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2013 MCNP6 Verification Study for the MCNPX_65 and MCNPX_EXTENDED Test Sets March 14, 2013

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ABSTRACT

Verification testing of the MCNP6 code has been performed in support of the MCNP/MCNPX code merger and the pending April, 2013 MCNP6 release. MCNP6 beta release version MCNP6_RELEASE1 (load date March 7, 2013 version 6.5.0) and MCNPX 2.7.0 were used to conduct the calculations. The tests were conducted using the models located in directories MCNPX_65 and MCNPX_EXTENDED. This test set consists of approximately 500 input decks and is designed to perform regression testing for MCNPX features. MCNP6 contains coding changes or additions that required changes to many of the test files to facilitate direct comparison of MCNP6 and MCNPX results. Many of the MCNP6 and v270 results compare well with each other. Results for some test problems contain significant discrepancies. This verification effort sought only to identify discrepancies, not to undertake corrections. This work parallels the effort conducted in late 2011 for the initial MCNP6 release as reported in LA-UR-12-00179.

KEYWORDS: MCNP6, MCNPX; MCNPX_65, MCNPX_EXTENDED, verification.

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Acronyms

LANL	Los Alamos National Laboratory
MCNP6	LANL Monte Carlo radiation transport code

1. INTRODUCTION

Los Alamos National Laboratory (LANL) develops and maintains the MCNP (Brown, 2003a; Brown, 2003b) and, prior to the merger, the MCNPX™ (Pelowitz, 2011) Monte Carlo N-Particle eXtended general-purpose radiation transport codes. The first merged version of MCNP and MCNPX, MCNP6, was released in 2012 (Goorley et al., 2012). A second release is scheduled to be issued in April, 2013.

Test problems from MCNPX were incorporated into the MCNP6 testbed as a part of the merger process. These problems are predominantly regression tests designed to test one or more features. These test problems are located in test directories MCNPX_65 and MCNPX_EXTENDED in the Testing subdirectory of the MCNP6 file set. In order to gain confidence in the Release 1 version of MCNP6, it was decided to test the answers produced from these problems in a side-by-side comparison of MCNPX 2.7.0 ("v270") and MCNP6. This test effort is termed "verification" because only functionality is examined. No validation testing is done, i.e., this suite contains no comparisons of calculated and experimental quantities.[1] This exercise was performed during a two-week period.

[1] In essence, the terminology "verification and validation" that was used in the report for the initial release (Durkee and James, 2012) is a misnomer. Therein no validation comparisons of code and experimental quantities were made.

2. MCNP6 VERIFICATION USING MCNPX TEST MODELS

The verification work was performed as follows. First, the MCNP6 executable was used to execute the test files located in directories MCNPX_65 and MCNPX_EXTENDED. As expected, there were essentially no differences between the template files (mctal, outp) and the new output files.

Second, MCNPX v270 was compiled with the Intel 10.0 compiler here with the name mxv270: [2]

```
/home/jdurkee/old_pete/MCNPXv270/blddgI/src/mcnpx
```

After renaming the MCNP6 executable mcnp6ref, the mcnpx executable was placed in the MCNP6/bin directory replacing the existing MCNP6 executable here:

```
/home/jdurkee/old_pete/MCNP6_Release1/bin
```

This (MCNPX v270) executable was then used to execute the test problems located in directories MCNPX_65 and MCNPX_EXTENDED. Each directory was run in turn by issuing the command 'make test EOL="" '.[3] It was also necessary to ensure that the files 'bertin' and 'phtlib', which are needed by MCNPX, were in the data path. The existing template files

[2] This is the same executable used for the initial release (Durkee and James, 2012).

[3] This command suppresses the "dev-test eol" commands in the "make" file that are used for MCNP6 execution. These commands are contained in file …/ MCNP6_Release/Testing/config/prundefine.mk.

included with the MCNP6 distribution and generated by MCNP6 served as the baseline for the comparison.

Comparison of the MCNP6 and v270 results was limited to mctal files. Contents of the mctal "dif" files produced by the "make" utility were viewed to assess differences. In many cases, the interpretation of the differences was trivial. Either no differences existed or differences were attributed to format differences in the MCNP6 and v270 mctal files.

