 236U, 237Np, 239Pu, 241Pu, 241Am, and 249Bk. The biggest differences are for 239Pu:

<u>*Multiplicities*</u>	LLNL		*fmult*	
	fissions	Fission neutrons	fissions	Fission neutrons
nu = 0	57805	0	80448	0
nu = 1	214797	214797	210640	210640
nu = 2	356797	713594	327371	654742
nu = 3	266637	799911	256968	770904
nu = 4	89619	358476	102006	408024
nu = 5	13422	67110	20412	102060
nu = 6	892	5352	2061	12366
nu = 7	31	217	91	637
nu = 8			3	24

<u>*Moments*</u>	<u>LLNL</u>		<u>*fmult*</u>	
nu	2.15946E+00	0.0005	2.15940E+00	0.0005
nu(nu-1)/2!	1.84267E+00	0.0011	1.94734E+00	0.0012
nu(nu-1)(nu-2)/3!	7.78258E-01	0.0022	9.13685E-01	0.0022
nu(nu-1) .... (nu-3)/4!	1.71194E-01	0.0047	2.38376E-01	0.0045
nu(nu-1) .... (nu-4)/5!	1.94250E-02	0.0125	3.48570E-02	0.0108
nu(nu-1) .... (nu-5)/6!	1.10900E-03	0.0443	2.78200E-03	0.0338
nu(nu-1) .... (nu-6)/7!	3.10000E-05	0.1796	1.15000E-04	0.1463

These spontaneous fission neutron results were all obtained with *Input 3* in the Appendix without the mode, f21:p. and e21 inputs at the end.

Photofission

The LLNL photofission has three advantages over the default ACE treatment:

1. prompt photofission gammas are produced;
2. photofission neutrons and gammas are correlated;
3. the correct multiplicity of photofission neutrons and gammas is used. The number of secondaries is correctly sampled rather than being the number just above or below the average.

The exact modeling of the photofission process enables coincidence counting of photofission neutrons and gammas.

The LLNL photofission model is only available for the following 39 isotopes 232Th, 233Th, 234Th, 234Pa, 233U, 234U, 235U, 236U, 237U, 238U, 239U, 240U, 236Np, 237Np, 238Np, 239Np, 237Pu, 238Pu, 239Pu, 240Pu, 241Pu, 242Pu, 243Pu, 244Pu, 242Am, 243Am, 244Am, 243Cm, 244Cm, 245Cm, 246Cm, 247Cm, 248Cm, 249Cm, 250Bk, 250Cf, 251Cf, 252Cf, and 253Cf. Further, the ENDF/B-VII photonuclear data library, ENDF7U, is required.

When the 7th entry, *illnlphfis = 1,* is set, photofission secondaries are sampled only when a photofission event occurs, and are not sampled when other photonuclear reactions occur. These other photonuclear reactions are not omitted, but treated with the default ACE table data method.

The LLNL photonuclear physics requires MCNPX photonuclear reactions be turned on.

PHYS:P 3j *ispn* 2j 1

The 4th entry, *ispn = -1,* is not the default and must be set to turn on analog photonuclear (*ispn = -1*) or biased photonuclear (*ispn =1*) events. Although the 2010 documentation stated that biased photonuclear did not work with LLNL photofission we found that it did. Consequently, the LLNL documentation has been updated and the MCNPX27D warning:

"LLNL photofission inactive when ispn!=-1 on PHYS:P card."

Has been replaced with the notification:

"Using LLNL Photofission Model"

The LLNL photofission enables the user to simulate the photofission process exactly, and therefore enables coincidence counting of photofission neutrons and gammas. This is different from the default settings of MCNPX, where secondary particles emitted by photonuclear interactions are only correct on average over a large number of interactions, because the numbers of secondary particles, as well as their energies and directions are averaged over all possible photonuclear interactions.

Figures 6 – 9 compare photonuclear results with the LLNL photofission model, both with analog and biased photonuclear production, to the default LANL ACE photonuclear and CEM model physics photonuclear.

