Multigroup 1D Diffusion Equation Derivation

Eugeny Sosnovsky, for 22.05/22.211

February 22, 2013

1 Introduction

This paper is based upon the quantities and the nomenclature defined in the *Fundamental Definitions* and *Neutron Transport Equation Derivation* documents, distributed with this one. It aims to summarize the following:

1. Derive the 1D form of the neutron transport equation (NTE).
2. Derive the continuous energy 1D neutron diffusion equation (NDE) from the 1D form of the NTE using the P_1 function expansion.
3. Demonstrate how the multigroup discretization works for all terms of the continuous energy 1D NDE.

Multidimensional diffusion and spherical harmonics are not treated in this paper. Some further simplifications of each of the equations listed above are also presented.

The initial simplifications, which apply to all forms of the NTE present in this paper, are the following:

- Precursor families are independent of the fissionable isotope.
- Double differential scattering cross section is dependent only on the scattering angle cosine $\hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}$, not independenly on $\hat{\mathbf{\Omega}}'$ and $\hat{\mathbf{\Omega}}$.
- There is no thermal feedback.

The NTE was derived with these simplifications in *Neutron Transport Equation Derivation*; it has the following form:

$$
\begin{aligned}
\frac{\partial}{\partial t} n\left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}}\right) = & -\nabla \cdot \hat{\mathbf{\Omega}} \varphi\left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}}\right) - \Sigma_t(\vec{\mathbf{x}}, E)\, \varphi\left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}}\right) + \\
& + \int_0^\infty dE' \iint_{4\pi} d\Omega' \left[\sum_{j=1}^{J} \Sigma_s^j\left(\vec{\mathbf{x}}, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right) \right] \varphi\left(t, \vec{\mathbf{x}}, E', \hat{\mathbf{\Omega}}'\right) + \\
& + \frac{1}{4\pi} \int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E', E)\, \nu_p^{j_f}(E')\, \Sigma_f^{j_f}(\vec{\mathbf{x}}, E') \right] \iint_{4\pi} d\Omega' \varphi\left(t, \vec{\mathbf{x}}, E', \hat{\mathbf{\Omega}}'\right) + \\
& + \frac{1}{4\pi} \sum_{m=1}^{M} \chi_{d,m}(E)\, \lambda_m c_m(t, \vec{\mathbf{x}}) + s_{ex}\left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}}\right).
\end{aligned}
\tag{1}
$$

The delayed neutron precursor equation (DNPE) becomes:

$$\frac{\partial}{\partial t} c_m(t, \vec{\mathbf{x}}) = \int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \nu_{d,m}^{j_f}(E') \, \Sigma_f^{j_f}(\vec{\mathbf{x}}, E') \right] \iint_{4\pi} d\Omega' \varphi\left(t, \vec{\mathbf{x}}, E', \hat{\mathbf{\Omega}}'\right) - $$
$$ - \lambda_m c_m(t, \vec{\mathbf{x}}) \quad \forall m \in [1, \ldots, M] \, . \tag{2}$$

2 1D Simplification of the NTE

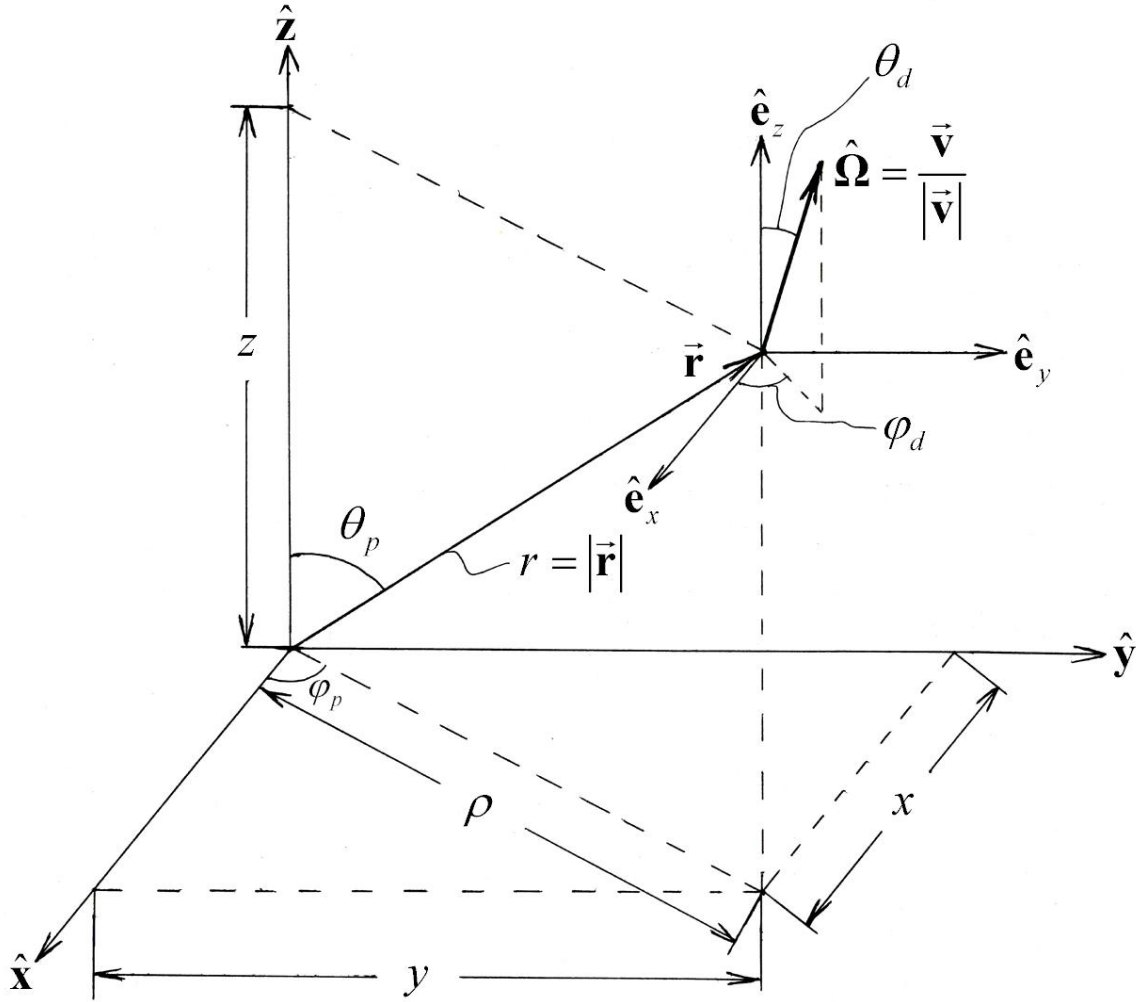The notation used in the *Fundamental Definitions* paper is repeated in Figure 1.