Some cases required that changes to inp files be made to enable proper v270 execution, including the "fmult," "tropt," and "mphys" cards. For fmult, the eleventh entry to the lca card was removed, the phys:n eighth entry was moved to the 5^{th} entry or the fmult card was replaced with settings on the phys:n 6^{th} entry to invoke the fission multiplicity treatment for v270. The eleventh entry was then changed to 66 to enable MCNP6 execution in MCNPX mode. The tropt option allows MCNP6 to stipulate transport options. The options are on by default in MCNPX v270. MCNPX does not recognize the tropt option, so this card was commented for v270 calculations. The mphys card allows the specification of model use in MCNP6. MCNPX does not recognize the tropt option, so this card was commented for v270 calculations.

In all tests where differences were apparent, subjective judgment was applied to interpret results as being with or without appreciable difference. Because the methodology is Monte Carlo, subjective assessment is perhaps complicated. In some instances, the input files seemed to be suitable for compatible MCNP6 and v270 execution but the default settings yielded results with notable differences. These calculations were re-executed using more histories (SDEF) or

cycles (kcode). In addition, differences in the outp files were examined for cases where mctal file differences were significant to develop additional insights into behavior.

The verification calculations were executed on the LANL Pete Linux cluster using an Intel serial build (make build CONFIG="intel plot acode noreportjob"). The executables are on the PETE cluster in this directory:

/home/jdurkee/old_pete/MCNP6_RELEASE1/bin

```
 [jdurkee@pete bin]$ ls -la
total 52320
drwxr-xr-x 3 jdurkee mcnpxdev     4096 Mar  7 14:21 .
drwxr-xr-x 7 jdurkee mcnpxdev     4096 Mar  7 11:13 ..
drwxr-xr-x 2 jdurkee mcnpxdev     4096 Mar  7 10:58 CVS
-rwxr-xr-x 1 jdurkee mcnpxdev     8690 Jun 28  2010 fpp
-rwxr-xr-x 1 jdurkee mcnpxdev 15905243 Mar  7 14:33 mcnp6
-rwxr-xr-x 1 jdurkee mcnpxdev 21660807 Mar  7 11:17 mcnp6old
-rwxr-xr-x 1 jdurkee mcnpxdev 15905243 Mar  7 14:20 mxv270
```

The test problems are located in these directories:

/home/jdurkee/old_pete/MCNP6_RELEASE1/Testing/MCNPX_65

/home/jdurkee/old_pete/MCNP6_RELEASE1/Testing/MCNPX_EXTENDED

No verification work was done using other compilers, execution platforms, or MPI executables.

3. VERIFICATION RESULTS

Results for the MCNPX_65 and MCNPX_EXTENDED test problems are presented in the following subsections.

3.1. Test Set 1: MCNPX_65 models

Good agreement was seen between mctal files for many problems. Discrepancies between MCNP6 and MCNPX v270 calculations were observed for the problems listed in Tables 1 and 2.

For model inp006 it was necessary to remove phys:n 8th entry. Files bertin and phtlib must be in the execution directory so that cross-section data for 6012.40c and 29000.02c are found. Otherwise, execution is attempted using models. MCNP6 issues a fatal and v270 executes using models. When bertin and phtlib are present, v270 executes. This MCNP6 build still fails with an inability to find 6012.40c and 29000.02c data.

For inp113 NPS was increased 100x the default values and differences were still noted. The difference arises from the fact that this is a FLUKA test problem and MCNP6 uses LAQGSM for high-energy modeling. Model inp102 contains a “6” in the eleventh entry of the lca card, which v270 does not accommodate. Execution of inp102 by MCNP6 in “X mode” (using a “66” in the eleventh entry of the lca card) and v270 (with the eleventh entry absent) resulted in good agreement when NPS was increased to 10^4.

Several models contain the “tropt” option, which is not treated by v270. The v270 calculations for these models failed to execute.

Table 1. Results for default MCNPX_65 test models.