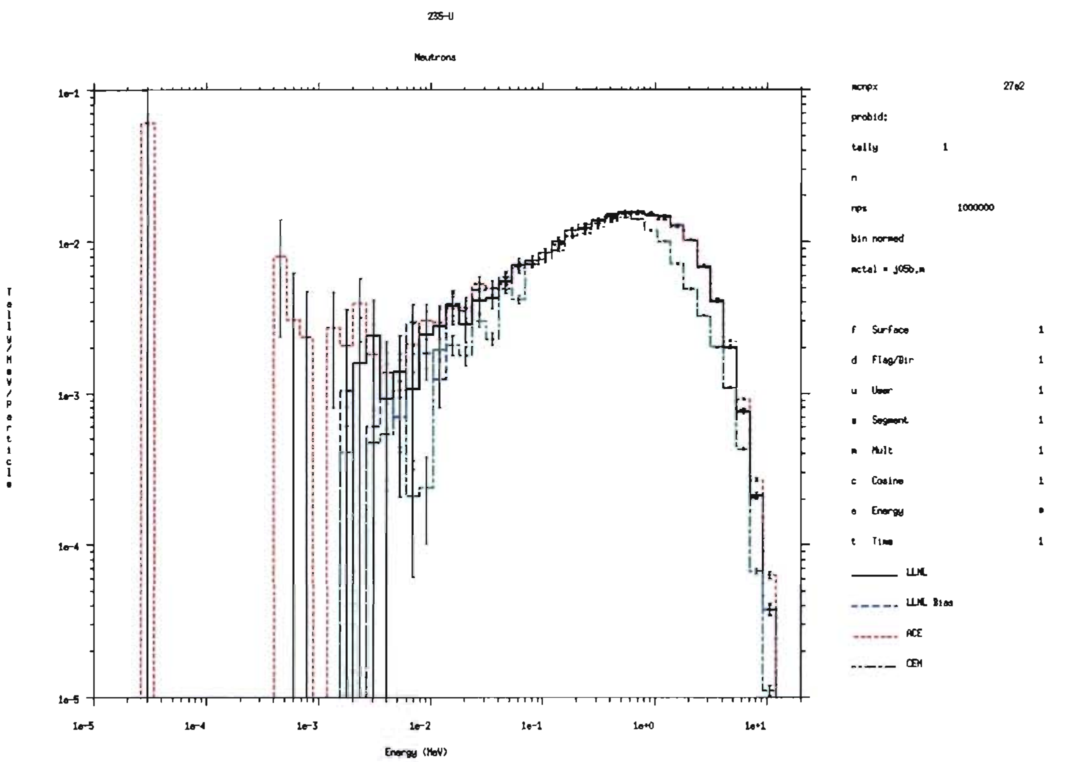

Figure 6. Neutrons emitted from 12-MeV photons incident upon U-235. LLNL photonuclear analog (black) and biased (blue) agree statistically. MCNPX default ACE physics (red) is close, but CEM model physics (green) is low.

Figures 6 and 8 show that the photo-neutron production is similar between the LLNL photonuclear model and the ACE default table physics and CEM model physics. Figures 7 and 9 show that the photo-photon production is similar between the LLNL photonuclear model and the ACE default table physics; it is quite different from the CEM model physics. In all cases the LLNL photonuclear model analog agreed with the biased photonuclear production options.

