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DELAYED-GAMMA SIGNATURE CALCULATION FOR NEUTRON-INDUCED FISSION AND ACTIVATION USING MCNPX. PART III. TRANSPORT THEORY.

by

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ABSTRACT

In Parts I and II, we presented the MCNPX Monte Carlo delayed-gamma theory and illustrative simulation results. The complexity and diversity of the relevant physics items can render the comprehension of their scope and interrelationship difficult. In Part III we augment the Monte Carlo formulation of Part I using transport theory as an means of showing the physics content for the MCNPX delayed-gamma feature.

KEYWORDS: MCNPX; CINDER'90; fission-product; delayed-gamma; activation; transport theory.

1. INTRODUCTION.

In Part I we examined the Monte Carlo formulation of the MCNPX (Pelowitz, 2008) delayed-gamma feature. This feature was seen to consist of an assortment of absorption, transmutation, and emission physics items for neutrons, photons, and radionuclides. These items were used to develop cumulative distribution functions (CDFs) that are used for sampling the number, energy, time, and direction of gammas arising from the radioactive decay of fission or activation products.

CDF formation and sampling is not necessarily an inherently complicated issue. However, because there are several physics items involved in the delayed-gamma feature, and because Monte Carlo does not involve the casting of these physics items into a transport-like equation, it can be a taxing exercise to visualize and understand how all of the physics items interrelate in the context of MCNPX simulation capability. The MCNPX User's Manual (Pelowitz, 2008) contains information about the physics items, but the information is limited to input-file "cards" and variable switches.

Here we cast the relevant MCNPX delayed-gamma physics items using a Boltzmann transport representation. Transport theory is a useful means of succinctly encapsulating transport physics into, for the case of the MCNPX delayed-gamma feature, a few coupled equations. We emphasize that MCNPX does not solve the transport equation—it performs Monte Carlo based simulation involving CDF sampling. But we offer the transport formulation as an alternative means of identifying the physics mechanisms involved in the MCNPX delayed-gamma feature.

2. MCNPX COUPLED NEUTRON-PHOTON TRANSPORT.

MCNPX treats many types of neutron and photon interactions when executed in coupled neutron-photon mode for fissioning systems, including the newest feature involving delayed-gamma line-emission by fission products created by neutron-induced fission. These interactions include the production of delayed neutrons and gammas due to fission induced by sub-20-MeV neutrons and, using LAHET (Los Alamos High-Energy Transport; Wilson et al., 1993; Waters, 1999; Pelowitz, 2008) higher-energy neutrons (> 20 MeV). MCNPX treats lower-energy photon interactions involving photoatomic interaction mechanisms (e.g., photoelectric absorption, Compton scatter, and pair production) with simulation options of simple or detailed models (which either ignore or include incoherent scattering and photoelectric-absorption fluorescent-photon creation). In addition, the LAHET component of MCNPX is used to model high-energy photoneutron and photofission interactions. When available, photofission is treated using photofission-yield data; otherwise, neutron-fission yield data (with an "A-1" correction) are used as an approximation for photofission yield data (Durkee et al., 2009). The equations given below, as well as the sampling-equation presentation given later in this paper, suitably characterize the basic theory for the current and prospective upgrades involving delayed-gamma line emission by both neutron- and photon-induced fission for MCNPX.

2.1. Boltzmann transport and isotopic-transmutation equations.

Although MCNPX is a Monte Carlo code, it is useful to view the classical* integrodifferential form of the coupled Boltzmann neutron and photon transport equations† and the associated delayed neutron and gamma precursor equations in order to better understand the assortment of coupled neutron-photon transport mechanisms treated by MCNPX. The MCNPX delayed-gamma capability is designed to execute in "fixed-source" mode rather than in "eigenfunction" mode. As such, the relevant source form of the linear Boltzmann equations‡ for coupled prompt and delayed neutron and photon transport (Keepin, 1965, pp. 161–162; Williams, 1966; Bell and Glasstone, 1970; Hetrick, 1971; Massimo, 1976; Liew and Ku, 1991) and the nuclide transmutation equations (England et al., 1976; Wilson et al., 1995) can be written as