Figure 1: Notation Summary

The z-axis will be used as the "principal axis", with the z dimension being used as the single positional independent variable.

The following simplifications reduce the NTE to a 1D slab reactor problem:

2

1. Properties and unknowns only vary along the z-dimension, which is the single positional independent variable.
2. The domain is infinite along the x- and y-dimensions, therefore there is no leakage or any variation in the xy-plane.
3. Directional quantities are therefore only dependent on θ_d, and not on φ_d, which results in complete axial ("azimuthal") symmetry about the z-axis.

Consider the energy-dependent angular neutron flux density $\varphi\left(t, z, E, \hat{\mathbf{\Omega}}\right)$. It is a function of θ_d and φ_d, the polar ("zenith") and azimuthal direction angles which $\hat{\mathbf{\Omega}}$ depends on. $\varphi\left(t, z, E, \hat{\mathbf{\Omega}}\right)$ is a density in direction; to integrate it over all directions, the following differentials and domain of integration are used:

$$\phi(t, z, E) = \int_0^{2\pi} d\varphi_d \int_0^{\pi} d\theta_d \sin\left(\theta_d\right) \varphi\left(t, z, E, \hat{\mathbf{\Omega}}\right). \tag{3}$$

For 1D neutron transport, it is more convenient to express the directional dependence on the zenith angle in terms of the zenith angle cosine $\mu = \cos\left(\theta_d\right)$, and modify the integration domain accordingly. Expressing θ_d in terms of μ:

$$\theta_d = \arccos(\mu), \tag{4}$$

differentiating:

$$d\theta_d = -\frac{1}{\sqrt{1 - \mu^2}} d\mu, \tag{5}$$

substituting into $\sin\left(\theta_d\right)$:

$$\sin\left(\theta_d\right) = \sqrt{1 - \mu^2}, \tag{6}$$

and substituting into the differential yields:

$$\sin\left(\theta_d\right) d\theta_d d\varphi_d = -d\mu d\varphi_d. \tag{7}$$

The limits are adjusted accordingly (flipped due to the minus sign on the differential):

$$\phi(t, z, E) = \int_{-1}^{1} d\mu \int_0^{2\pi} d\varphi_d \varphi\left(t, z, E, \hat{\mathbf{\Omega}}\right). \tag{8}$$

By the above simplifications, $\varphi\left(t, z, E, \hat{\mathbf{\Omega}}\right)$ is axisymmetric, and depends only on μ, not on φ_d. Integrating it over all azimuthal directions yields:

$$\varphi(t, z, E, \mu) = \int_0^{2\pi} d\varphi_d \varphi\left(t, z, E, \hat{\mathbf{\Omega}}\right) = 2\pi\varphi\left(t, z, E, \hat{\mathbf{\Omega}}\right), \tag{9}$$

in which $\varphi(t, z, E, \mu)$ is the neutron flux density in energy and zenith angle cosine. This quantity serves as the unknown in 1D neutron transport. It can be thought of as follows: $\frac{1}{V_n(E)}\varphi(t, z, E, \mu)\, d\mu$ is the density of neutrons in position and energy, moving through the
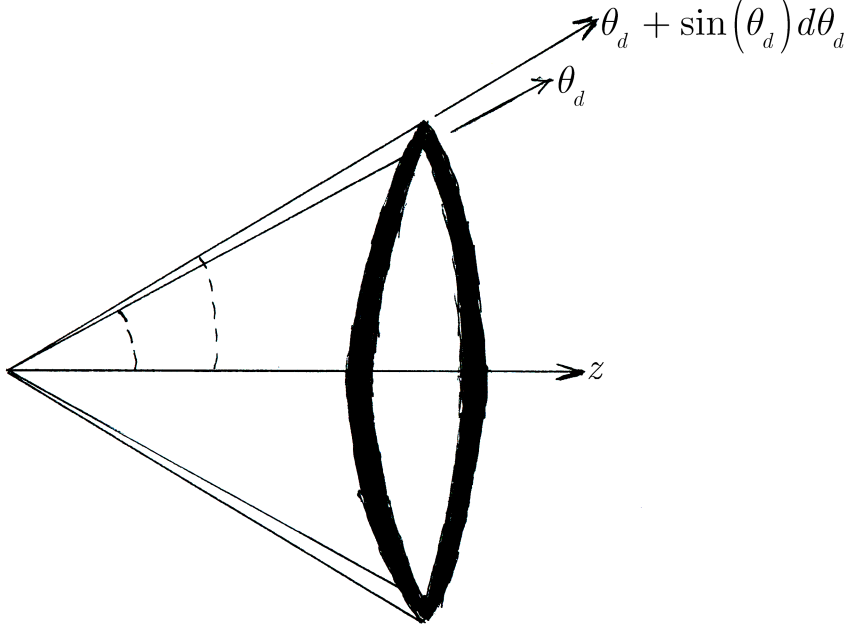
Figure 2: $\varphi(t, z, E, \mu)$ Illustration

cone spanned by zenith angle cosine interval $[\mu, \mu + d\mu]$, which is equivalent to the zenith angle interval $\left[\theta_d, \theta_d + \sin\left(\theta_d\right)d\theta_d\right]$. This cone is illustrated in Figure 2.

To express the NTE in terms of $\varphi(t, z, E, \mu)$, therefore reducing it to 1D, we integrate Eq. (1) over all azimuthal directions.