Test Model	Results for MCNP6 and v270
inp006	Differences
inp102	lca card 11th entry
inp103	Uses tropt-only MCNP6 has this option
inp105	Uses tropt-only MCNP6 has this option
inp106	Uses tropt-only MCNP6 has this option
inp107	Uses tropt-only MCNP6 has this option
inp108	Uses tropt-only MCNP6 has this option
inp110	Uses tropt-only MCNP6 has this option
inp111	Uses tropt-only MCNP6 has this option
inp112	Uses tropt-only MCNP6 has this option
inp113	Uses tropt-only MCNP6 has this option
inp114	Uses tropt-only MCNP6 has this option
inp115	Uses tropt-only MCNP6 has this option
inp116	Uses tropt-only MCNP6 has this option
inp117	Uses tropt-only MCNP6 has this option
inp118	Uses tropt-only MCNP6 has this option
inp123	Uses tropt-only MCNP6 has this option
inp129	Uses tropt-only MCNP6 has this option
inp201	Using mphys-only MCNP6 has this option
inp203	Uses tropt-only MCNP6 has this option
inp215	Uses tropt-only MCNP6 has this option
inp216	Uses tropt-only MCNP6 has this option
inp250	Bad character in column 34
inp303	Uses tropt-only MCNP6 has this option
inp304	Uses tropt-only MCNP6 has this option
inp305	Uses tropt-only MCNP6 has this option
inp306	Uses tropt-only MCNP6 has this option
inp309	Uses tropt-only MCNP6 has this option
inp329	Uses tropt-only MCNP6 has this option

Subdirectory INPREF was created to house the reference inp files. Subdirectory INPCTROPT was created to house the inp files with the commented lines containing the tropt keywords. These

files were copied to the Inputs subdirectory and the calculations executed using ‘make test EOL=”” ‘ from the MCNPX_65 subdirectory.

Table 2 summarizes results for inp files with commented tropt cards. Most of the differences were resolved.

Table 2. Results for modified MCNPX_65 test models.

Test Model	Results for MCNP6 and v270
inp006	Fatal – MCNP6 fails to find 6012.40c, 29000.42c data
inp102	Ok for MCNP6 run in X mode NPS=10k, v270 w/o 11th
inp103	Ok
inp105	Ok
inp106	Ok
inp107	Ok
inp108	Ok
inp110	Ok
inp111	Ok
inp112	Ok
inp113	Differences for ref & 100x NPS
inp114	Ok
inp115	Many differences. 256-MeV protons on U238.
inp116	Many differences. 1000-MeV protons on Pb208.
inp117	Ok
inp118	Ok

inp123	Differences. MCNP6 runs. MCNPX:
	`bad trouble in xact in routine expunge`
	`92238.70c is completely wiped out.`

inp129	Ok
inp201	Ok
inp203	Ok
inp215	Many differences. 256-MeV protons on U238.
inp216	Many differences. 1000-MeV protons on Pb208.
inp250	Bad character in column 34. MCNP6 runs, X fails.
inp303	Ok
inp304	Ok
inp305	Ok
inp306	Ok
inp309	Ok
inp329	Ok

3.2. Test Set 2: MCNPX_EXTENDED Models

Calculations were executed for all subdirectories. However, 144 of the test problems have either an "mphys" or "tropt" keyword. Test problem inp07 in testdndg has a "rand" keyword. Execution of v270 failed for these models. Copies of the reference inp files were modified to comment the mphys, tropt, or rand line. Re-execution using v270 then succeeded. Results with appreciable differences in these subdirectories are summarized as follows. For the most part, no appreciable differences were found for test problems in subdirectories avr, class, classgeom, classvar, heavyions, mbody, phys, push, test27a, test27b, testburn, testmcnp, and testmesh. The results are summarized as follows

Table 3 contains results for the avr07 model. The reference ("ref") deck contains a mphys card. After this card was comment, v270 executed and no notable differences between the MCNP6 and v270 mctal files were noted.

Table 3. Results for MCNPX_EXTENDED avr test models.

Test Model	Results for MCNP6 and v270
avr07 – ref	Using mphys-only MCNP6 has this option
avr07 – no mphys	Ok

Table 4 list results for the class models exhibiting notable differences.

Table 4. Results for MCNPX_EXTENDED class test models.

Test Model	Results for MCNP6 and v270
test57:godiva6a	Differences
test58:godiva6b	Differences

Table 5 summarizes results for the three classvar models exhibiting notable differences.

Table 5. Results for MCNPX_EXTENDED classvar test models.

Test Model	Results for MCNP6 and v270
var4a	Differences
var4b	Differences
var4c	Differences

Initial execution of the heavyions models failed because of the use of tropt cards and “6” in the eleventh entry of the lca card. To continue, (1) the tropt card was commented to permit v270 execution, (2) the eleventh lca card entry set to 66 to cause MCNP6 execution in MCNPX mode, and (3) the eleventh lca card entry was omitted for v270 calculations. With these modifications, calculations for all heavyions models resulted in no appreciable differences between MCNP6 and v270 as indicated in Table 6.