Neutron flux

$$
\begin{aligned}
\frac{1}{\mathrm{v}}\frac{\partial\Phi}{\partial t} = & -\hat{\Omega}\cdot\vec{\nabla}\Phi(\vec{r},E_n,\hat{\Omega}_n,t) - [\Sigma_{n,\vec{T}}(\vec{r},E_n,t)+\Sigma_{n,\gamma}(\vec{r},E_n,t)]\Phi(\vec{r},E_n,\hat{\Omega}_n,t) \\
& + \int\int\sum_{x\neq f}\Sigma_{n,x}(\vec{r},E'_n,t)f_{n,x}(\vec{r};E'_n\to E_n,\hat{\Omega}'_n\to\hat{\Omega}_n;t)\Phi(\vec{r},E'_n,\hat{\Omega}'_n,t)d\hat{\Omega}'_n dE'_n \\
& + \int\int\chi_{n,n}(E'_n\to E_n)[1-\beta_{n,n}(\vec{r},E'_n)]\nu_{n,n}(\vec{r},E'_n)\Sigma_{n,f}(\vec{r},E'_n,t)\Phi(\vec{r},E'_n,\hat{\Omega}'_n,t)d\hat{\Omega}'_n dE'_n \\
& + \int\int\chi_{\gamma,n}(E'_\gamma\to E_n)[1-\beta_{\gamma,n}(\vec{r},E'_\gamma)]\nu_{\gamma,n}(\vec{r},E'_\gamma)\Sigma_{\gamma,f}(\vec{r},E'_\gamma,t)\Gamma(\vec{r},E'_\gamma,\hat{\Omega}'_\gamma,t)d\hat{\Omega}'_\gamma dE'_\gamma \\
& + \sum_{i=1}^{I}\sum_{p=1}^{P_i}N_{i:p}(\vec{r},t)\lambda_{i:p}p_{n:i:p}(E_n,\hat{\Omega}_n) + \sum_{j=1}^{J}\sum_{q=1}^{Q_j}N_{j:q}(\vec{r},t)\lambda_{j:q}p_{n:j:q}(E_n,\hat{\Omega}_n) \\
& + \Sigma_{\gamma,n}(\vec{r},E_\gamma,t)\Gamma(\vec{r},E_\gamma,\hat{\Omega}_\gamma,t) + S_n(\vec{r},E_n,\hat{\Omega}_n,t)
\end{aligned}
\tag{1}
$$

---

* Quantum effects are neglected.

† Neither the equations nor the boundary conditions contain any random element. Thus, although traditionally the term "deterministic" has been considered as a property of the numerical solution methods, with the advent of stochastic transport equations the formulation is sometimes termed deterministic (Dubi, 1986; Morel, 2007; Williams, 2007) . For a discussion of stochastic transport theory, see Bell (1965), Williams (2006), Levermore et al. (1986), Adams et al. (1989), and Munoz-Cubo and Verdu (2003).

‡ MCNPX treats all particles as point particles.

Photon flux

$$
\begin{aligned}
\frac{1}{c}\frac{\partial \Gamma}{\partial t} = & -\hat{\Omega}\cdot\vec{\nabla}\Gamma(\vec{r},E_\gamma,\hat{\Omega}_\gamma,t) - [\Sigma_{\gamma,\vec{r}}(\vec{r},E_\gamma,t)+\Sigma_{\gamma,n}(\vec{r},E_\gamma,t)]\Gamma(\vec{r},E_\gamma,\hat{\Omega}_\gamma,t) \\
& + \int\int\sum_{x\neq f}\Sigma_{\gamma,x}(\vec{r},E_\gamma,t) f_{\gamma,x}(\vec{r};E'_\gamma \to E_\gamma,\hat{\Omega}'_\gamma \to \hat{\Omega}_\gamma;t)\Gamma(\vec{r},E'_\gamma,\hat{\Omega}'_\gamma,t)d\hat{\Omega}'_\gamma dE'_\gamma \\
& + \int\int\chi_{\gamma,\gamma}(E'_\gamma \to E_\gamma)[1-\beta_{\gamma,\gamma}(\vec{r},E'_\gamma)]\nu_{\gamma,\gamma}(\vec{r},E'_\gamma)\Sigma_{\gamma,f}(\vec{r},E'_\gamma,t)\Gamma(\vec{r},E'_\gamma,\hat{\Omega}'_\gamma,t)d\hat{\Omega}'_\gamma dE'_\gamma \\
& + \int\int\chi_{n,\gamma}(E'_n \to E_\gamma)[1-\beta_{n,\gamma}(\vec{r},E'_n)]\nu_{n,\gamma}(\vec{r},E'_n)\Sigma_{n,f}(\vec{r},E'_n,t)\Phi(\vec{r},E'_n,\hat{\Omega}'_n,t)d\hat{\Omega}'_n dE'_n \\
& + \underline{\sum_{i=1}^{I}\sum_{p=1}^{P_i} N_{i:p}(\vec{r},t)\lambda_{i:p}p_{\gamma:i:p}(E_\gamma,\hat{\Omega}_\gamma)} + \underline{\sum_{j=1}^{J}\sum_{q=1}^{Q_j} N_{j:q}(\vec{r},t)\lambda_{j:q}p_{\gamma:j:q}(E_\gamma,\hat{\Omega}_\gamma)} \\
& + \Sigma_{n,\gamma}(\vec{r},E_n,t)\Phi(\vec{r},E_n,\hat{\Omega}_n,t) + S_\gamma(\vec{r},E_\gamma,\hat{\Omega}_\gamma,t)
\end{aligned}
\tag{2}
$$