The time derivative term integrates trivially:

$$\int_0^{2\pi} d\varphi_d \frac{\partial}{\partial t} n\left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}}\right) = \frac{1}{V_n(E)} \frac{\partial}{\partial t} \varphi(t, z, E, \mu). \tag{10}$$

The streaming term integrates as follows:

$$\int_0^{2\pi} d\varphi_d \nabla \cdot \hat{\mathbf{\Omega}} \varphi\left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}}\right) = \int_0^{2\pi} d\varphi_d \begin{bmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{bmatrix} \cdot \left(\begin{bmatrix} \sin(\theta_d)\cos(\varphi_d) \\ \sin(\theta_d)\sin(\varphi_d) \\ \cos(\theta_d) \end{bmatrix} \varphi\left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}}\right) \right). \tag{11}$$

$\hat{\mathbf{\Omega}}$ and $\varphi\left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}}\right)$ do not depend on x or y, so the first two terms of the dot product are canceled out. Substituting μ into the third term and taking the integral yields the 1D form of the streaming term:

$$\int_0^{2\pi} d\varphi_d \frac{\partial}{\partial z} \left(\cos(\theta_d) \varphi\left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}}\right) \right) = \mu \frac{\partial}{\partial z} \varphi(t, z, E, \mu). \tag{12}$$

4

The total reaction term integrates trivially:

$$\int_0^{2\pi} d\varphi_d \Sigma_t(\vec{\mathbf{x}}, E) \, \varphi\left(t, \vec{\mathbf{x}}, E, \hat{\boldsymbol{\Omega}}\right) = \Sigma_t(z, E) \, \varphi(t, z, E, \mu) \,. \tag{13}$$

The inscattering term is a sum of J identical terms, one per isotope j. One element of such sum is treated below.

The double differential scattering cross section depends on $\hat{\boldsymbol{\Omega}}' \cdot \hat{\boldsymbol{\Omega}}$, which is the scattering angle cosine: the cosine of the angle between the source direction $\hat{\boldsymbol{\Omega}}'$ and the target direction $\hat{\boldsymbol{\Omega}}$. The double differential scattering cross section $\Sigma_s^j\left(\vec{\mathbf{x}}, E' \to E, \hat{\boldsymbol{\Omega}}' \cdot \hat{\boldsymbol{\Omega}}\right)$ is a macroscopic (scattering) cross section density in (target) energy and (target) direction, therefore it has the units of $\mathrm{cm}^{-1}/\mathrm{eVsr}$. Because we are attempting to characterize the scattering rate between two cones ($\mu' \to \mu$), we want the double differential scattering cross section to account for all target azimuthal directions, therefore yielding a cross section density in target energy and target zenith angle cosine. Such differential cross section characterizes scattering from a cone of directions to a cone of directions, not from a particular direction to other particular directions. We will denote this new double differential cross section as $\Sigma_{s*}^j(z, E' \to E, \mu_0)$, in which μ_0 is the scattering angle cosine. μ_0 is a function of φ_d and φ_d', as well as μ and μ'; the azimuthal angle dependence can be simplified out, using the azimuthal symmetry of the source flux, as will be demonstrated in section 3 below.

Because $\Sigma_{s*}^j(z, E' \to E, \mu_0)$ is a macroscopic cross section density in target energy and target zenith angle cosine, it must have the units of $\mathrm{cm}^{-1}/\mathrm{eVcos(rad)}$, which is dimensionally the same as $\mathrm{cm}^{-1}/\mathrm{eVrad}$.

$\Sigma_s^j\left(z, E' \to E, \hat{\boldsymbol{\Omega}}' \cdot \hat{\boldsymbol{\Omega}}\right)$ and $\Sigma_{s*}^j(z, E' \to E, \mu_0)$ are related as follows:

$$\frac{1}{2\pi} \int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi_d' \Sigma_s^j\left(z, E' \to E, \hat{\boldsymbol{\Omega}}' \cdot \hat{\boldsymbol{\Omega}}\right) = \Sigma_{s*}^j(z, E' \to E, \mu_0) \,, \tag{14}$$

in which μ_0 is a function of only μ and μ', since $\Sigma_{s*}^j(z, E' \to E, \mu_0)$ characterizes cone-to-cone scattering, and not scattering between two individual directions.

The source energy-dependent angular flux density $\varphi\left(t, \vec{\mathbf{x}}, E', \hat{\boldsymbol{\Omega}}'\right)$ is, by the above simplifications, axisymmetric. Therefore, we can postulate, for now, that the inscattering rate directional density (into the cone μ) is also axisymmetric. This will be proven, and the expression for $\Sigma_{s*}^j(z, E' \to E, \mu_0)$ will be provided, in section 3. Using this postulate yields:

$$\int_0^{2\pi} d\varphi_d \iint_{4\pi} d\Omega' \Sigma_s^j\left(\vec{\mathbf{x}}, E' \to E, \hat{\boldsymbol{\Omega}}' \cdot \hat{\boldsymbol{\Omega}}\right) \varphi\left(t, \vec{\mathbf{x}}, E', \hat{\boldsymbol{\Omega}}'\right) =$$
$$= \int_{-1}^1 d\mu' \Sigma_{s*}^j(z, E' \to E, \mu_0(\mu, \mu')) \, \varphi(t, z, E', \mu') \,. \tag{15}$$

Note, that without this postulate (and the above simplifications), Eq. (15) is not necessarily true, because it may not be possible to formulate an appropriate $\Sigma_{s*}^j(z, E' \to E, \mu_0)$ which can characterize scattering from the entire cone μ' into the entire target cone μ. The

dependence of μ_0 on μ and μ' is, from here, implied. Integrating Eq. (15) over all source energies, and summing over all present isotopes j yields the 1D form of the scattering kernel:

$$\int_0^{2\pi} d\varphi_d \int_0^\infty dE' \iint_{4\pi} d\Omega' \left[\sum_{j=1}^J \Sigma_s^j \left(\vec{\mathbf{x}}, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}} \right) \right] \varphi \left(t, \vec{\mathbf{x}}, E', \hat{\mathbf{\Omega}}' \right) =$$

$$= \sum_{j=1}^J \int_0^\infty dE' \int_{-1}^1 d\mu' \Sigma_{s*}^j(z, E' \to E, \mu_0) \, \varphi(t, z, E', \mu') \,. \tag{16}$$