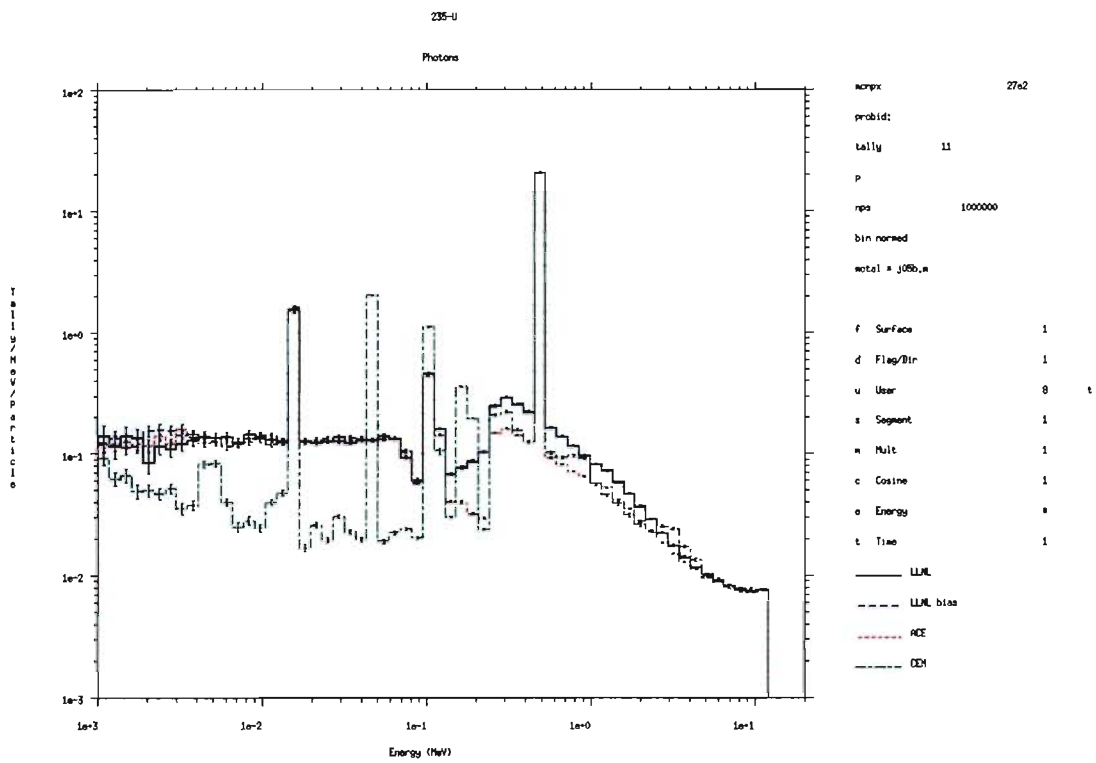

Figure 7. Photons emitted from 12-MeV photons incident upon U-235. LLNL photonuclear analog (black) and biased (blue) agree statistically. MCNPX default ACE physics (red) and particularly CEM model physics (green) are significantly different.