and, for $i=1,\ldots,I;\, p=1,\ldots,P_i$ and $j=1,\ldots,J;\, q=1,\ldots,Q_j$,

Nuclide density stemming from neutron-induced transmutation and decay

$$
\begin{aligned}
\frac{\partial N_{i:p}(\vec{r},t)}{\partial t} = & \int\int\left[\sum_{k\neq p}^{P_i} N_k(\vec{r},t)\sigma_{k\to p}(\vec{r},E_n) - N_{i:p}(\vec{r},t)\sigma_{n,a}(\vec{r},E_n)\right]\Phi(\vec{r},E_n,\hat{\Omega}_n,t)d\hat{\Omega}_n dE_n \\
& + \int\int\sum_{m=1}^{M} y_{n:m\to i}(\vec{r},E_n)\Sigma_{n,f:m}(\vec{r},E_n,t)\Phi(\vec{r},E_n,\hat{\Omega}_n,t)d\hat{\Omega}_n dE_n \\
& + \sum_{k\neq p}^{P_i}\lambda_{k\to i:p}N_k(\vec{r},t) - \lambda_{i:p}N_{i:p}(\vec{r},t)
\end{aligned}
\tag{3}
$$

Nuclide density stemming from photon-induced transmutation and decay

$$
\begin{aligned}
\frac{\partial N_{j:q}(\vec{r},t)}{\partial t} = & \int\int\left[\sum_{l\neq q}^{Q_j} N_l(\vec{r},t)\sigma_{l\to q}(\vec{r},E_\gamma) - N_{j:q}(\vec{r},t)\sigma_{\gamma,a}(\vec{r},E_\gamma)\right]\Gamma(\vec{r},E_\gamma,\hat{\Omega}_\gamma,t)d\hat{\Omega}_\gamma dE_\gamma \\
& + \int\int\sum_{m=1}^{M} y_{\gamma:m\to j}(\vec{r},E_\gamma)\Sigma_{\gamma,f:m}(\vec{r},E_\gamma,t)\Gamma(\vec{r},E_\gamma,\hat{\Omega}_\gamma,t)d\hat{\Omega}_\gamma dE_\gamma \\
& + \sum_{l\neq q}^{Q_j}\lambda_{l\to j:q}N_l(\vec{r},t) - \lambda_{j:q}N_{j:q}(\vec{r},t)
\end{aligned}
\tag{4}
$$

2.2. Variable definitions.

In this section, the various variable definitions and conventions used in Eqs.(1)–(4) are provided. We define

$\Phi(\vec{r}, E_n, \hat{\Omega}_n, t)$ = time-dependent angular neutron flux (neutrons/m^2-sr-s-MeV)

$\Gamma(\vec{r}, E_\gamma, \hat{\Omega}_\gamma, t)$ = time-dependent angular photon flux (photons/m^2-sr-s-MeV)

t = is time (s)

$\vec{r}$ = position (m)

v = neutron speed (m s^{-1})

c = speed of light (m s^{-1})

E_n = neutron energy (MeV)

E_γ = gamma energy (MeV)

$\hat{\Omega}_n$ = neutron direction vector

$\hat{\Omega}_\gamma$ = photon direction vector

$f_{n,x}(\vec{r}; E_n' \to E, \hat{\Omega}_n' \to \hat{\Omega}_n; t)$ = neutron transfer probabilities (neutrons/sr-MeV)

$f_{\gamma,x}(\vec{r}; E_\gamma' \to E_\gamma, \hat{\Omega}_\gamma' \to \hat{\Omega}_\gamma; t)$ = photon transfer probabilities (photons/sr-MeV)

$S_n(\vec{r}, E_n, \hat{\Omega}_n, t)$ = inhomogeneous neutron sources (neutrons/m^3-sr-s-MeV)

$S_\gamma(\vec{r}, E_\gamma, \hat{\Omega}_\gamma, t)$ = inhomogeneous photon (photons/m^3-sr-s-MeV)

$\nu_{n,n}(\vec{r},E_n')$ = expected total number of neutrons emitted per fission at $\vec{r}$ due to a neutron of energy E_n'

$\nu_{\gamma,n}(\vec{r},E_\gamma')$ = expected total number of neutrons emitted per fission at $\vec{r}$ due to a photon of energy E_γ'

$\nu_{\gamma,\gamma}(\vec{r},E_\gamma')$ = expected total number of photons emitted per fission at $\vec{r}$ due to a photon of energy E_γ'

$\nu_{n,\gamma}(\vec{r},E_n')$ = expected total number of photons emitted per fission at $\vec{r}$ due to a neutron of energy E_n'

$\beta_{n,n}(\vec{r},E_n')$ = fraction of the total numbers of neutrons that come from the pth neutron precursor due to neutron fission (delayed neutrons/neutron)

$\beta_{\gamma,\gamma}(\vec{r},E_\gamma')$ = fraction of the total numbers of photons that come from the qth photon precursor due to photofission (delayed photons/photon)

$\beta_{\gamma,n}(\vec{r},E_\gamma')$ = fraction of the total numbers of neutrons that come from the pth neutron precursor due to photofission (delayed neutrons/photon)

$\beta_{n,\gamma}(\vec{r},E_n')$ = fraction of the total numbers of photons that come from the pth neutron precursor due to neutron fission (delayed photons/neutron)

$N_{i;p}(\vec{r},t)$ = delayed-particle precursor isotopic concentrations for the $i=1,\ldots,I$ fission products (or residual nuclides) created by neutron-induced fission (atoms/m^3); subscript p indicates that there are $p=1,\ldots,P_i$ radioactive decay products for the ith fission product (or residual nuclide).