Table 6. Results for MCNPX_EXTENDED heavyions test models.

Test Model	Results for MCNP6 and v270
inp74 – ref inp74 – no tropt	Using tropt-only MCNP6 has this option Ok
inp75 – ref inp75 – no tropt	Using tropt-only MCNP6 has this option Ok
inp80 – ref inp80 – no tropt, 11th	Using tropt-only MCNP6 has this option Lca card 11th entry 6 Ok

Table 7 summarizes the notable differences for the phys models.

Table 7. Results for MCNPX_EXTENDED phys test models.

Test Model	Results for MCNP6 and v270
inpw04 – ref inpw04 – no mphys	Using mphys-only MCNP6 has this option Ok
inpw05: 20 keV el on W	Differences of about 50% in some values
inpw11	Differences, some negative values
inpw17	Differences of about 50% in some values

Table 8 summarizes the differences for the phys models.

Table 8. Results for MCNPX_EXTENDED push test models.

Test Model	Results for MCNP6 and v270
inp06	Pertubation & dxtran incompatible Mat keyword of pert 8 requires sd 1 for tal 6
inp08: kcode in hex	Differences
inp16 – ref inp16 – no mphys	Using mphys-only MCNP6 has this option Ok

Table 9 summarizes the differences for the test27a models.

Table 9. Results for MCNPX_EXTENDED test27a test models.

Test Model	Results for MCNP6 and v270
inp01 – ref inp01 – no mphys	Using mphys-only MCNP6 has this option Ok
inp03 – ref inp03 – no mphys	Using mphys-only MCNP6 has this option
inp05 – ref inp05 – no mphys	Using mphys-only MCNP6 has this option Ok
inp09 – ref inp09 – no mphys	Using mphys-only MCNP6 has this option Ok
inp11 – ref inp11 – no mphys	Using mphys-only MCNP6 has this option Fatal - Spontaneous photons need DGs activated
inp12 – ref	Fatal - Spontaneous photons need DGs activated

Table 10 summarizes the differences for the test27b models.

Table 10. Results for MCNPX_EXTENDED test27b test models.

Test Model	Results for MCNP6 and v270
inp01 – ref inp01 – no tropt	Using tropt-only MCNP6 has this option Ok
inp04 – ref inp04 – no tropt	Using tropt-only MCNP6 has this option Ok
inp05 – ref inp05 – no tropt	Using tropt-only MCNP6 has this option Ok
inp07 – ref inp07 – no tropt	Using tropt-only MCNP6 has this option Ok
inp13 – ref inp13 – no tropt	Using tropt-only MCNP6 has this option Ok

Table 11 summarizes the differences for the test27c models.

Table 11. Results for MCNPX_EXTENDED test27c test models.

Test Model	Results for MCNP6 and v270
inp01 – ref inp01 – no tropt	Using tropt-only MCNP6 has this option Ok
inp02 – ref inp02 – no tropt	Using tropt-only MCNP6 has this option Ok
inp03 – ref inp03 – no mphys	Using mphys-only MCNP6 has this option Ok
inp06 – ref inp06 – no tropt	Using tropt-only MCNP6 has this option Ok
inp07 – ref inp07 – no tropt	Using tropt-only MCNP6 has this option Ok
inp08 – ref inp08 – no tropt	Using tropt-only MCNP6 has this option Ok

The test27d results exhibit differences. Several models inp12, inp13, and inp15 contain the tropt and FMULT cards. Problem inp14 fails – it uses a phys:n eighth entry in a way that is suspect and may be a mistake in the input file and it has a zero neutron importance in cells where the photon importance is zero. MCNP6 and MCNPX interpret the eighth entry differently. In MCNPX is should be ignored, in MCNP6 it serves as the *tabl* transition energy. Table 12 summarizes the differences for the test27d models.

Table 12. Results for MCNPX_EXTENDED test27d test models.