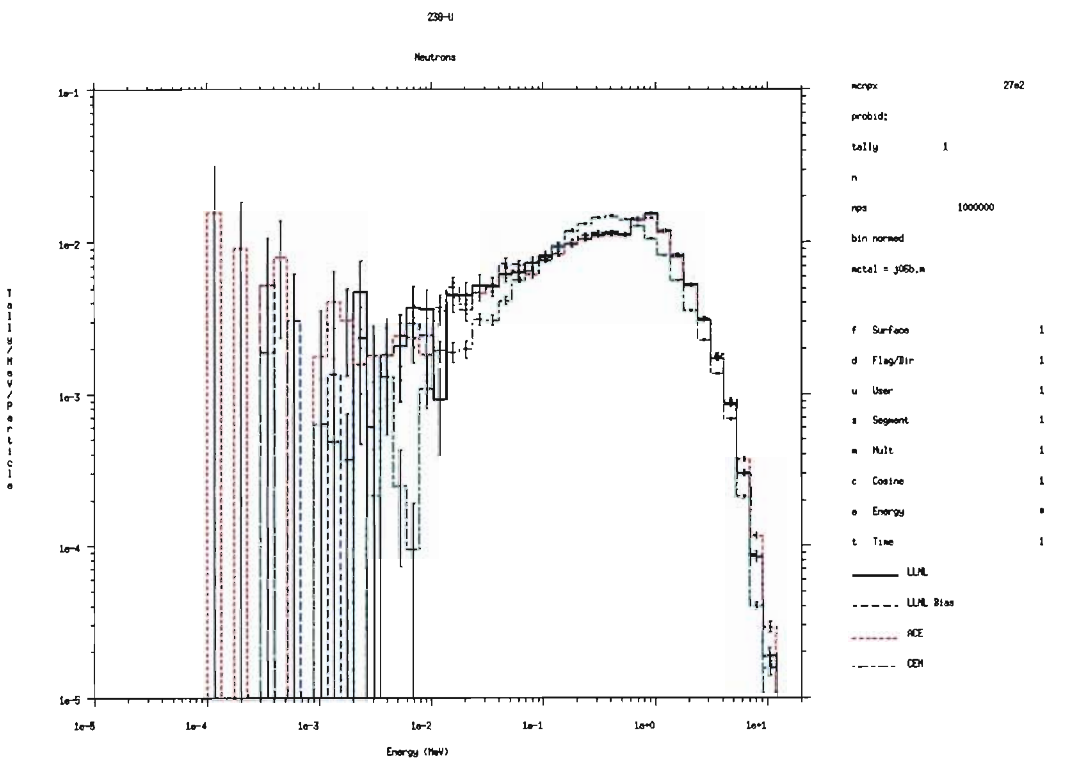

Figure 8. Neutrons emitted from 12-MeV photons incident upon U-238. LLNL photonuclear analog (black) and biased (blue) agree statistically. MCNPX default ACE physics (red) is close, but CEM model physics (green) is low.

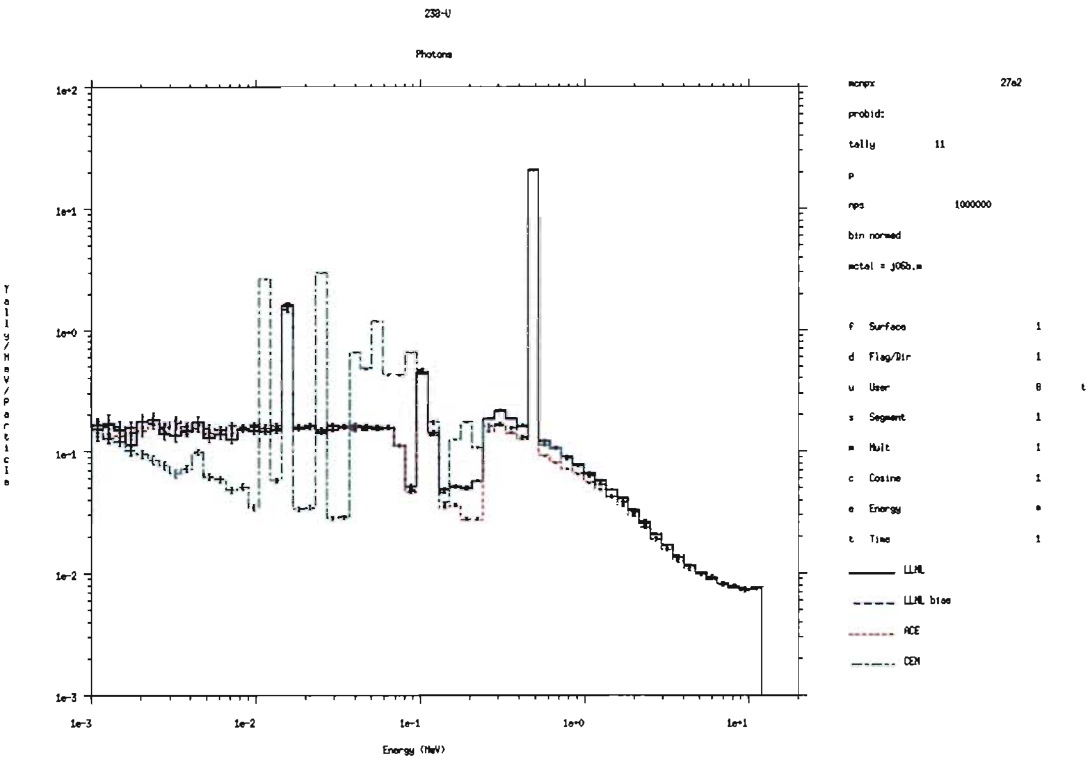

Figure 9. Photons emitted from 12-MeV photons incident upon U-238. LLNL photonuclear analog (black) and biased (blue) agree statistically. MCNPX default ACE physics (red) and particularly CEM model physics (green) are significantly different.

Resolved Issues

The following issues have been resolved:

Compilation

Compilation of the v27E model results in a large number of compiler messages. I do not know if these are a problem. Jerome Verbeke, LLNL, and I were unsuccessful at finding a way to eliminate them. However, we feel they are not a problem.

Tracking

The v27E model tracks the v27D model exactly. Douglas Wright and Jerome Verbeke, LLNL, confirm that this is expected.