$N_{j;q}(\vec{r},t)$ = delayed-particle precursor isotopic concentrations for the $j=1,\ldots,J$

fission products (or residual nuclides) created by photofission (atoms/m^3); subscript q indicates that there are $q = 1, \ldots, Q_q$ radioactive decay products for the jth photofission product (or residual nuclide).

$\lambda_{i:p}$ = radioactive decay constants for the P_i delayed-neutron precursors (decay/atom-s)

$\lambda_{j:q}$ = radioactive decay constants for the Q_j delayed-photon precursors (decay/atom-s)

$\chi_{n,n}(E_n' \rightarrow E_n)$ = prompt-neutron emission spectra due to neutron fission (neutrons/MeV-sr-prompt neutron)

$\chi_{\gamma,n}(E_\gamma' \rightarrow E_n)$ = prompt-neutron emission spectra due to photofission (neutrons/MeV-sr-prompt neutron)

$\chi_{\gamma,\gamma}(E_\gamma' \rightarrow E_\gamma)$ = prompt-photon emission spectra due to photofission (photons/MeV-sr-prompt photon)

$\chi_{n,\gamma}(E_n' \rightarrow E_\gamma)$ = prompt-photon emission spectra due to neutron fission (photons/MeV-sr-prompt photon)

$p_{n:i:p}(E_n, \hat{\Omega}_n)$ = delayed-neutron spectra as a function of the emerging neutron energy E_n due to the decay of fission products created by neutron fission (neutrons/decay-sr-MeV)

$p_{n:j:q}(E_n, \hat{\Omega}_n)$ = delayed-neutron spectra as a function of the emerging neutron energy E_n due to the decay of fission products created by photofission (neutrons/decay-sr-MeV)

$p_{\gamma:i:p}(E_\gamma, \hat{\Omega}_\gamma)$ = delayed-gamma emission spectra due to the decay of fission products created by neutron fission (photons/decay-sr-MeV)[†]

$p_{\gamma:j:q}(E_\gamma, \hat{\Omega}_\gamma)$ = delayed-gamma emission spectra due to the decay of fission products created by photofission (photons/decay-sr-MeV)

$\Sigma_{n,\bar{T}}(\vec{r}, E_n, t)$ = total macroscopic neutron cross sections excluding radiative capture (neutrons/m)

$\Sigma_{\gamma,\bar{T}}(\vec{r}, E_\gamma, t)$ = total macroscopic photon cross sections excluding radiative capture (photons/m)

$\Sigma_{n,\gamma}(\vec{r}, E_n, t)$ = macroscopic radiative-capture cross section (neutrons/photon-m)

$\Sigma_{\gamma,n}(\vec{r}, E_\gamma, t)$ = macroscopic photoneutron-production cross section (photons/neutron-m)

$\Sigma_{n,x}(\vec{r}, E'_n, t)$ = total macroscopic neutron-interaction cross sections excluding fission (neutrons/m)

$\Sigma_{\gamma,x}(\vec{r}, E_\gamma, t)$ = total macroscopic photon-interaction cross sections excluding fission (photons/m)

$\Sigma_{n,f:m}(\vec{r}, E_n, t)$ = macroscopic neutron fission cross sections for the $m = 1, \ldots M$ fissioning nuclides (fissions/neutron-m)

$\Sigma_{\gamma,f:m}(\vec{r}, E_\gamma, t)$ = macroscopic photofission cross sections for the $m = 1, \ldots M$ fissioning nuclides (fissions/photon-m)

$\Sigma_{n,f}(\vec{r}, E'_n, t)$ = total macroscopic neutron fission cross section (fissions/neutron-m)

[†] The emission spectra for neutrons and photons for each fission product are dependent on the mechanism inducing the fission. Therefore, the subscripts p and q serve to distinguish those chains that are created by neutron fission and photofission.

$\Sigma_{\gamma,f}(\vec{r},E'_\gamma,t)$ = total macroscopic photofission cross section (fissions/photon-m)

$y_{n:m\to i}(\vec{r};E_n)$ = neutron-induced fission-product yield data (atoms/fission)

$y_{\gamma:m\to j}(\vec{r};E_\gamma)$ = photon-induced fission-product yield data (atoms/fission)