The prompt fission source term integrates trivially:

$$\int_0^{2\pi} d\varphi_d \frac{1}{4\pi} \int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E', E) \, \nu_p^{j_f}(E') \, \Sigma_f^{j_f}(\vec{\mathbf{x}}, E') \right] \iint_{4\pi} d\Omega' \varphi \left(t, \vec{\mathbf{x}}, E', \hat{\mathbf{\Omega}}' \right) =$$

$$= \frac{1}{2} \int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E', E) \, \nu_p^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \int_{-1}^1 d\mu' \varphi(t, z, E', \mu') \,. \tag{17}$$

The delayed neutron source term integrates similarly:

$$\int_0^{2\pi} d\varphi_d \frac{1}{4\pi} \sum_{m=1}^M \chi_{d,m}(E) \, \lambda_m c_m(t, \vec{\mathbf{x}}) = \frac{1}{2} \sum_{m=1}^M \chi_{d,m}(E) \, \lambda_m c_m(t, z) \,. \tag{18}$$

Lastly, we integrate the external source term, converting it from an energy-dependent angular neutron source density to an energy-dependent neutron source density in space and zenith angle cosine:

$$\int_0^{2\pi} d\varphi_d s_{ex} \left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}} \right) = s_{ex}(t, z, E, \mu) \,. \tag{19}$$

Combining the terms from Eqs. (10), (12), (13), (16), (17), (18) and (19) yields the 1D simplification NTE for slab geometry:

$$\frac{1}{V_n(E)} \frac{\partial}{\partial t} \varphi(t, z, E, \mu) = -\mu \frac{\partial}{\partial z} \varphi(t, z, E, \mu) - \Sigma_t(z, E) \, \varphi(t, z, E, \mu) +$$

$$+ \sum_{j=1}^J \int_0^\infty dE' \int_{-1}^1 d\mu' \Sigma_{s*}^j(z, E' \to E, \mu_0) \, \varphi(t, z, E', \mu') +$$

$$+ \frac{1}{2} \int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E', E) \, \nu_p^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \int_{-1}^1 d\mu' \varphi(t, z, E', \mu') +$$

$$+ \frac{1}{2} \sum_{m=1}^M \chi_{d,m}(E) \, \lambda_m c_m(t, z) + s_{ex}(t, z, E, \mu) \,. \tag{20}$$

To simplify the DNPE into its 1D form, we simply make use of the azimuthal symmetry to partially integrate $\varphi\left(t, \vec{\mathbf{x}}, E', \hat{\mathbf{\Omega}}'\right)$ in Eq. (2), which yields:

$$\frac{\partial}{\partial t} c_m(t, z) = \int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \nu_{d,m}^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \int_{-1}^1 d\mu' \varphi(t, z, E', \mu') - $$
$$- \lambda_m c_m(t, z) \quad \forall m \in [1, \dots, M]\,. \tag{21}$$

This concludes the 1D simplification of the neutron transport and the delayed neutron precursor equations. We can now proceed to angular discretization.

3 1D Angular Discretization of the NTE

To discretize the 1D NTE in direction, we must discretize all of its terms in μ. μ ranges in $[-1, 1]$, so Legendre polynomials are usually used as the basis functions for the expansion of the angular quantities. Such discretization is known as the P_n discretization in 1D. The first three Legendre polynomials are given by:

$$P_0(\mu) = 1, \tag{22a}$$
$$P_1(\mu) = \mu, \tag{22b}$$
$$P_2(\mu) = \frac{1}{2}\left(3\mu^2 - 1\right). \tag{22c}$$

Legendre polynomials with $n > 0$ satisfy the recursion relation:

$$(2n+1)\,\mu P_n(\mu) = (n+1)\,P_{n+1}(\mu) + n P_{n-1}(\mu)\,. \tag{23}$$

Legendre polynomials are also orthogonal to each other (not orthonormal), with the following orthogonality relation:

$$\int_{-1}^1 d\mu P_l(\mu)\,P_n(\mu) = \frac{2\delta_{ln}}{2n+1}, \tag{24}$$

in which δ_{ln} is the Kronecker delta:

$$\delta_{ln} = \begin{cases} 1 & \text{if } l = n, \\ 0 & \text{if } l \neq n. \end{cases} \tag{25}$$

Let $f(\mu)$ be a function that we want to expand in terms of Legendre polynomials. The expansion is given by:

$$f(\mu) = \sum_{n=0}^N \frac{2n+1}{2} f_n P_n(\mu)\,, \tag{26}$$

in which f_n, the nth Legendre moment of $f(\mu)$, is calculated according to:

$$f_n = \int_{-1}^{1} d\mu f(\mu) P_n(\mu). \tag{27}$$

Equation (26) is exact when $N \to \infty$. It can be shown, that the power series in it is convergent, therefore we can postulate (and experimentally demonstrate) that a finite N can adequately (within a bounded error) approximate any $f(\mu)$.

The inscattering term in Eq. (20) accounts for inscattering into the target cone with zenith angle cosine μ. However, fundamentally, as was shown in section 2, the differential scattering cross section $\Sigma_s^j \left(\vec{\mathbf{x}}, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}} \right)$ is a density in target direction, and not in target zenith angle cosine. In section 2, the density in target zenith angle cosine arose from the postulated axial symmetry of the inscattering term. To rigorously prove this axial symmetry, it will be necessary to use the Spherical Harmonics Addition Theorem, given by Eq. (28), and using the associated Legendre polynomials defined by Eq. (29). In Eq. (28), $\mu_0 = \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}$. It will be used to expand $\Sigma_s^j \left(\vec{\mathbf{x}}, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}} \right)$ using Eqs. (26) and (27).

$$P_n(\mu_0) = P_n(\mu) P_n(\mu') + 2 \sum_{l=1}^{n} \frac{(n-l)!}{(n+l)!} P_n^l(\mu') P_n^l(\mu) \cos \left[l \left(\varphi_d - \varphi_d' \right) \right] \tag{28}$$

$$P_n^l(\mu) = \left(1 - \mu^2 \right)^{l/2} \frac{d^l P_n(\mu)}{d\mu^l} \tag{29}$$

To derive the continuous energy 1D neutron diffusion equation, we perform the following steps on each term of Eq. (20):

Step 1. Expand $\varphi(t, z, E, \mu)$ using Eq. (26).