Additional Test Results

Eighteen variations of three input files (see Inputs 5, 6, 7 in the Appendix below) were run with various combinations of these parameters to compare results with and without the LLNL fission model. The LLNL fission model treatment (*fism* = 5 and/of *illnlfis* = 1) is referred to as "LLNL. Results with the LLNL fission model turned off are referred to as "LLNL off." The results can be summarized as follows:

- Neutron-induced fission, 235-U:
  - The LLNL fission model is the only way in MCNPX to produce prompt fission gammas. For 235-U, LLNL produced 40% more prompt gammas, presumably because LLNL includes fission gammas.
  - Neutron-induced fission generates similar amounts of both prompt and delayed neutrons regardless of whether or not the LLNL fission model is used;
  - The LLNL fission model produces no delayed fission gammas. The only way to get delayed fission gammas in MCNPX is the use models for activation and decay (ACT card) which is independent of the LLNL fission model.
- Spontaneous Fission, 240-Pu:
  - The LLNL fission model is the only way in MCNPX to produce prompt spontaneous fission gammas. For 240-Pu, the LLNL model produced 3.0149 prompt spontaneous fission gammas per fission.
  - Because spontaneous fission occurs over time there is no such thing as delayed fission neutrons.
  - Delayed gammas from spontaneous fission can generated with the spontaneous photon source (SDEF par = sp) in MCNPX which is independent of the LLNL fission model.
- Photonuclear, 238-U:
  - The LLNL fission model is the only way in MCNPX to produce prompt photofission gammas.
  - Photonuclear neutron production, prompt photofission neutron production, and photonuclear photon production are all unaffected by the LLNL fission model.
  - The only way to get photonuclear delayed fission neutrons and gammas in MCNPX is to use models for activation and decay (ACT card) which is independent of the LLNL fission model.

Note that MCNPX 27E had to use the fatal option for no delayed neutrons (*dnb* = 0) and LLNL fission (*fism* = 5): PHYS:N 3J 0 J 5. It should only be a fatal error if *dnb* > 0. This has been corrected in MCNPX 2.7.0.

User Interface

The key MCNPX input parameters are:

PHYS:N 3J *dnb* J *fism*
PHYS:P 3J *ispn* 2J *illnlphfis*

Note that in the MCNPX documentation, *illnlphfis* is referred to as *fism*. It is referred to here as *illnlphfis* (the variable name in the code) to avoid confusion with *fism* on the PHYS:N card. These parameters have many values, but the ones utilized in this study are:

> *dnb* = 0 / -1 / -101 = no / analog / model physics delayed neutrons;
> *ispn* = -1 = analog photonuclear physics turned on;
> *fism* = 0 = no fission multiplicity: if nu = 2.7 then 2 neutrons are produced 30% of the time and 3 neutrons are produced 70% of the time;
> *fism* = 1 = each fission results in 0 – 10 fission neutrons using FMULT data;
> *illnlphfis* = 0 (this entry was unavailable before MCNPX 27D).

For the LLNL fission model,

> *fism* = 5 = turn on LLNL neutron fission multiplicity;
> *illnlphfis* = 1 = turn on LLNL photofission.

Input 5 - Neutron Induced Fission for 235-U

Source: WATT fission default neutron spectrum, single-collision and then transport without further interaction (LCA 7J -2)

Fission model	LLNL off	LLNL off	LLNL off	LLNL on	LLNL on	LLNL on
fism	1	1	1	5	5	5
dnb	analog	model	none	analog	model	none
dnb	-1	-101	0	-1	-101	0
source neutrons	1	1	1	1	1	1
N/fission (nubar)	2.66652	2.66652	2.66652	2.66546	2.66546	2.66546
fissions	0.162413	0.16233	0.16241	0.161951	0.161769	0.161952
prompt	0.43038	0.430012	0.433077	0.429148	0.428646	0.43168
delayed	0.002697	0.003065	0	0.002528	0.00303	0
n t>1e3 sh	0.002697	0.003065	0	0.002528	0.00303	0
**DN/fission	0.016606	0.018881	0	0.01561	0.01873	0
β (DN fraction)	0.006228	0.007077	0	0.005856	0.007019	0
prompt gammas	1.8921	1.8921	1.8921	2.6512	2.6525	2.6512
gam time>1e3 sh	0*	0*	0*	0*	0*	0*

** DN/fission = .01668 Duderstadt & Hamilton, *Nuclear Reactor Analysis*, John Wiley (1976)

*The only way in MCNPX to get delayed gammas is to use physics models (ACT card) which are independent of the LLNL fission model and work whether it is on or off.