The quantities $\beta_{n,n}(\vec{r},E'_n)$ and $\beta_{\gamma,\gamma}(\vec{r},E'_\gamma)$ satisfy

$$\beta_{n,n}(\vec{r},E'_n)=\sum_{p=1}^{P}\beta_{n,n:p}(\vec{r},E'_n),\quad \beta_{\gamma,\gamma}(\vec{r},E'_\gamma)=\sum_{q=1}^{Q}\beta_{\gamma,\gamma:q}(\vec{r},E'_\gamma)\,, \tag{5}$$

while the quantities $\beta_{\gamma,n}(\vec{r},E'_\gamma)$ and $\beta_{n,\gamma}(\vec{r},E'_n)$ satisfy

$$\beta_{\gamma,n}(\vec{r},E'_\gamma)=\sum_{q=1}^{Q}\beta_{\gamma,n:q}(\vec{r},E'_\gamma),\quad \beta_{n,\gamma}(\vec{r},E'_n)=\sum_{p=1}^{P}\beta_{n,\gamma:p}(\vec{r},E'_n)\,. \tag{6}$$

2.3. Equation descriptions.

Equations (1) and (2) are the coupled time-dependent Boltzmann equations for the neutron and photon angular fluxes. Equations (3) and (4) are representations of the isotopic-chain delayed-particle precursor equations for neutron- and photon-induced reactions. Brief termwise descriptions are presented in Tables 1-4, with in-depth descriptions presented in the ensuing sections. Please note that the descriptions pertain to the delayed-gamma upgrades. This means that some terms are not calculated or are treated approximately, e.g., the flux-induced isotopic transmutation terms.

Table 1. Equation 1 termwise descriptions

Line	Term	Description	Calculated in MCNPX
1	1	Time rate of change of neutron angular flux	Y
	2	Neutron streaming	Y
	3	Loss by neutron absorption	Y
2	1	Prompt nonfission neutron source	Y
3	1	Prompt neutron source due to neutron fission	Y
4	1	Prompt neutron source due to photofission	Y
5	1	Delayed-neutron production due to precursors formed by neutron fission	Y
	2	Delayed-neutron production due to precursors formed by photofission	Y
6	1	Photonuclear neutron production	Y
	2	Inhomogeneous source	Y

Table 2. Equation 2 termwise descriptions

Line	Term	Description	Calculated in MCNPX
1	1	Time rate of change of photon angular flux	Y
	2	Photon streaming	Y
	3	Loss by photon absorption	Y
2	1	Prompt nonfission photon source	Y
3	1	Prompt photon source due to photofission	Y
4	1	Prompt photon source due to neutron fission	Y
5	1	Delayed-photon production due to precursors formed by neutron fission	Y
	2	Delayed-photon production due to precursors formed by photofission	Y
6	1	Radiative-capture photon production	Y
	2	Inhomogeneous source	Y

Table 3. Equation 3 termwise descriptions

Line	Term	Description	Calculated in MCNPX
1	1	Time rate of change of precursors created by neutron fission	Y
	2	Neutron-induced transmutation source	Y†
	3	Neutron-induced transmutation loss	Y†
2	1	Neutron-induced fission source	Y
3	1	Decay source	Y
	2	Decay loss	Y

†Simple-multi-particle reactions are treated. See the following section for details.

Table 4. Equation 4 termwise descriptions

Line	Term	Description	Calculated in MCNPX
1	1	Time rate of change of precursors created by photofission	Y
	2	Photon-induced transmutation source	Y
	3	Photon-induced transmutation loss	N
2	1	Photon-induced fission source	Y
3	1	Decay source	Y
	2	Decay loss	Y

Equation 1: Neutron flux.

Terms 1–3 in line 1 represent the time rate of change of the angular neutron flux, streaming, and neutron loss due to absorption, respectively. The absorption term is separated into a piece for mechanisms other than prompt radiative capture production and another that explicitly shows this mechanism. All terms are treated by MCNPX.

Line 2 represents the source of prompt neutrons at $\vec{r};t$ due to the integrated contribution of all non-fission interactions at $\vec{r};E_n';t$ and all angular neutron flux directions $\hat{\Omega}_n'$. This term is treated by MCNPX.

Lines 3 and 4 represent the prompt-neutron production due to fission induced by neutrons and photons, respectively. MCNPX calculates both terms using library data.

Term 1 in Line 5 is the delayed-neutron production due to the decay of precursors formed by neutron fission. For Monte Carlo delayed-neutron energy emission, this term is integrated over all position, direction, and time and is integrated to some randomly sampled energy to calculate particle emission energy. Currently, this energy sampling is handled approximately in MCNPX using a set of pre-integrated values (Madland-Nix formalism, Madland 1988; http://t2.lanl.gov) that are cast in six precursor groups ($P = 6$) and 300 energy groups. These data are stored in data statements (in routine **CID**) for use during execution. This energy-sampling technique differs from the technique used for delayed gammas (see Section 5). However, upgrades are now scheduled to produce the necessary $p_{n:i:p}(E_n)$ experimental data and the MCNPX upgrades to make the delayed-neutron sampling technique commensurate with the delayed-gamma capability.