Step 2. Multiply the resulting term by $P_n(\mu)$.

Step 3. Integrate the resulting term over $\mu \in [-1, 1]$.

Step 4. Simplify the resulting expression using Eq. (24). The streaming and inscattering terms also make use of Eqs. (23) and (28), respectively.

All individual terms of Eq. (20) are now treated below.

Performing steps 1–3 on the time derivative term yields:

$$\int_{-1}^{1} d\mu \frac{1}{V_n(E)} \frac{\partial}{\partial t} \sum_{l=0}^{L} \left[\frac{2l+1}{2} \varphi_l(t, z, E) P_l(\mu) \right] P_n(\mu) =$$

$$= \frac{1}{V_n(E)} \sum_{l=0}^{L} \frac{\partial}{\partial t} \varphi_l(t, z, E) \left[\frac{2l+1}{2} \int_{-1}^{1} d\mu P_l(\mu) P_n(\mu) \right], \tag{30}$$

which simplifies, using Eq. (24), as follows:

$$\frac{1}{V_n(E)} \sum_{l=0}^{L} \frac{\partial}{\partial t} \varphi_l(t, z, E) \left[\frac{2l+1}{2} \int_{-1}^{1} d\mu P_l(\mu) P_n(\mu) \right] =$$

$$= \frac{1}{V_n(E)} \sum_{l=0}^{L} \frac{\partial}{\partial t} \varphi_l(t, z, E) \left[\frac{2l+1}{2} \frac{2\delta_{ln}}{2n+1} \right] = \frac{1}{V_n(E)} \frac{\partial}{\partial t} \varphi_n(t, z, E). \tag{31}$$

8

Note, that that the subscript n in $V_n(E)$ simply indicates "neutron" (speed), while in all other terms, it is the index of the Legendre moment the term is a part of.

Next, we perform steps 1–3 on the streaming term:

$$\int_{-1}^{1} d\mu \mu \frac{\partial}{\partial z} \sum_{l=0}^{L} \left[\frac{2l+1}{2} \varphi_l(t,z,E) \, P_l(\mu) \right] P_n(\mu) =$$
$$= \sum_{l=0}^{L} \frac{\partial}{\partial z} \varphi_l(t,z,E) \left[\frac{2l+1}{2} \int_{-1}^{1} d\mu P_l(\mu) \, \mu P_n(\mu) \right]. \tag{32}$$

For $n = 0$, recognizing that $P_1(\mu) = \mu$, Eq. (32) reduces as follows:

$$\sum_{l=0}^{L} \frac{\partial}{\partial z} \varphi_l(t,z,E) \left[\frac{2l+1}{2} \int_{-1}^{1} d\mu P_l(\mu) \, \mu P_0(\mu) \right] =$$
$$= \sum_{l=0}^{L} \frac{\partial}{\partial z} \varphi_l(t,z,E) \left[\frac{2l+1}{2} \int_{-1}^{1} d\mu P_l(\mu) \, P_1(\mu) \right] = \frac{\partial}{\partial z} \varphi_1(t,z,E). \tag{33}$$

For $n > 0$, we replace $\mu P_n(\mu)$ using Eq. (23), which yields:

$$\sum_{l=0}^{L} \frac{\partial}{\partial z} \varphi_l(t,z,E) \left[\frac{2l+1}{2} \int_{-1}^{1} d\mu P_l(\mu) \, \mu P_n(\mu) \right] =$$
$$= \sum_{l=0}^{L} \frac{\partial}{\partial z} \varphi_l(t,z,E) \frac{2l+1}{2} \left[\frac{n+1}{2n+1} \int_{-1}^{1} d\mu P_l(\mu) \, P_{n+1}(\mu) + \frac{n}{2n+1} \int_{-1}^{1} d\mu P_l(\mu) \, P_{n-1}(\mu) \right]. \tag{34}$$

By Eq. (24), the first term of the sum in Eq. (34) is nonzero only for $l = n+1$, and the second term only for $l = n-1$. For a given $n > 0$, this reduces Eq. (34) to:

$$\sum_{l=0}^{L} \frac{\partial}{\partial z} \varphi_l(t,z,E) \frac{2l+1}{2} \left[\frac{n+1}{2n+1} \int_{-1}^{1} d\mu P_l(\mu) \, P_{n+1}(\mu) + \frac{n}{2n+1} \int_{-1}^{1} d\mu P_l(\mu) \, P_{n-1}(\mu) \right] =$$
$$= \frac{n+1}{2n+1} \frac{\partial}{\partial z} \varphi_{n+1}(t,z,E) + \frac{n}{2n+1} \frac{\partial}{\partial z} \varphi_{n-1}(t,z,E). \tag{35}$$

Performing steps 1–4 on the total reaction term yields:

$$\int_{-1}^{1} d\mu \Sigma_t(z,E) \sum_{l=0}^{L} \left[\frac{2l+1}{2} \varphi_l(t,z,E) \, P_l(\mu) \right] P_n(\mu) =$$
$$= \Sigma_t(z,E) \sum_{l=0}^{L} \varphi_l(t,z,E) \left[\frac{2l+1}{2} \int_{-1}^{1} d\mu P_l(\mu) \, P_n(\mu) \right] =$$
$$= \Sigma_t(z,E) \, \varphi_n(t,z,E). \tag{36}$$

One element of the inscattering term's sum of J isotopes' contributions is treated below. We will start with the unsimplified inscattering term from Eq. (1), to prove that, under the simplifications in section 2, the inscattering rate directional density is axisymmetric.