Observations:

- The number of gammas from the LLNL fission model neutron-induced fission is 40% higher than when LLNL is not used, presumably because LLNL includes prompt fission gammas that otherwise are neglected.
- All gammas from neutron-induced fission (either from ACE data and the LLNL fission model) are prompt.

Input 6 - Spontaneous Fission for 240-Pu

Source: par=SF

The MCNPX spontaneous fission source MCNPX uses FMULT data for fission yields, so the LLNL fission model does not affect the number of spontaneous fissions per nuclide. Further, the FMULT data and the data used by the LLNL fission model for spontaneous fission multiplicity generally come from the same data bases. Consequently, the average number of spontaneous fission neutrons, *nu*, is statistically the same for all but 252-Cf where it is .42% different. The multiplicity distributions and moments are nearly identical for 233U, 238U, 238Pu, 240Pu, 242Pu, 242Cm, and 244Cm. They are statistically different, but similar (within 1%) for 252Cf. But they are quite different for 232Th, 232U, 234U, 235U, 236U, 237Np, 239Pu, 241Pu, 241Am, and 249Bk. The biggest differences are for 239Pu. Whereas spontaneous fission has no time = 0, there is no such thing as prompt and delayed.

The significant advantage for spontaneous fission with the LLNL fission model is that it is the only means in MCNPX of producing spontaneous fission gammas. For 240-Pu, there were 3.0149 prompt gammas per spontaneous fission.

Input 7 - Photonuclear for 238-U

Source: par=P erg=12 (12-MeV photons)

Photofission model	LLNL off	LLNL on
illnlphfis	0	1
fism	any	any
fism	0/-1/-101	0/-1/-101
dnb	-1	-1
source photons	1	1
photonuclear abs	0.012394	0.012394
photofission	0.004354	0.004354
photonuclear photons	0.052893	0.052864
photofission photons	0	0.033900
photonuclear neutrons	0.014344	0.014335
photofission neutrons	0.014413	0.014415
neutron time>1e3 sh	0*	0*
gamma time>1e3 sh	0*	0*

*The only way in MCNPX to get delayed neutrons and gammas from photonuclear reactions is to use physics models (ACT card) which are independent of the LLNL fission model and work whether it is on or off.

Observations:

- The LLNL photofission model is the only way to produced prompt fission gammas in MCNPX.
- Regardless of whether or not the LLNL photonuclear model is used, the neutron fission treatment (with or without the LLNL fission model) has no effect on the generation of photoneutrons or photofission neutrons. Photonuclear reactions tracked regardless of *fism* = 0, 1, or 5 or *dnb* on the PHYS:N card. There were neither delayed neutrons nor delayed photons from photonuclear reactions.
- Regardless of whether or not the LLNL photonuclear model is used, photonuclear neutron production, prompt photofission neutron production, and photonuclear photon production are unchanged.

Appendix A
Sample Input Files

Input 1 - Effect of delayed neutron biasing

Thermal 2.53e-8 MeV neutrons on Pu, single collision, spectra out. Prompt (time < 1e4 shakes) and delayed (time > 1e4 shakes). Toggle:

```
PHYS:N 3J -1 J 1   $ ACE, DNB off
PHYS:N 3J  1 J 1   $ ACE, DNB on
PHYS:N 3J -1 J 5   $ LLNL, DNB off
PHYS:N 3J  1 J 5   $ LLNL, DNB on
```

```
LLNL fission multiplicity w/o delayed bias
1 101 -20    -1
2 0           1

1 sph 0 0 0 .01

mode n
nps 1000000
prdmp 2J -1 3
cut:n 2J 0 0
phys:n 3J 1 J 5
m101 94239 1
imp:n 1 0
fcl:n -1 0
sdef erg=2.53e-8
c
f01:n 1
e01 1e-11 15iLog 1e-4 200iLOG 20 30
em01 0 15r 1 202R
```

```
t01 1e4 1e30
c
f11:n 1
e11 1e-11 15iLog 1e-4 200iLOG 20 30
t11 1e4 1e30
c
f21:n 1
t21 1e2 1e4 50ilog 1e11 1e12 1e15
tm21 0 1 53R
fq21 t f
c
f31:n 1
t31 1 3ilog 1e4 50ilog 1e11 1e12 1e15 1e20
fq31 t f
```