Term 1 in Line 5 is evaluated for Monte Carlo delayed-neutron time emission by integrating over all position, direction, and energy, followed by integration to some randomly sampled time. Data are available (in cinder.dat) for the energy-integrated isotropic emission probabilities $p_{n:i:p} = \int_0^\infty p_{n:i:p}(E_n)dE_n$. Thus, sampling distributions for

delayed-neutron emission time are calculated in MCNPX by integrating $\sum_{i=1}^{I}\sum_{p=1}^{P_i} N_{i:p}(\vec{r},t)\lambda_{i:p}p_{n:i:p}$ to times t_j. This time-CDF calculation procedure is similar to the delayed gamma treatment, but, as is indicated in term 1 of line 5 in Eq. (2) and as will be detailed in Section 5, the individual line-emission values are used for delayed gammas. Once the new $p_{n:i:p}(E_n)$ data are available, the time-CDF treatment for delayed neutrons will be modified to conform to the delayed-gamma treatment.

Term 2 in line 5 is the delayed-neutron production due to the decay of precursors formed by photofission. This term is treated in the same manner as that for term 1 of line 5.

Line 6, term 1 is photonuclear neutron production, which is calculated using mix and match, using table data when available and physics models otherwise.

Term 2 of line 6 is the inhomogeneous neutron source. The MCNPX code user stipulates this term via the MCNPX "sdef" source card. Its content can range from a simple monoenergetic single-pulse point source to complicated energy-, space-, and time-dependent neutron sources.

The atom densities embedded in the macroscopic cross sections in the terms in lines 1–4 and in term 1 of line 6 are the cell-based material atom densities (stipulated in the MCNPX input file) that are used to do MCNPX particle transport. Currently, these densities are treated as invariant as a function of time for the delayed-gamma

calculations. That is, the input-file material densities are not transmuted. For pulsed or low-flux simulations (relevant to many detection scenarios), time-dependent changes in these materials should be relatively negligible. Future upgrades to MCNPX will be required to calculate flux-induced transmutation dependence by linking the delayed-gamma and burn (Fensin et al., 2006) capabilities. A combined decay and flux-induced transmutation capability would permit simulations of applications involving reactor fuel burn, etc. Time-dependence of the atom densities in line 5, i.e., the fission-product atom densities, is treated using CINDER'90 in the delayed-gamma upgrade.

Equation 2: Photon flux.

Terms 1–3 in line 1 represent the time rate of change of the angular photon flux, streaming, and photon loss due to absorption, respectively. Term 3 represents loss for mechanisms such as photoelectric absorption, whereas term 4 connotes photoneutron creation. These terms are treated by MCNPX.

Line 2 represents the source of prompt photons at $\vec{r};t$ due to the integrated contribution of all non-fission interactions at $\vec{r};E'_\gamma;t$ and all angular photons flux directions $\hat{\Omega}'_\gamma$. This term is treated by MCNPX.

Lines 3 and 4 represent the prompt-photon production due to photofission and neutron fission, respectively. These terms are treated by MCNPX using library data.

Line 5 contains terms for the delayed-photon production due to neutron fission and photofission. Term 1 of line 5, which is underscored, is the central focus of this article—its Monte Carlo treatment is addressed in detail in the following sections. Summation extends over all I fission products (or residual nuclides) and their associated P_i radioactive decay progeny. Delayed-gamma emission is assumed to be isotropic in the laboratory system. The term is nonzero for a fission event caused by a neutron. When the Monte Carlo CDF is sampled, zero or a finite number of delayed photons may be created.

Term 2 of line 5 (also underscored) is treated in the same manner as term 1. This term contributes to a photofission event that produces delayed photons.

Term 1 of line 6 is neutron radiative-capture photon production, which is calculated using table data augmented by physics models.

Term 2 of line 6 is the inhomogeneous photon source, which is stipulated by the user using the MCNPX "sdef" card. As with neutron sources, the photon-source specification can be either simple or have an exotic mixture of space, energy, direction, and time dependencies. Moreover, the user may specify sources consisting of both neutrons and photons for $S_n(\vec{r}, E_n, \hat{\Omega}_n, t)$ and $S_\gamma(\vec{r}, E_\gamma, \hat{\Omega}_\gamma, t)$.

Comments pertaining to the treatment of atom-density time dependence for Eq. (1) are relevant here. Thus, the transport-related densities are treated as time invariant, whereas the precursor densities are time dependent.

Equations (3) and (4): Neutron- and photon-induced isotopic transmutation equations.

Experimentation has revealed that a large number of delayed-neutron precursors are created by fission (England and Rider, 1994).[1] Experience has shown that delayed-neutron creation can be suitably modeled by lumping the behavior into a few precursor groups for creation by both neutron- and photon-induced production (Keepin, 1965; Bell and Glasstone, 1970, p. 467; Duderstadt and Hamilton, 1976).

As mentioned previously, MCNPX currently uses this simplification for sampling delayed-neutron spectra. For delayed-neutron emission-time and number sampling and for all delayed-gamma sampling needs, CINDER'90 is used to calculate explicitly the isotopic concentrations for 3400 radionuclides. The two isotopic-transmutation equations, Eqs. (3) and (4), are written to represent delayed neutron and gamma production due to neutron- and photon-induced fission and isotopic transmutation, respectively.