Test Model	Results for MCNP6 and v270
inp04 – ref inp04 – no mphys	Using mphys-only MCNP6 has this option Still has differences
inp08 – ref inp08 – no tropt	Using tropt-only MCNP6 has this option Ok
inp09 – ref inp09 – no tropt	Using tropt-only MCNP6 has this option Ok
inp10 – ref inp10 – no tropt	Using tropt-only MCNP6 has this option Ok
inp12 – ref inp12 – no tropt,fmult	Using tropt, fmult method-only MCNP6 has this option Still has 50% differences
inp13 – ref inp13 – no tropt,fmult	Using tropt & fmult method-only MCNP6 has this option Still has 50% differences
inp14 – ref inp14 – no tropt	Using mphys-only MCNP6 has this option Errors: zero n importance while nonzero p importance.
inp15 – ref inp15 – no tropt,fmult	Using tropt,fmult method-only MCNP6 has this option Ok
inp16 – ref inp16 – no tropt	Using tropt-only MCNP6 has this option Ok
inp17 – ref inp17 – no mphys	Using mphys-only MCNP6 has this option Ok
inp18 – ref inp18 – no mphys	Using mphys-only MCNP6 has this option Ok

The test27e results had many differences. Test models inp01, inp02, and inp03 include the LLNL fission multiplicity which requires changing input deck to invoke the LLNL Fission model from the phys:n card.[4] Deck inp15 tests fission and activation by 20-MeV protons, inp16 fission by 22-MeV neutrons, and inp17 fission by 2000-MeV protons. Table 13 summarizes the differences for the test27e models.

[4] Comment "fmult method = 5" and set the 6th entry of the phys:n card to 5, "phys:n 3J j j 5".

Table 13. Results for MCNPX_EXTENDED test27e test models.

Test Model	Results for MCNP6 and v270
inp01 – ref inp01 – no fmult	Using fmult method-only MCNP6 has this option Ok
inp02 – ref inp02 – no fmult	Using fmult method-only MCNP6 has this option Ok
inp03 – ref inp03 – no fmult	Using fmult method-only MCNP6 has this option Ok, perhaps small differences
inp04 – ref inp04 – no fmult	Using tropt-only MCNP6 has this option Ok
inp11 – ref: bkd srcs	Notable diffs in tallys 1 and 11
inp12 – ref inp12 – no tropt,fmult	Using tropt-only MCNP6 has this option Still has 50% differences
inp15 – ref: MG DG	Ok, perhaps small differences
inp16 – ref: MG DG	Ok, perhaps small differences
inp17 – ref: MG DG	Some differences
inp18 – ref	Using swapb-only MCNP6 has this option
inp19 – ref	Using swapb-only MCNP6 has this option
inp20 – ref	Using swapb-only MCNP6 has this option
inp21 – ref	Using swapb-only MCNP6 has this option
inp22 – ref: LLNL PF	Many differences
inp30 – ref: DN,G,B	No delayed beta v270
inp31 – ref: DN,G,B	No delayed beta v270
inp33 – ref: DN,G,B	No delayed beta v270
inp40 – ref phys:n 3J j j 5	Using fmult method-only MCNP6 has this option Using ft cap edep-only MCNP6 has this option (fatal)
inp41 – ref	Using ft cap edep-only MCNP6 has this option (fatal)
inp42 – ref phys:n 3J j j 5	Using fmult method-only MCNP6 has this option Using ft cap edep-only MCNP6 has this option (fatal)
inp43 – ref phys:n 3J j j 5	Using fmult method-only MCNP6 has this option Using ft cap edep-only MCNP6 has this option (fatal)
inp44 – ref	Fatal: he3-1, bf3-1, tdep, zns-1, lii-1, etc.
inp45 – ref	Fatal: tdep
inp46 – ref	Fatal: fft
inp47 – ref	Fatal: fft
inp48 – ref	Fatal: wrong number of parameters for ft geb

Several testburn input files contain the mphys, fmult, and/or rand card, which are not recognized by v270. Test models inp41 and inp42 initially failed to execute v270 due to a data value ("6") in the eleventh place of the lca card. Consequently, direct comparison of MCNP6 with v270 results was not possible. Further testing was done by 1) executing MCNP6 using the eleventh lca card entry set to 66, which caused MCNP6 execution in MCNPX mode, and 2) removing the eleventh lca card entry for v270 calculations.

Table 14 summarizes the MCNP6 and v270 results. Other reports (Durkee, 2011a; Durkee, 2011b; Durkee, 2011c) contain extensive descriptions of delayed-particle v&v.

Table 14. Results for MCNPX_EXTENDED testdndg test models.