Input 2 - Gamma production with LLNL fission model

Thermal 2.53e-8 MeV neutrons on Pu or 2-Mev neutrons on 235-U. Single collision, spectra out. Prompt (time < 1e4 shakes) and delayed (time > 1e4 shakes). Neutron results are similar but photon tally 211 shows significantly different gamma production spectra.

Toggle:

```
PHYS:N 3J -1 J 1  $ ACE
PHYS:N 3J -1 J 5  $ LLNL

m101 92235 1          sdef  erg=2
m101 94239 1          sdef  erg=2.53e-8
```

```
LLNL fission multiplicity and prompt fission gammas
1 101 -20   -1
2 0          1

1 sph 0 0 0 .01

imp:n 1 0
mode n p
nps 1000000
prdmp 2J 1 3
cut:n 2J 0 0
print  -10 -30 -85 -86
lca 7j -2
m101 94239 1
phys:n 3J -1 J 5
sdef erg=2.53e-8
c
f11:n 1
```

```
e11 1e-11 15iLog 1e-4 200iLOG 20 30
t11 1e4 1e30
c
f31:n 1
t31 1 3ilog 1e4 50ilog 1e11 1e12 1e15 1e20
fq31 t f
c
f211:p 1
e211 1e-4 200iLOG 20 30
t211 1e4 1e30
c
f231:p 1
t231 1 3ilog 1e4 50ilog 1e11 1e12 1e15 1e20
fq231 t f
c
+F306 1
```

Input 3 - Spontaneous fission with LLNL fission model

Spontaneous fission was run on all spontaneous fission nuclides (default *fmult* table) comparing spectra, heating, and multiplicity. The *nonu* option eliminated the effect of induced fission. The spectra and heating were nearly the same comparing the LLNL fission model with the default *fmult* model for each nuclide. The multiplicities and moments were nearly the same for 233U, 238U, 238Pu, 240Pu, 242Pu, 242Cm, 244Cm. and 252Cf, but differed significantly for other nuclides.

The spontaneous photon runs used the last three inputs in this file: mode, f21, and e21. These were emitted to get the spontaneous fission neutron results quoted.

Toggle:

PHYS:N 3J -1 J 1 $ ACE
PHYS:N 3J -1 J 5 $ LLNL

m101 *nnnnn* 1 $ *nnnnn* = all *fmult* spontaneous fission nuclides.

```
LLNL spontaneous fission
1 101 -0.1  -1
2 0          1

1 sph 0 0 0 .001

imp:n 1 0
nps 1000000
prdmp 2J -1 3
cut:n 2J 0 0
print -10 -30 -85 -86
```

```
m101 90232 1
phys:n 3J -1 J 5
sdef par=sf
c
f11:n 1
e11 1e-11 15iLog 1e-4 200iLOG 20 30
c
+F306 1
Nonu

mode n p
f21:p 1
e21 .001 200ilog 20
```

Input 4 - Photonuclear with LLNL fission model

Photonuclear reactions were run for 235-U and 238-U. Comparisons were made for the LLNL photonuclear model with analog photonuclear and biased photonuclear (one photonuclear reaction per neutron collision). Comparisons were also made with the default ACE treatment (biased photonuclear) and model physics (biased photonuclear) which is uses the CEM model for photonuclear.

