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GENXS Expansion to Include Fragment Spectra of Heavy Ions

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1 Introduction

The GENXS Card allows for various cross sections to be tallied in MCNP6 (see LA-UR-11-02146 by Richard Prael). Previously, double differential cross sections (cross section per emitted fragment energy and angle) were only available for fragments up to ^4He . This upgrade includes the ability to tally and output double differential cross sections for any heavy ion (with valid ZAID). It also includes the ability to tally and output angle-integrated cross sections per emitted fragment energy for any ZAID.

2 MCNP6 and GENXS Example Input Files

A sample MCNP6 input using GENXS is displayed below:

MCNP6 test: Spectra from 200 MeV p + Al27 by CEM03.03

1 1 1.0 -1 2 -3

2 0 -4(1:-2:3)

3 0 4

c _____

1 cz 4.0

2 pz -1.0

3 pz 1.0

4 so 50.0

c _____

m1 13027 1.0

sdef erg=200 par=H dir=1 pos=0 0 0 vec 0 0 1

imp:h 1 1 0

phys:h 300

mode h n a #

LCA 8j 1 \$ use CEM03.03

tropt genxs inxcp200al nreact on nescat off

c _____

print 40 110 95

nps 10000000

prdmp 2j -1

This example simulates the nuclear spallation reaction of 200 MeV protons striking ^{27}Al . Note that in order to tally double differential cross sections of heavy ions, heavy ions (#) must be added to the MODE card. As explained in LA-UR-11-02146, the GENXS card requires a second input file. This line, `tropt genxs inxcp200al nreact on nescat off` specifies the use of GENXS and names the GENXS input file as `inxcp200al`. The file `inxcp200al` appears below:

MCNP6 test: p, d, t, LF spectra from 200 MeV p + Al27 by CEM03.03

```
1 1 1 /
Cross Section Edit
72 -11 15 /
5. 10. 15. 20. 25. 30. 35. 40. 45. 50. 55. 60. 65. 70. 75. 80.
85. 90. 95. 100. 120. /
155. 145. 115. 105. 95. 85. 55. 45. 25. 15. 0. /
1 5 21 22 23 24 2006 3006 3007 3008 3009 4007 4009 4010 5010 /
```

See LA-UR-11-02146 for a full explanation of the GENXS input file. Note that the last line,

```
1 5 21 22 23 24 2006 3006 3007 3008 3009 4007 4009 4010 5010 /
contains the particle types to be tallied and output. Numbers 1 – 24 refer to the
MCNP6 particle types, as used in the previous GENXS version. With this ex-
pansion, heavy ions may now be tallied, according to their ZAID ( $Z * 1000 + A$ ).
Therefore, numbers > 1000 refer to the ZAID of a particular heavy ion. As an
example, this GENXS input instructs MCNP6 to tally
1 5 21 22 23 24 2006 3006 3007 3008 3009 4007 4009 4010 5010
n p d t 3He 4He 6He 6Li 7Li 8Li 9Li 7Be 9Be 10Be 10B.
```

Fig. 1 displays an excerpt of the double differential cross section output for ⁶Li (ZAID 3006). Note that instead of showing “mu max” for the emission direction, GENXS now outputs the angles in “degrees+/-spread”. We believe this will be easier and more intuitive for users, and help avoid user error and misinterpretation. Angle-integrated spectra and energy-integrated spectra are also calculated, as well as the total angle- and energy-integrated production cross section.

Figs 2 and 3 show plots of the example spectra from MCNP6 compared to results by CEM03.03, for the reaction 200 MeV p + ²⁷Al. The results between MCNP6 and CEM03.03 are consistent. In addition, other “test” reactions studied revealed the expected consistency between MCNP6 and CEM03.03.

The MCTAL tallies have also been updated so that angle-integrated cross section spectra of specified heavy ions may be viewed from within `mcplot`, similar to how specified nucleons and light fragments were viewed in the previous version of GENXS (see Fig. 4).

Lastly, up to 50 heavy ions can be tallied. This limit is according to the parameter, `heavymax`, in `xs_mod.F90`, and can be easily altered in subsequent versions.

3006 production cross section

E (MeV)	167.5deg+/-12.5	150.0deg+/-5.0	130.0deg+/-15.0	110.0deg+/-5.0	100.0deg+/-5.0	90.0deg+/-5.0	70.0deg+/-15.0					
5.000000E+00	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000					
1.000000E+01	8.301E-06.040	9.325E-06.039	1.165E-05.016	1.442E-05.023	1.529E-05.022	1.614E-05.021	1.893E-05.012					
1.500000E+01	2.598E-07.037	2.822E-07.051	3.920E-06.028	6.006E-06.036	7.040E-06.032	8.988E-06.028	1.277E-05.014					
2.000000E+01	6.928E-07.019	6.303E-07.015	1.011E-06.056	1.791E-06.065	2.538E-06.054	3.180E-06.047	5.867E-06.021					
2.500000E+01	1.999E-07.028	1.146E-07.034	2.865E-07.015	5.259E-07.120	6.760E-07.104	1.110E-06.080	2.287E-06.034					
3.000000E+01	9.327E-08.378	2.865E-08.707	1.039E-07.1174	1.601E-07.218	2.308E-07.131	3.724E-07.139	7.161E-07.060					
3.500000E+01	0.000E+00.000	1.432E-08.1000	3.463E-08.302	3.049E-08.500	6.545E-08.737	1.003E-07.267	2.490E-07.102					
4.000000E+01	1.332E-08.1000	0.000E+00.000	9.445E-09.500	7.622E-09.1000	1.454E-08.300	2.865E-08.500	6.673E-08.196					
4.500000E+01	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	7.162E-09.1000	1.283E-08.447					
5.000000E+01	0.000E+00.000	0.000E+00.000	6.297E-09.707	0.000E+00.000	0.000E+00.000	0.000E+00.000	2.567E-09.1000					
5.500000E+01	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000					
6.000000E+01	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000					
6.500000E+01	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000					