Test Model	Results for MCNP6 and v270
inp07 – ref inp07 – no mphys,fmult,r	Using mphys,fmult,rand-only MCNP6 has these options Base NPS poor. NPS 10^5 ok.
inp21 – ref	`Fatal. spontaneous photons needs delayed gammas activated. But act NONFISS=p dg=line`
inp22 – ref	`Fatal. spontaneous photons needs delayed gammas activated. But act NONFISS=p dg=line`
inp23 – ref inp23 – no mphys	Using mphys-only MCNP6 has this option `Fatal. spontaneous photons needs delayed gammas activated. But act NONFISS=p dg=line`
inp24 – ref inp24 – no mphys,tropt	Using mphys, tropt -only MCNP6 has these options `Fatal. spontaneous photons needs delayed gammas activated. But act NONFISS=p dg=line`
inp25 – ref	`Fatal. spontaneous photons needs delayed gammas activated. But act NONFISS=p dg=line`
inp41 – ref inp41 – no tropt,lca 6	Using tropt-only MCNP6 has this option. 11^{th} lca=6 lca card. Ok for MCNP6 run in X mode.
inp42 – ref inp42 – no mphys, lca 6	Using mphys-only MCNP6 has this option. 11^{th} lca=6 lca card. Ok for MCNP6 run in X mode.

Calculations for all testincl models produced the following findings. Models inp03, inp21 – inp29, inp102 – inp114, inp117 – inp120, inp124, and inp134 failed v270 execution because of the tropt card. Models inp22, inp25, inp28, inp86, inp96, and inp108 would not execute v270 due to a data value ("6") in the eleventh place of the lca card. Consequently, direct comparison of MCNP6 with v270 results was not possible. Further testing was done by 1) executing MCNP6 using the eleventh lca card entry set to 66, which caused MCNP6 execution in MCNPX mode, and 2) removing the eleventh lca card entry for v270 calculations.

Results for the testincl models with tropt of lca cards are listed in Table 15. Results for the other decks show no differences between MCNP6 and v270.

Table 15. Results for MCNPX_EXTENDED testincl test models.

Test Model	Results for MCNP6 and v270
inp03 – ref inp03 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp21 – ref inp21 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp22 – ref inp22 – no 11th	Using tropt, 11th entry lca card – 270 fatal Ok for MCNP6 run in X mode.
inp23 – ref inp23 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp24 – ref inp24 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp25 – ref inp25 – no tropt, 11th	Using tropt, 11th entry lca card – 270 fatal Ok for MCNP6 run in X mode.
inp26 – ref inp26 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp27 – ref inp27 – no tropt	Using tropt-only MCNP6 has this option. Differences
inp28 – ref inp28 – no tropt, 11th	Using tropt, lca card 11th entry – 270 fatal Ok for MCNP6 run in X mode.
inp29 – ref inp29 – no tropt	Using tropt-only MCNP6 has this option. Differences
inp86 – ref inp86 – no 11th	lca card 11th entry – 270 fatal. Ok
inp96 – ref inp96 – no 11th	lca card 11th entry – 270 fatal. Ok
inp103 – ref inp103 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp104 – ref inp104 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp105 – ref inp105 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp106 – ref inp106 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp107 – ref inp107 – no tropt	Using tropt-only MCNP6 has this option. Ok

Table 15 (contd). Results for MCNPX_EXTENDED testincl test models.

Test Model	Results for MCNP6 and v270
inp108 – ref inp108 – no tropt, 11th	Using tropt, lca card 11th entry – 270 fatal Ok for MCNP6 run in X mode.
inp109 – ref inp109 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp110 – ref inp110 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp111 – ref inp111 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp112 – ref inp112 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp113 – ref inp113 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp114 – ref inp114 – no tropt	Using tropt-only MCNP6 has this option. Differences
inp117 – ref inp117 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp118 – ref inp118 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp119 – ref inp119 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp120 – ref inp120 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp124 – ref inp124 – no tropt	Using tropt-only MCNP6 has this option. Fatal – more than 1 particle type on tally card
inp134 – ref inp134 – no tropt	Using tropt-only MCNP6 has this option. Fatal – more than 1 particle type on tally card

Table 16 summarizes the MCNP6 and v270 results for testmesh. Problem inp08 appears to have discrepancies in the mctal files.

Table 16. Results for MCNPX_EXTENDED testmesh test models.

