Title: MCNP6 Enhancements to Alpha Particle Production and Transport

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MCNP6 Enhancements to Alpha Particle Production and Transport

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INTRODUCTION

Recent interest in improved alpha-particle production and transport as well as the availability of ACE alpha cross-section data has led to several new features in the all-energy, all-particle transport code MCNP. In early 2004, work began on a physics model that would use the CINDER90 depletion code in conjunction with a delayed-particle library to allow for production of delayed neutrons, gammas, and betas and has recently been expanded to allow for delayed alpha production.[1] Delayed-neutrons data can be sampled from two sources by using the DN keyword on the ACT card.[2] The sampling may be taken from ACE library data for fission only or model data for fission and/or activation. There are also options to use a combination of both and to treat all neutrons as prompt. The sampling of delayed gammas also can be taken from two sources via the DG keyword on the ACT card. The sampling can be taken from the original 25 group model data or have the model data augmented by line emission data from ENDF/B-VII. Delayed-beta and now alpha-particle production is done solely with ENDF/B-VII data populated into the latest version of DELAY_LIBRARY.DAT in a 10 keV bin structure. The isotope spectra to be sampled for delayed betas and alphas are calculated by CINDER90. The type of delayed-particle creation can be controlled using the FISSION and NONFISS keywords on the ACT card. The FISSION keyword allows the user to select which, if any, of the 4 available delay particles will be produced from induced fission products and their decay chains, as calculated by CINDER90. The NONFISS keyword allows the user to select which, if any, of the 4 delay particles to sample from non-fission nuclear reactions or spontaneous decay. In addition to these new production capabilities, MCNP6.1.1 now allows for library cross-sections to be used in the transport of alpha particles which greatly increases the types of sources that can be modeled. Light ion transport has traditionally been achieved through model physics for atomic and nuclear interactions. For low energy coulombic interactions the continuous slowing down approximation (CSDA) is used to compute stopping power tables for each particle/material combination, (Table 85 in MCNP output). The stopping powers are calculated using the Bethe-Bloch model with the Sternheimer and Peierls density effect correction for energies above 5.24 MeV/AMU as well as the SPAR model for energies below 1.31 MeV/AMU with linear interpolation between the two models.[3] The energy spacing of the stopping powers computed as well as choice of scattering model can be selected using the PHYS card. The transition energies and model selection options for the high energy nuclear physics models is controlled with the LCA, LCB, LEA, LEB, and LCC cards.[2] While the nuclear physics models are very useful, their accuracy is highly dependent on the energies being sampled. This, along with the speed loss when using models is the motivation for using good library cross-sections. This data now available in the ACE-formatted files such as TENDL 2012 can be used in the transport of alpha particles. Utilizing the new production capability for delayed alphas along with the ability to use cross-section data for (α,n) reactions allows for much broader modeling capability within MCNP6. In particular, this work will show how neutron generators like plutonium-beryllium (PuBe) sources can be modeled using the spontaneous alpha decay feature along with the (α,n) production cross-section data from TENDL 2012. An MCNP6 PuBe source has been benchmarked to SOURCES 4C as well as benchmarking of the TENDL 2012 (α,n) yields to illustrate where possible sources of error lie.

DESCRIPTION OF ACTUAL WORK

Spontaneous Decay Time Integration

Previous versions of MCNP had large errors (~100%) when sampling the spontaneous-decay spectrum from a decay chain with a large spread in half-lives. This problem has been addressed by setting all decay constants to unity. This does not affect the physics since the spontaneous-decay option assumes equilibrium. This allows for uniformly spaced time bins from 1e-3 to 20 s which greatly reduces the error (~20%). If a limited number of progeny in the decay chain are required, the upper limit of the time bins can be changed from 20 s to a user input on the DBCN 55th entry. Delayed particle emission can be integrated in two ways. The default integrates over 10^{10} s with 99 time steps. However, for longer half-lives the DBCN 10th entry can be set to the half-life of the longest lived isotope of interest which increases the number of time steps to 234. The results of the uniform time binning and time integration change can be seen in Figs. 1 and 2.