E (MeV)	50.0deg+/-5.0	35.0deg+/-10.0	20.0deg+/-5.0	7.5deg+/-7.5								
5.000000E+00	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000								
1.000000E+01	1.901E-05.022	1.826E-05.019	1.853E-05.034	1.825E-05.045								
1.500000E+01	1.709E-05.023	1.932E-05.018	2.134E-05.031	2.213E-05.041								
2.000000E+01	8.508E-06.033	1.070E-05.024	1.315E-05.040	1.392E-05.051								
2.500000E+01	3.852E-06.049	4.644E-06.037	6.638E-06.056	6.778E-06.074								
3.000000E+01	1.683E-06.075	2.125E-06.054	2.680E-06.088	2.528E-06.120								
3.500000E+01	4.862E-07.139	8.711E-07.085	1.026E-06.143	1.429E-06.160								
4.000000E+01	2.618E-07.189	2.632E-07.154	8.863E-07.189	5.862E-07.250								
4.500000E+01	6.544E-08.378	1.128E-07.236	7.282E-08.577	2.198E-07.408								
5.000000E+01	2.905E-08.577	3.134E-08.447	6.285E-08.577	1.009E-07.577								
5.500000E+01	0.000E+00.000	2.507E-08.500	0.000E+00.000	0.000E+00.000								
6.000000E+01	0.000E+00.000	0.000E+00.000	0.000E+00.000	0.000E+00.000								
6.500000E+01	0.000E+00.000	6.267E-09.1000	0.000E+00.000	3.604E-08.1000								

E (MeV)	angle integrated	mu max	deg min	energy integrated
5.000000E+00	0.000E+00.000	-0.906307787037	155.00000000	5.949E-05.033
1.000000E+01	1.928E-04.006	-0.819132504269	145.00000000	6.467E-05.033
1.500000E+01	1.267E-04.008	-0.422618261741	115.00000000	8.510E-05.014
2.000000E+01	5.770E-05.012	-0.258819045103	105.00000000	1.147E-04.018
2.500000E+01	2.335E-05.018	-0.087155427248	95.00000000	1.297E-04.017
3.000000E+01	9.052E-06.029	0.087155427248	85.00000000	1.496E-04.015
3.500000E+01	2.325E-06.049	0.573576436351	55.00000000	2.062E-04.008
4.000000E+01	1.184E-06.081	0.707106781187	45.00000000	2.549E-04.014
4.500000E+01	3.608E-07.147	0.906307787037	25.00000000	2.818E-04.011
5.000000E+01	1.726E-07.213	0.965925826289	15.00000000	3.204E-04.018
5.500000E+01	3.922E-08.447	1.000000000000	0.00000000	3.299E-04.024
6.000000E+01	7.844E-09.1000			
6.500000E+01	2.353E-08.577			

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Figure 2: Comparison of emitted ³He and ⁶Li angle-integrated fragment spectra for the reaction 200 MeV p + ²⁷Al, calculated by MCNP6 (red dashed lines) and CEM03.03 (blue solid lines).

Figure 3: Comparison of emitted ${}^6\text{Li}$ double differential spectra for the reaction 200 MeV p + ^{27}Al , at an emission angle of 20° , calculated by MCNP6 (red dashed lines) and CEM03.03 (blue solid lines).

Figure 4: Example of MCTAL production cross section plot. Comparison of emitted ${}^6\text{Li}$ double differential spectra for the reaction 200 MeV $p + {}^{27}\text{Al}$, at an emission angle of 20° , calculated by MCNP6 (red dashed lines) and CEM03.03 (blue solid lines).

3 Further Tests

We additionally tested this GENXS heavy-ion expansion with several different event generators (CEM03.03, Bertini+Dresner+RAL, INCL+ABLA, and LAQGSM03.03). Results of this test appear in Fig. 5. Results are as we expect.

Furthermore, we tested MCNP6 with the GENXS heavy-ion expansion on a nucleus-induced reaction using the LAQGSM03.03 event generator. Results of this simulation compared with experimental data are seen in Fig. 6. Similar results were found in Example 6.5 of the MPI Testing Primer (LA-UR-13-26944).

We also tested our GENXS expansion running MPI, as well as with the 1400+ test suite. We conclude that this expansion works as expected across several different event generators and for both nucleon- and nucleus-induced reactions.

Figure 5: Comparison of emitted ${}^3\text{He}$ and ${}^4\text{He}$ angle-integrated fragment spectra for the reaction 200 MeV p + ${}^{27}\text{Al}$, calculated by MCNP6 with CEM03.03 (blue solid lines), with Bertini (red dashed lines), with LAQGSM03.03 (purple dash-dotted lines), and with INCL-ABLA (green dotted lines), all run with the GENXS expansion for heavy ions discussed in this paper.

Figure 6: Comparison of emitted neutron double differential spectra for the reaction 600 MeV/A $^{28}\text{Si} + {}^{\text{nat}}\text{Cu}$, at an emission angle of 20° , calculated by MCNP6 with LAQGSM03.03 with this GENXS heavy-ion expansion (blue solid line), compared to results by Heilbronn, et al (green points).