Test Model	Results for MCNP6 and v270
inp04 – ref inp04 – no tropt	Using tropt-only MCNP6 has this option Ok
inp05 – ref inp05 – no tropt	Using tropt-only MCNP6 has this option Ok
inp06 – ref inp06 – no tropt	Using tropt-only MCNP6 has this option Ok
inp07 – ref inp07 – no tropt	Using tropt-only MCNP6 has this option Ok
inp08 – ref	Differences in mctal files
inp09 – ref	Ok
inp10 – ref inp10 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp11 – ref inp11 – no mphys	Using mphys-only MCNP6 has this option. Ok

Almost all testmix models contain either a tropt, mphys, or lca 11th card. Commenting these cards resulted in calculations with no appreciable differences between MCNP6 and v270 as indicated in Table 17.

Table 17. Results for MCNPX_EXTENDED testmix test models.

Test Model	Results for MCNP6 and v270
inp01 – ref inp01 – no tropt	Using tropt-only MCNP6 has this option Ok
inp02 – ref inp02 – no tropt	Using tropt-only MCNP6 has this option Ok
inp03 – ref inp03 – no tropt, 11th	Using tropt-only MCNP6 has this option, lca 11th Ok
inp04 – ref inp04 – no mphys	Using mphys-only MCNP6 has this option Ok
inp05 – ref inp05 – no mphys	Using mphys-only MCNP6 has this option Ok
inp08 – ref inp08 – no tropt	Using tropt-only MCNP6 has this option Ok
inp09 – ref inp09 – no mphys	Using mphys-only MCNP6 has this option Ok
inp10 – ref inp10 – no tropt	Using tropt-only MCNP6 has this option Ok
inp11 – ref inp11 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp12 – ref inp12 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp13 – ref inp13 – no tropt	Using tropt-only MCNP6 has this option. Ok

The testpht directory (Durkee and James, 2012) no longer exists.

Table 18 summarizes results for the testxnew models. Several models have differences in the mctal file contents for the tally fluctuation charts.

Table 18. Results for MCNPX_EXTENDED testxnew test models.

Test Model	Results for MCNP6 and v270
inp01 – ref	Differences in tally fluctuation charts
inp02 – ref	Differences in tally fluctuation charts
inp03 – ref	Differences in tally fluctuation charts
inp04 – ref	Differences in tally fluctuation charts
inp08 – ref	Differences in tally fluctuation charts
inp14 – ref inp14 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp15 – ref inp15 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp16 – ref inp16 – no tropt	Using tropt-only MCNP6 has this option. Ok

Calculations for all testxold models resulted in no notable differences between MCNP6 and v270 as noted in Table 19.

Table 19. Results for MCNPX_EXTENDED testxold test models.

Test Model	Results for MCNP6 and v270
inp01 – ref inp01 – no tropt	Using tropt-only MCNP6 has this option Ok
inp02 – ref inp02 – no tropt	Using tropt-only MCNP6 has this option Ok
inp03 – ref inp03 – no tropt	Using tropt-only MCNP6 has this option Ok
inp05 – ref inp05 – no tropt	Using tropt-only MCNP6 has this option Differences
inp06 – ref inp06 – no tropt	Using tropt-only MCNP6 has this option Differences
inp30 – ref inp30 – no tropt	Using tropt-only MCNP6 has this option Ok
inp31 – ref inp31– no mphys	Using mphys-only MCNP6 has this option Ok
inp32 – ref inp32 – no tropt	Using tropt-only MCNP6 has this option Ok
inp33 – ref inp33 – no tropt, 11th	Using tropt-only MCNP6 has this option. lca 11th Ok
inp35 – ref inp35 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp36 – ref inp36 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp37 – ref inp37 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp38 – ref inp38 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp39 – ref inp39 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp40 – ref inp40 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp41 – ref inp41 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp42 – ref inp42 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp73 – ref inp73 – no tropt	Using tropt-only MCNP6 has this option. Ok

The zrecoil models contain an assortment of "tropt" and "fmult method" cards. The tropt cards were commented for v270 execution. Test models with the "fmult method" were changed to invoke the LLNL fission model from the phys:n card.[5] Table 20 summarizes the zrecoil results. No differences between the MCNP6 and v270 results were observed for other models.

Table 20. Results for MCNPX_EXTENDED zrecoil test models.