In line 1, term 1 on the right-hand side of Eq. (3) is the neutron-induced transmutation source of all nuclides to nuclide *i:p*, while term 2 is the neutron-induced loss of nuclide *i:p*. These terms are currently treated approximately in the MCNPX delayed-gamma upgrade . In particular, all 34 standard ENDF/B-VI types simple-multi-particle reactions[†] are treated (Durkee et al., 2009). However, this treatment does not include mass conservation.[‡] The upgrade is thus primarily suitable for characterization using pulsed or

[1] Data for 271 delayed-neutron precursors are presented in this reference.
[†] e.g., (n,p), (n,alpha), etc.
[‡] The simple-multi-particle reactions are treated in subroutine colidn.F rather than in CINDER'90. No mass treatment is done in colidn.F, whereas it is done in CINDER'90.

low-flux systems. Additional future work is necessary to accommodate prolonged flux exposure and eigenfunction (MCNPX "kcode") calculations.

Line 2 of Eq. (3) is the neutron-fission source for nuclide *i:p*. This term is nonzero for the fission products and zero for their decay progeny. As was discussed in Section 2, in MCNPX, tabulated fission-yield data are used (in **CID**) to sample the products of each fission for several fissioning nuclides in the presence of thermal, fission, and 14-MeV neutron spectra. For higher energies, LAHET provides a list of residual nuclides.

Term 1, line 3 of Eq. (3) is the source of nuclide *i:p* due to the radioactive decay of all contributing nuclides. Term 2 is the loss of nuclide *i:p* due to its decay.

Time-dependent nuclide densities for delayed neutron and photon production due to neutrons are thus calculated (for this upgrade) by CINDER'90 using the contributions from lines 2 and 3 in Eq. (3). For each fission, the identities of the sampled fission products are sent from **CID** to CINDER'90. CINDER'90 then calculates the densities for each nuclide in the decay chain for each fission product. Spatial dependence is accommodated on a cellwise basis.

The terms in Eq. (4) pertain to flux-induced transmutation and fission by photons, as well as the radioactive decay of the nuclides. Photon-flux-induced transmutation term is treated by photonuclear models. The photofission source, line 2, is treated for some

nuclides† using new photofission-yield data, $y_{\gamma:m\to j}(\vec{r};E_\gamma)$ (Durkee et al., 2009). For other nuclides, the term is approximately treated only by using neutron-fission yield data, $y_{n:m\to i}(\vec{r};E_n)$. The decay terms in line 3 are treated.

In MCNPX, for each fission event, either the neutron-induced, delayed-precursor contribution, Eq. (3), or the photon-induced, delayed-precursor concentrations, Eq. (4), are used to calculate the fission-product chains and the delayed-neutron and/or delayed-gamma CDFs and transport. Thus, only the terms in line 5 of Eqs. (1) and/or (2) corresponding to neutron- or photon-induced fission can contribute for that fission event. If the sampling results in no delayed neutrons and/or photons, then the respective term in Eq. (1) and/or (2) is zero for that fission event.

The precursors are presumed to be fixed in space; thus, terms involving convection or diffusion are absent in Eqs. (3) and (4).

2.4. Equation solution.

Equations (1)–(4) are statements of neutron, photon, and nuclide conservation for an infinitesimal element of volume, energy, and direction at time *t*. The quantities $\Phi(\vec{r};E_n,\hat{\Omega}_n;t)d^3r\,d\hat{\Omega}_n dE_n$ and $\Gamma(\vec{r};E_\gamma,\hat{\Omega}_\gamma;t)d^3r\,d\hat{\Omega}_\gamma dE_\gamma$ are the probabilities that a single neutron and a single photon are in the differential volume elements $d^3r\,d\hat{\Omega}_n dE_n$ and $d^3r\,d\hat{\Omega}_\gamma dE_\gamma$, respectively. These probabilities contain no information other than the

† The data are available for ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{241}Am, and ^{243}Am.

expected values (Bell, 1965). At a finite level, a deterministic solution (e.g., discrete ordinates) of Eqs.(1)–(2) provides information about only the expected neutron and photon behavior. In contrast, a Monte Carlo solution conveys information about the statistical behavior of the neutrons and photons.

Deterministic (discrete ordinates and spherical harmonics) numerical solutions to Eqs. (1)–(2) involve the discretization of the space, energy, direction, and time dependencies, as well as the derivatives and integrals. The resulting set of algebraic expressions is solved for angular fluxes throughout the spatial mesh at each timestep. Cross-section data are represented in a multigroup format and require a preparation account for self-shielding (in energy and space) and heterogeneity effects for individual models to preserve reaction-rate conservation. Geometrical modeling capabilities tend to be limited, and solutions contain no statistical information. Results are valid for the average behavior of a large number of particles. The memory requirements for discretized solutions can be very large and computer-memory intensive, particularly for multidimensional models. The treatment involves approximation due to discretization and multigroup cross-section treatments (Bell and Glasstone, 1970; Duderstadt and Hamilton, 1976, pp. 117–123; O'Dell and Alcouffe, 1987; Durkee et al., 1999). We are unaware of any deterministic numerical codes that are capable of treating delayed-gamma line emission due to fission.