Isotope j contribution to the inscattering term is given by:

$$\int_0^\infty dE' \iint_{4\pi} d\Omega' \Sigma_s^j\left(\vec{\mathbf{x}}, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right) \varphi\left(t, \vec{\mathbf{x}}, E', \hat{\mathbf{\Omega}}'\right). \tag{37}$$

Because $\varphi\left(t, \vec{\mathbf{x}}, E', \hat{\mathbf{\Omega}}'\right)$ and $\Sigma_s^j\left(\vec{\mathbf{x}}, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right)$ are axisymmetric, by Eq. (9), we can replace $\varphi(t, z, E', \mu')$ into Eq. (37) as follows:

$$\begin{aligned}
\int_0^\infty dE' \iint_{4\pi} d\Omega' \Sigma_s^j\left(\vec{\mathbf{x}}, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right) \varphi\left(t, \vec{\mathbf{x}}, E', \hat{\mathbf{\Omega}}'\right) = \\
= \int_0^\infty dE' \iint_{4\pi} d\Omega' \Sigma_s^j\left(z, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right) \frac{1}{2\pi} \varphi(t, z, E', \mu').
\end{aligned} \tag{38}$$

As in section 2, to reduce the inscattering term to 1D, we replace the source direction differential $d\Omega'$ and the corresponding integration limits using Eqs. (7) and (8), and integrate Eq. (38) over all target azimuthal directions:

$$\begin{aligned}
\int_0^{2\pi} d\varphi_d \int_0^\infty dE' \iint_{4\pi} d\Omega' \Sigma_s^j\left(z, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right) \frac{1}{2\pi} \varphi(t, z, E', \mu') = \\
= \frac{1}{2\pi} \int_0^\infty dE' \int_{-1}^1 d\mu' \varphi(t, z, E', \mu') \int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi'_d \Sigma_s^j\left(z, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right).
\end{aligned} \tag{39}$$

Next, we treat the inner double integral in Eq. (39) separately. Recognizing that, by definition, $\mu_0 = \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}$, we expand $\Sigma_s^j\left(z, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right)$ using Eqs. (26) and (27):

$$\begin{aligned}
\int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi'_d \Sigma_s^j\left(z, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right) = \\
= \int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi'_d \sum_{k=0}^L \frac{2k+1}{2} \Sigma_{s,k}^j(z, E' \to E) P_k(\mu_0) = \\
= \sum_{k=0}^L \frac{2k+1}{2} \Sigma_{s,k}^j(z, E' \to E) \int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi'_d P_k(\mu_0),
\end{aligned} \tag{40}$$

in which $\Sigma_{s,k}^j(z, E' \to E)$ is the kth Legendre moment of the double differential scattering cross section, computed according to Eq. (27). $\Sigma_{s,k}^j(z, E' \to E)$ is a single differential scattering cross section, a scattering cross section density in target energy.

Using the Spherical Harmonics Addition Theorem (Eq. (28)) in the double integral in

10

Eq. (40) yields:

$$\int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi_d' P_k(\mu_0) =$$

$$= \int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi_d' \left[P_k(\mu) P_k(\mu') + 2 \sum_{l=1}^{k} \frac{(k-l)!}{(k+l)!} P_k^l(\mu') P_k^l(\mu) \cos\left[l\left(\varphi_d - \varphi_d'\right)\right] \right] = \quad (41)$$

$$= 4\pi^2 P_k(\mu) P_k(\mu') + 2 \sum_{l=1}^{k} \frac{(k-l)!}{(k+l)!} P_k^l(\mu') P_k^l(\mu) \int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi_d' \cos\left[l\left(\varphi_d - \varphi_d'\right)\right].$$

For all integers $l \geq 1$, the following holds:

$$\int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi_d' \cos\left[l\left(\varphi_d - \varphi_d'\right)\right] = 0 \quad \forall l \geq 1, \quad (42)$$

which significantly simplifies Eq. (41):

$$\int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi_d' P_k(\mu_0) = 4\pi^2 P_k(\mu) P_k(\mu'). \quad (43)$$

Substituting Eq. (43) into Eq. (40) yields:

$$\int_0^{2\pi} d\varphi_d \int_0^{2\pi} d\varphi_d' \Sigma_s^j\left(z, E' \to E, \hat{\Omega}' \cdot \hat{\Omega}\right) = 4\pi^2 \sum_{k=0}^{L} \frac{2k+1}{2} \Sigma_{s,k}^j(z, E' \to E) P_k(\mu) P_k(\mu'), \quad (44)$$

substituting which into Eq. (39) yields:

$$\int_0^{2\pi} d\varphi_d \int_0^{\infty} dE' \iint_{4\pi} d\Omega' \Sigma_s^j\left(z, E' \to E, \hat{\Omega}' \cdot \hat{\Omega}\right) \frac{1}{2\pi} \varphi(t, z, E', \mu') =$$

$$= \frac{1}{2\pi} \int_0^{\infty} dE' \int_{-1}^{1} d\mu' \varphi(t, z, E', \mu') 4\pi^2 \sum_{k=0}^{L} \frac{2k+1}{2} \Sigma_{s,k}^j(z, E' \to E) P_k(\mu) P_k(\mu') =$$

$$= \int_0^{\infty} dE' \int_{-1}^{1} d\mu' \varphi(t, z, E', \mu') 2\pi \sum_{k=0}^{L} \frac{2k+1}{2} \Sigma_{s,k}^j(z, E' \to E) P_k(\mu) P_k(\mu'). \quad (45)$$