Test Model	Results for MCNP6 and v270
inp01 – ref inp01 – no tropt	Using tropt-only MCNP6 has this option Ok
inp02 – ref inp02 – no tropt	Using tropt-only MCNP6 has this option Ok
inp03 – ref inp03 – no tropt	Using tropt-only MCNP6 has this option Ok
inp04 – ref inp04 – phys:n 3J j j 5	Using fmult method-only MCNP6 has this option Ok
inp05 – ref inp05 – phys:n 3J j j 5	Using fmult-only MCNP6 has this option Ok
inp06 – ref inp06 – phys:n 3J j j 5	Using fmult-only MCNP6 has this option Ok
inp11 – ref inp11 – no tropt	Using tropt-only MCNP6 has this option Ok
inp12 – ref inp12 – no tropt	Using tropt-only MCNP6 has this option Ok
inp13 – ref inp13 – no tropt	Using tropt-only MCNP6 has this option Ok
inp14 – ref light ion recoil inp14 – no tropt	Using tropt-only MCNP6 has this option. Differences
inp15 – ref inp15 – no tropt	Using tropt-only MCNP6 has this option. Differences
inp16 – ref inp16 – phys:n 3J j j 5	Using fmult-only MCNP6 has this option. Ok

[5] Comment "fmult method = 5" and set the 6th entry of the phys:n card to 5, "phys:n 3J j j 5".

Table 20 (contd). Results for MCNPX_EXTENDED zrecoil test models.

Test Model	Results for MCNP6 and v270
inp17 – ref inp17 – phys:n 3J j j 5	Using fmult-only MCNP6 has this option. Ok
inp18 – ref inp18 – phys:n 3J j j 5	Using fmult-only MCNP6 has this option. Ok
inp21 – ref inp21 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp22 – ref inp22 – phys:n 3J j j 5	Using fmult-only MCNP6 has this option. Ok
inp25 – ref inp25 – phys:n 3J j j 5	Using fmult-only MCNP6 has this option. Ok
inp26 – ref inp26 – phys:n 3J j j 5	Using fmult-only MCNP6 has this option. Ok
inp30 – ref inp30 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp31 – ref inp31 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp35 – ref inp35 – no tropt	Using tropt-only MCNP6 has this option. Ok
inp64 – ref	`Fatal.  more than one particle-type designator`
inp65 – ref	`Fatal.  more than one particle-type designator`
inp66 – ref	`Fatal.  more than one particle-type designator`

4. SUMMARY AND CONCLUSIONS

In support of the MCNP6 Release 1 effort scheduled for April, 2013, a verification study has been conducted to identify appreciable discrepancies between MCNP6 and MCNPX v2.7.0 results using MCNPX test problems located on directories MCNPX_65 and MCNPX_EXTENDED. The code versions used were MCNP6 beta release version MCNP6_RELEASE1 (load date March 7, 2013 version 6.5.0) and MCNPX 2.7.0.

The screening of significant discrepancies was done by comparing mctal files. In some instances, no differences in mctal files created by MCNP6 and v270 were noted. In others, trivial differences were noted regarding simple format changes in MCNP6 and v270 files.

For some results, differences were noted for the default number of histories or kcode settings. For such cases, the execution was redone using more histories, often 100 times more, or refined kcode parameters. This refinement sometimes resulted in reductions in the differences between MCNP6 and v270 to permit the qualitative assessment of agreement. Other times, differences remained.

Some input files contained a “6” in the eleventh location of the lca card. v270 does not accommodate this entry. Consequently, a direct comparison of MCNP6 and v270 was not possible. Comparison of MCNP6 execution in “X mode” was done by changing the “6” to a “66” for MCNP6. Companion v270 execution was done by omitting the entry in the eleventh column

of the lca card. In many instances, execution of MCNP6 in "X mode" resulted in insignificant differences. In other instances, differences remained.

Some test models contain the "tropt" option. This option is treated by MCNP6 but is not treated by MCNPX. Direct comparison of results for such models was not possible. Indirect comparison was made by commenting the tropt card and executing v270.

Since these test sets were primarily used for regression testing, it was not practical to identify which results were significant in each case. The methodology was also subjective for identifying "significant" differences in test answers. Overall, there are a number of test problems on test directories MCNPX_65 and MCNPX_EXTENDED for which appreciable discrepancies exist between MCNP6 and v270 results. However, for the majority of test problems, the codes run equivalently and give (essentially) the same answers.

This effort did not always extend to the identification of the underlying causes of the discrepancies. Differences have been noted for future attention.

The verifications test results here are a companion to results obtained for the delayed-particle feature (Durkee, 2011; Durkee et al., 2013).

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