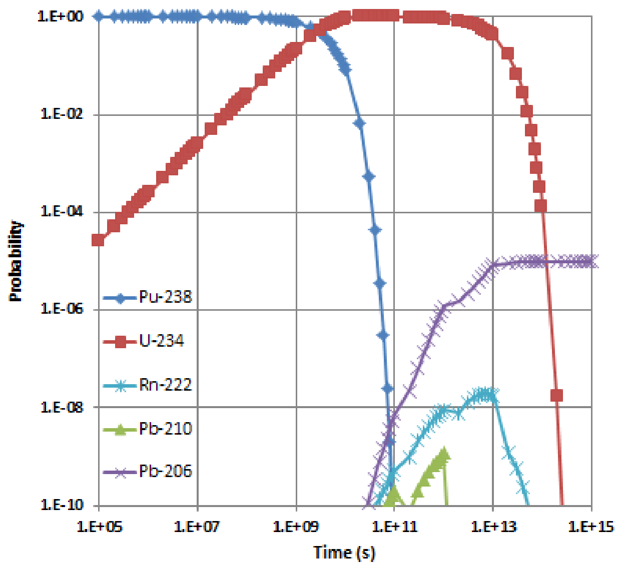

Fig. 1. CINDER90 time-dependent atom densities for the decay of Pu-238, using the refined time-bin structure (1e-6 to 1e20 s, every whole number of every decade).

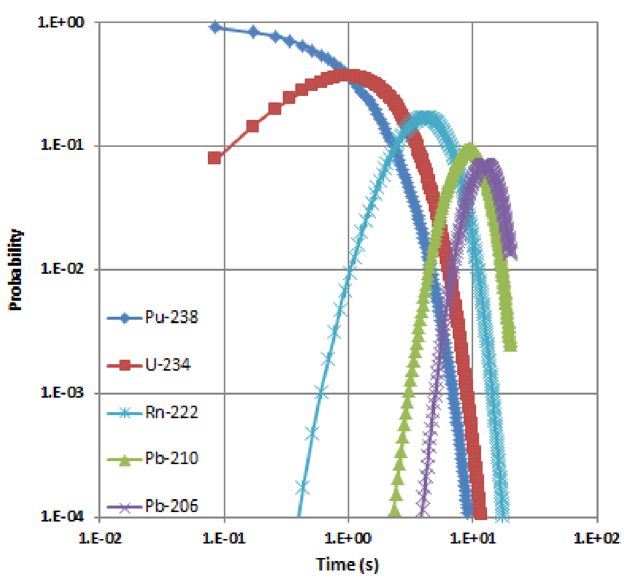

Fig. 2. CINDER90 time-dependent atom densities for the decay of Pu-238, using unity for all decay constants and 234 bins within 20 s.

Delayed Alpha Sources

The delayed-alpha source option can be accessed in two ways. The first option is to use the PAR=SA keyword which will calculate via CINDER any radioactive isotopes in the material cards and sample their spectra from the DELAY_LIBRARY.DAT file. The second method is to specify the isotope the user wishes to decay using the PAR=ZAID and ERG=0 keywords. Using this method also requires heavy ion transport to be turned on by placing # on the MODE card.[2] By decreasing the time interval to be integrated over from 26 orders of magnitude to at most 4 when using 20 s greatly improves the accuracy of the spectrum as can be seen in Fig 3. Using the old time interval (1e-6 – 1e20 s), with 99 bins, results in larger statistical errors as well as an integral alpha production of ~1 alpha/decay. Using the new time interval (1e-3 – 20 s), with 99 bins, results in ~6 alphas/decay and using the 234 bin structure results in ~7 alphas/decay.

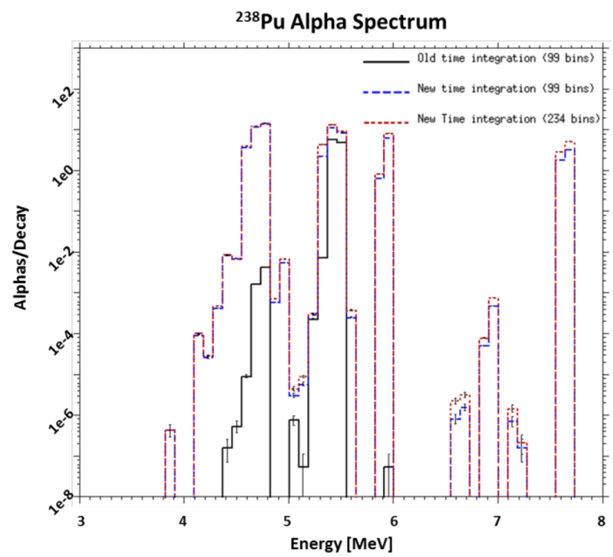

Fig. 3. Alpha spectrum of ^{238}Pu decay illustrating the results of decreasing the integrated time interval to 20 s, as well as increasing the number of time bins used for integration. Old time interval utilizing 99 bins resulted in ~1 alpha/decay while the new time interval using 99 and 234 bins resulted in ~6 and ~7 alphas/decay respectively.