Dividing Eq. (44) by 2π and comparing the result to Eq. (14) yields the expression for $\Sigma_{s*}^j(z, E' \to E, \mu_0)$:

$$\Sigma_{s*}^j(z, E' \to E, \mu_0) = 2\pi \sum_{k=0}^{L} \frac{2k+1}{2} \Sigma_{s,k}^j(z, E' \to E) P_k(\mu) P_k(\mu'), \quad (46)$$

which can be substituted into Eq. (45) to yield (also using Eq. (38)):

$$\int_0^{2\pi} d\varphi_d \iint_{4\pi} d\Omega' \Sigma_s^j\left(\vec{\mathbf{x}}, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right) \varphi\left(t, \vec{\mathbf{x}}, E', \hat{\mathbf{\Omega}}'\right) =$$

$$= \int_{-1}^1 d\mu' \Sigma_{s*}^j(z, E' \to E, \mu_0) \, \varphi(t, z, E', \mu') =$$

$$= \int_{-1}^1 d\mu' \left[2\pi \sum_{k=0}^L \frac{2k+1}{2} \Sigma_{s,k}^j(z, E' \to E) \, P_k(\mu) \, P_k(\mu') \right] \varphi(t, z, E', \mu') = \tag{47}$$

$$= \int_{-1}^1 d\mu' \left[\sum_{k=0}^L \frac{2k+1}{2} \Sigma_{s*,k}^j(z, E' \to E) \, P_k(\mu) \, P_k(\mu') \right] \varphi(t, z, E', \mu') \, .$$

$\Sigma_{s*,k}^j(z, E' \to E)$ is the kth azimuthally-integrated Legendre moment of the double differential scattering cross section, given by:

$$\Sigma_{s*,k}^j(z, E' \to E) = 2\pi \Sigma_{s,k}^j(z, E' \to E) \, . \tag{48}$$

Equation (47) is the same as Eq. (15), which serves as proof (through Legendre polynomial expansion) of the postulate made in section 2. Equation (46) provides the expression for $\Sigma_{s*}^j(z, E' \to E, \mu_0)$, the special cone-to-cone differential scattering cross section discussed in section 2. Equation (47) clearly does not contain φ_d or φ_d', which makes sense, since the expression characterizes scattering from all direction cones μ' to a direction cone μ.

Most of the steps presented in the derivation above are normally skipped in literature. The difference between $\Sigma_{s*}^j(z, E' \to E, \mu_0)$ and $\Sigma_s^j\left(z, E' \to E, \hat{\mathbf{\Omega}}' \cdot \hat{\mathbf{\Omega}}\right)$ — a cone-to-cone versus a direction-to-direction cross section — is often ignored. It is also often stated that in 1D, $P_k(\mu_0) = P_k(\mu) \, P_k(\mu')$; this is not correct however — instead, Eq. (43) is. Not ignoring such differences is what resulted in the above lengthy (but rigorous) derivation; from this point, it is much more conventional.

Performing step 1 on $\varphi(t, z, E', \mu')$ in Eq. (47) using Eq. (26) yields:

$$\int_{-1}^1 d\mu' \left[\sum_{k=0}^L \frac{2k+1}{2} \Sigma_{s*,k}^j(z, E' \to E) \, P_k(\mu) \, P_k(\mu') \right] \varphi(t, z, E', \mu') =$$

$$= \int_{-1}^1 d\mu' \left[\sum_{k=0}^L \frac{2k+1}{2} \Sigma_{s*,k}^j(z, E' \to E) \, P_k(\mu) \, P_k(\mu') \right] \left[\sum_{l=0}^L \frac{2l+1}{2} \varphi_l(t, z, E') \, P_l(\mu') \right] . \tag{49}$$

Using Eq. (24) on Eq. (49) drops most of the terms of the sums, greatly simplifying the equation:

$$\int_{-1}^1 d\mu' \left[\sum_{k=0}^L \frac{2k+1}{2} \Sigma_{s*,k}^j(z, E' \to E) \, P_k(\mu) \, P_k(\mu') \right] \left[\sum_{l=0}^L \frac{2l+1}{2} \varphi_l(t, z, E') \, P_l(\mu') \right] =$$

$$= \sum_{l=0}^L \frac{2l+1}{2} \Sigma_{s*,l}^j(z, E' \to E) \, \varphi_l(t, z, E') \, P_l(\mu) \, . \tag{50}$$

Performing steps 2–4 on Eq. (50), we multiply it by $P_n(\mu)$, integrate it over $\mu \in [-1, 1]$, and use Eq. (24) to further simplify it:

$$\int_{-1}^{1} d\mu P_n(\mu) \sum_{l=0}^{L} \frac{2l+1}{2} \Sigma_{s*,l}^{j}(z, E' \to E) \varphi_l(t, z, E') P_l(\mu) =$$

$$= \sum_{l=0}^{L} \Sigma_{s*,l}^{j}(z, E' \to E) \varphi_l(t, z, E') \left[\frac{2l+1}{2} \int_{-1}^{1} d\mu P_n(\mu) P_l(\mu) \right] = \quad (51)$$

$$= \Sigma_{s*,n}^{j}(z, E' \to E) \varphi_n(t, z, E').$$

Integrating Eq. (51) over all source energies and summing over all present isotopes j yields the 1D continuous energy P_n-discretized inscattering term:

$$\sum_{j=1}^{J} \int_{0}^{\infty} dE' \Sigma_{s*,n}^{j}(z, E' \to E) \varphi_n(t, z, E'). \quad (52)$$

To treat the prompt fission source term, we first recognize that, because $P_0(\mu) = 1$:

$$\int_{-1}^{1} d\mu' \varphi(t, z, E', \mu') = \phi(t, z, E') = \varphi_0(t, z, E'), \quad (53)$$

that is, the 0th Legendre moment of the flux is the scalar flux. The 1st Legendre moment also has physical meaning, discussed in section 4.

The prompt fission source term is isotropic in μ (that is, not a function of μ), so it can be viewed as being multiplied by $P_0(\mu)$. Performing steps 2–4 on it is therefore trivial:

$$\int_{-1}^{1} d\mu P_n(\mu) P_0(\mu) \frac{1}{2} \int_{0}^{\infty} dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E', E) \nu_p^{j_f}(E') \Sigma_f^{j_f}(z, E') \right] \varphi_0(t, z, E') =$$

$$= \begin{cases} \int_{0}^{\infty} dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E', E) \nu_p^{j_f}(E') \Sigma_f^{j_f}(z, E') \right] \varphi_0(t, z, E') & \text{if } n = 0, \\ 0 & \text{if } n \neq 0. \end{cases} \quad (54)$$