To switch between 235-U and 238-U toggle 92235 or 92238:

```
M1    92235 1      pnlib=.70u
full   -1 0.00004 92000.00003 92235.00005 92000.00005
        92235.00018 1e10
```

To switch between LLNL photonuclear and ACE or CEM:

```
PHYS:P j 1 j  1 2j j    $ for ACE or CEM
PHYS:P j 1 j  1 2j 1    $ for LLNL Photonuclear
PHYS:P j 1 j -1 2j 1    $ for LLNL Photonuclear, analog
MX1:p  model            $ for CEM
```

```
Test LLNL photofission secondaries
1  1  -19.0     -1  imp:n=1
2  0             1  imp:n=0

1  so  1.0

mode n p
m1   92238 1
mx1:p  model
PHYS:P j 1 j  1 2j j
sdef par=p erg=12
LCA  7j -2
print -85 -86 -161 -162
```

```
prdmp 2j -1
nps   100000
f1:n  1
e1    1e-6 59log 12
f11:p 1
e11   1e-3 59log 12
ft11  tag 3
fu11  -1 0.00004 92000.00003 92235.00005
      92000.00005 92235.00018 1e10
fq11  e u
```

The MCNPX *command* file for making the plots in Figures 6 – 9 is:

```
rmc j06b.m loglog xlim 1e-5 20 title 1 "238-U" title 2 "Neutrons"
rmc j06b.m tal 1 lab "LLNL" cop rmc j06c.m tal 1 lab "LLNL Bias" &
cop rmc j06a.m tal 1 lab "ACE" cop rmc j06d.m tal 1 lab "CEM"
pause
xlim 1e-3 20  title 2 "Photons" &
rmc j06b.m tal 11 lab "LLNL" cop rmc j06c.m tal 11 lab "LLNL bias" &
cop rmc j06a.m tal 11 lab "ACE" cop rmc j06d.m tal 11 lab "CEM"
pause
end
end
```

Input 5 - Additional Test Results - Neutron Induced Fission for 235-U

```
Induced fission: LLNL
1 101 -20    -1
2 0           1

1 sph 0 0 0 .01

imp:n 1 0
mode n p
nps 1000000
prdmp 2J 1 3
cut:n 2J 0 0
print  -10 -30 -85 -86
lca 7j -2
m101 92235 1
phys:n 3J -1 J 5
sdef erg=d1
sp1 -3
c
f11:n 1
t11 1e3 1e12
fq11 t f
c
f211:p 1
```

```
t211 1e3 1e30
fq211 t f
```

Toggle:

```
phys:n 3J   -1 J 1
phys:n 3J    0 J 1
phys:n 3J -101 J 1
phys:n 3J   -1 J 5
phys:n 3J    0 J 5
phys:n 3J -101 J 5
```

Input 6 - Additional Test Results - Spontaneous Fission for 240-Pu

```
Spontaneous Fission: LLNL
1 101 1e-5  -1
2 0          1

1 sph 0 0 0 .01

imp:n 1 0
fcl:n 1
mode n p
nps 1000000
prdmp 2J 1 3
cut:n 2J 0 0
print  -10 -30 -85 -86
m101 94240 1
phys:n 3J -1 J 5
sdef par=sf
c
f11:n 1
t11 1e3 1e12
ft11 inc
fu11 0 1 2 100 T
fq11 u t
c
f211:p 1
t211 1e3 1e12
ft211 inc
fu211 0 1 2 100 T
fq211 u t
```

Toggle:

```
phys:n 3J -1 J 1
phys:n 3J -1 J 5
```

```
and
phys:n 3J      0 J 1
phys:n 3J     -1 J 1
phys:n 3J   -101 J 1
```

Input 7 - Additional Test Results - Photonuclear for 238-U

```
Test LLNL photofission secondaries
1  1  -19.0      -1  imp:n=1
2  0              1  imp:n=0

1  so  1.0

mode n p
m1   92238 1  pnlib=.70u
PHYS:N 3j -1 J 0
PHYS:P j 1 j -1 2j 1
sdef par=p erg=12
LCA  7j -2
print -85 -86 -161 -162
prdmp 2j 1
nps   1000000
c
f1:n  1
e1    1e-6 59log 12
t1    1e3 1e12
c
f21:p  1
e21    1e-6 59log 12
t21    1e3 1e12
c
f211:p 1
e211   1e-3 59log 12
ft211  tag 3
fu211  -1 0.00004 92000.00003 92235.00005 92000.00005
92235.00018 1e10
fq211  e u
```

Toggle:

```
PHYS:P j 1 j -1 2j J
PHYS:P j 1 j -1 2j 1
and
PHYS:N 3j -1 J 0
PHYS:N 3j -1 J 1
PHYS:N 3j -1 J 5
```