Various interpretations of the so-called MCNPX Monte Carlo solution to Eqs. (1)–(2) can be offered. The MCNPX solution can be interpreted as being obtained by integrating the terms in these equations over space, direction, energy, and time to obtain an integral form

of the transport equation. The individual integral terms constitute cumulative distribution functions. The CDFs (integrals) are randomly sampled on a particle-by-particle basis to simulate creation, destruction, and transport. It should be noted that MCNPX can solve many types of transport problems. For particle-density-based estimates, it can be shown by integration over the transport process that the mean particle densities are described by the Boltzmann transport equation. That is, the Boltzmann transport equation describes the average behavior of a Monte Carlo calculation. However, a transport equation need not be written in order to solve a particle-transport problem using Monte Carlo.[†]

The necessary MCNPX data (e.g., cross sections and fission yields) are represented in either tabular or polynomial form or by theoretical model functions. The treatment is almost exact because there is no discretization of the transport parameters, and point cross-section data are used; some approximation for delayed-gamma analysis enters via the presumed linear behavior of isotopic concentrations with time for the CDF calculation (see Section 5). The creation of a computational model tends to be more complicated and time consuming than a deterministic numerical counterpart. However, geometrical modeling capabilities tend to be extensive, and the solutions contain important statistical information. Information can be gleaned on an individual-particle basis. Simulations can be conducted which involve small numbers of particles, thereby enabling studies in

[†] MCNP/MCNPX "solves" the Boltzmann transport equation in a similar sense that an NBA player "solves" Newton's law of motion to put a basketball through the hoop. Note that the Monte Carlo practitioner need never have considered, nor even know of, the Boltzmann transport equation to solve his transport problems, just as the NBA player need never have considered, nor even know of, Newton's law of motion to put a basketball through the hoop. It is doubtful that most people would consider the ball's motion as "solving" Newton's law. Certainly the ball's trajectory can be *described* by Newton's law in the same sense that (some aspects of) a Monte Carlo calculation can be *described* by the Boltzmann transport equation, but does the fact that an equation describes a process really mean that the process is "solving" the equation (Booth, 2007)?

regimes wherein the Boltzmann equation is invalid. MCNPX computer-memory demands for calculations excluding delayed-gamma emission are typically a fraction of their deterministic counterparts, allowing time-dependent, 3D models to be solved on modern personal computers. However, MCNPX delayed-gamma calculations are memory and CPU-time intensive; thus, execution of such models on clusters or large mainframe computers is preferable.

If a fission product or residual nuclide is created by neutron fission, neutron fission-yield data are used and Eq. (3) is solved by CINDER'90 (see Section 2 of Part I) to supply the isotopic concentrations for all of the decay products of each fission product created by neutron fission. These isotopic concentrations are supplied to MCNPX for use in CDF calculations of delayed neutron and gamma emission caused by neutron-induced fission. If photofission occurred, then Eq. (4) is solved.

For the fission branch (not the residual-nuclide branch), sampling is performed for the first fission-product after **CID** is entered. The identity of the second fission product is determined by mass conservation, taking into account whether the fission was induced by a neutron or photon as well as the number of prompt fission neutrons produced.

3. SUMMARY AND CONCLUSIONS.

As is discussed in Part I, the new MCNPX delayed-gamma Monte Carlo technique involves the creation and sampling of CDFs for the fission products or residual nuclides,

the number of delayed gammas produced for an event, and the energy, time, and direction of emission. Processing involves the treatment of low- and high-energy regimes for reaction initiation using various library or model data capabilities. For lower energies, fission products are determined (sampled) using fission-yield data for thermal, fission-spectrum (fast), and high-energy (>14 MeV) source-neutron energies. Interactions for neutrons having energies in excess of 20 MeV are calculated using LAHET, which is also an integral piece of MCNPX, to produce a list of residual nuclides. For each fission or activation event, time-dependent concentrations for decay-chain nuclides are calculated by CINDER'90 using the sampled fission products.

The interrelationship of these physics items can be a challenge to comprehend. The motivation behind Part III has been to address the complexity issue using an alternative paradigm. In particular, in this paper we have augmented the MCNPX Monte Carlo theory presentation contained in Part I by utilizing the coupled neutron/photon Boltzmann transport equations with delayed neutrons and gammas as a means of coordinating a discussion of the transport mechanisms that are treated by MCNPX for the delayed-gamma upgrade. This presentation should be particularly useful for those readers that have a background in transport theory.

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Table 1. Equation 1 termwise descriptions

Table 2. Equation 2 termwise descriptions

Table 3. Equation 3 termwise descriptions

Table 4. Equation 4 termwise descriptions

LIST OF FIGURE CAPTIONS

None.