Thick Target (α,n) Yields

The new alpha transport library capability in MCNP6 was recently used to benchmark the TENDL 2012 alpha cross-section library by comparing thick target (α,n) yields.[4] The results varied by target and incident alpha energy. Beryllium was of particular interest for the application of modeling neutron sources which very often use ^{9}Be for (α,n) neutron generation as well as (n,2n) neutron multiplication. Fig 4 shows the percent relative errors for ^{9}Be neutron production over the published energy spectrum. The errors are shown to be high, especially around 4 MeV. This library was used to benchmark a PuBe source against SOURCES 4C to show the capability while acknowledging the accuracy will be based on the quality of the data libraries used.

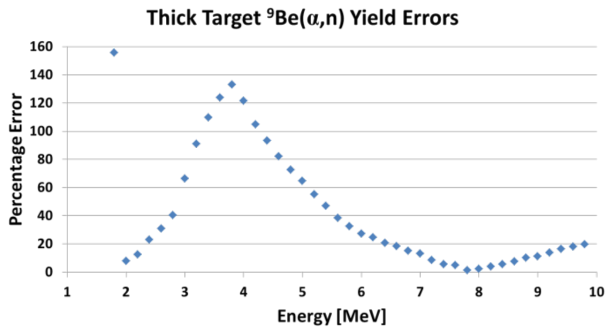

Fig. 4. Percentage error in the MCNP6 thick target (α,n) yields for ^{9}Be as compared to published values. Data taken from *Comparing Measured (a,n) Thick Target Yields to MCNP6 using TENDL 2012 Libraries.*[4]

PuBe Source Benchmark

To demonstrate both the spontaneous-alpha decay feature as well as the alpha library cross-section transport, a PuBe source was modeled and the neutron spectrum was compared with the SOURCES 4C code as well as experimental data. The SOURCES 4C code produces neutron production rates and spectra from (α,n) reactions, spontaneous fission, and delayed neutron emission from radioactive isotope decay.[5] SOURCES 4C is well benchmarked and has very fast computational times, but in doing so leaves out details that are very important to some users. For example, SOURCES 4C does not give the spectra of any of the decay progeny, only the parent isotope. In order to replicate this in MCNP6 the 55th entry on the DBCN card is used. The 55th entry controls the time interval to be integrated over. In the new time-integration method all decay constants are set to unity and therefore setting the DBCN 55th entry to ~1.5 s will sample almost exclusively the first decay only. For most users this can be used to select how far down a decay chain a user wishes to sample. In order to replicate SOURCES 4C and not sample any of the daughter nuclides the DBCN 55th entry was set to the minimum value of 1e-3 s. By setting the time integration interval less than 1 the results had to be renormalized by a factor of 1000 to maintain the output in neutrons per decay. The final MCNP6 tally was also multiplied by the activity of the PuBe source and divided by the volume of the source to obtain results in neutrons per second per cm^3 as to compare to SOURCES 4C output. The resulting spectra are shown in Fig 5 and the integral flux results are tabulated in Table 1.

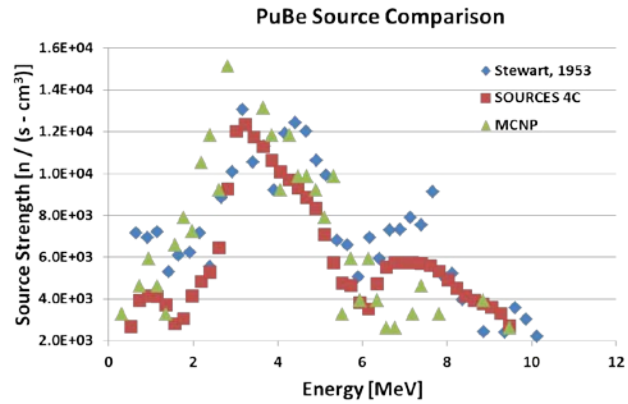

Fig. 5. MCNP6 PuBe source comparison to SOURCES 4C and Stewart's experimental data.[6] Data was normalized to n/(s-cm^3) to match SOURCES 4C output.

Table 1. Integral neutron Source Strength

Experiment	Source Strength n/(s-cm^3)	Relative Error
Stewart, 1953[6]	2.2e5	-
SOURCES 4C	2.7e5	22.3 %
MCNP6	2.9e5	28.9 %

CONCLUSIONS

New enhancements to alpha-particle production and transport have been added to the Monte Carlo transport code MCNP6. These enhancements include the sampling of delayed-alpha particles from the decay of activated materials, a refined time integration method to more accurately sample delayed alphas, and the ability to use ACE-formatted cross-section libraries for the transport of alpha particles. These enhancements allow the full modeling of neutron sources such as PuBe sources with reduced computational times using libraries rather than models for transport. The accuracy of these models will depend highly on the quality of the cross-section data used.

ENDNOTES

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