The delayed neutron source term is also isotropic in μ, and so steps 2–4 are performed on it similarly to yield:

$$\int_{-1}^{1} d\mu P_n(\mu) P_0(\mu) \frac{1}{2} \sum_{m=1}^{M} \chi_{d,m}(E) \lambda_m c_m(t, z) = \begin{cases} \sum_{m=1}^{M} \chi_{d,m}(E) \lambda_m c_m(t, z) & \text{if } n = 0, \\ 0 & \text{if } n \neq 0. \end{cases} \quad (55)$$

The external source term does depend on μ, and so step 1 consists of expanding it according to Eqs. (26) and (24):

$$s_{ex}(t, z, E, \mu) = \sum_{l=0}^{L} \frac{2l+1}{2} s_{ex,l}(t, z, E) P_l(\mu). \quad (56)$$

13

Performing steps 2–4 on it yields:

$$\int_{-1}^{1} d\mu P_n(\mu) \sum_{l=0}^{L} \frac{2l+1}{2} s_{ex,l}(t,z,E) P_l(\mu) = s_{ex,n}(t,z,E). \tag{57}$$

Combining the terms from Eqs. (31), (33), (35), (36), (52), (54), (55) and (57) yields the 1D continuous energy P_n equations:

$$\frac{1}{V_n(E)} \frac{\partial}{\partial t} \varphi_0(t,z,E) = -\frac{\partial}{\partial z} \varphi_1(t,z,E) - \Sigma_t(z,E) \varphi_0(t,z,E) +$$

$$+ \sum_{j=1}^{J} \int_0^{\infty} dE' \Sigma_{s^*,0}^j(z, E' \to E) \varphi_0(t,z,E') +$$

$$+ \int_0^{\infty} dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E',E) \nu_p^{j_f}(E') \Sigma_f^{j_f}(z,E') \right] \varphi_0(t,z,E') + \tag{58a}$$

$$+ \sum_{m=1}^{M} \chi_{d,m}(E) \lambda_m c_m(t,z) + s_{ex,0}(t,z,E) \quad \text{for } n = 0,$$

$$\frac{1}{V_n(E)} \frac{\partial}{\partial t} \varphi_n(t,z,E) = -\frac{n+1}{2n+1} \frac{\partial}{\partial z} \varphi_{n+1}(t,z,E) - \frac{n}{2n+1} \frac{\partial}{\partial z} \varphi_{n-1}(t,z,E) -$$

$$- \Sigma_t(z,E) \varphi_n(t,z,E) + \sum_{j=1}^{J} \int_0^{\infty} dE' \Sigma_{s^*,n}^j(z, E' \to E) \varphi_n(t,z,E') + \tag{58b}$$

$$+ s_{ex,n}(t,z,E) \quad \forall n \in [1,\ldots,N].$$

In Eq. (58b), N indicates the maximum Legendre moment to which the expansion occurs. Because the streaming term of the $n = N$ equation then contains $\varphi_{N+1}(t,z,E)$, which is unknown, the equations are closed by setting $\frac{\partial}{\partial z} \varphi_{N+1}(t,z,E)$ to zero. Because, as stated above, the Legendre moment expansion (Eq. (26)) is a converging series, $\frac{\partial}{\partial z} \varphi_{N+1}(t,z,E) = 0$ does not introduce an inaccuracy assuming a sufficiently high N is used.

Equation (53) can be used to convert the 1D DNPE into the P_n-supporting form:

$$\frac{\partial}{\partial t} c_m(t,z) = \int_0^{\infty} dE' \left[\sum_{j_f=1}^{J_f} \nu_{d,m}^{j_f}(E') \Sigma_f^{j_f}(z,E') \right] \varphi_0(t,z,E') - \tag{59}$$

$$- \lambda_m c_m(t,z) \quad \forall m \in [1,\ldots,M].$$

This concludes the angular discretization of the 1D neutron transport and the 1D delayed neutron precursor equations. We can now proceed to the continuous energy 1D neutron diffusion equation derivation.

4   1D Neutron Diffusion Equation Derivation

To derive the continuous energy 1D NDE, we take Eqs. (58) and limit N to 1. Dropping $\frac{\partial}{\partial z}\varphi_2(t, z, E)$, Eq. (58b) becomes:

$$
\frac{1}{V_n(E)}\frac{\partial}{\partial t}\varphi_1(t, z, E) = -\frac{1}{3}\frac{\partial}{\partial z}\varphi_0(t, z, E) - \Sigma_t(z, E)\,\varphi_1(t, z, E) +
$$
$$
+ \sum_{j=1}^{J}\int_0^\infty dE'\Sigma_{s*,1}^j(z, E' \to E)\,\varphi_1(t, z, E') + s_{ex,1}(t, z, E)\,.
\tag{60}
$$

Let $J(t, z, E)$ be the energy dependent net current density. The 1D diffusion approximation approximates $J(t, z, E)$ as follows:

$$
J(t, z, E) = -D(z, E)\,\frac{\partial}{\partial z}\phi(t, z, E)\,,
\tag{61}
$$

in which $D(z, E)$ is the diffusion coefficient, derived below.

As shown in the *Fundamental Definitions* document, the energy dependent current density is given by (in 3D):

$$
\vec{\mathbf{J}}(t, \vec{\mathbf{x}}, E) = \iint_{4\pi} d\Omega\hat{\mathbf{\Omega}}\varphi\left(t, \vec{\mathbf{x}}, E, \hat{\mathbf{\Omega}}\right)\,,
\tag{62}
$$

which, with the simplifications in section 2, simplifies to:

$$
J(t, z, E) = \int_{-1}^{1} d\mu\mu\varphi(t, z, E, \mu)\,.
\tag{63}
$$

By Eqs. (22b), (27) and (63), $J(t, z, E)$ can be shown to be the 1st Legendre moment of the flux:

$$
J(t, z, E) = \varphi_1(t, z, E)\,,
\tag{64}
$$

therefore, additionally using Eq. (53), Eq. (61) becomes:

$$
\varphi_1(t, z, E) = -D(z, E)\,\frac{\partial}{\partial z}\varphi_0(t, z, E)\,.
\tag{65}
$$

To define $D(z, E)$, we need to make several additional approximations to Eq. (60), listed below.

1. Current density fractional variation can be treated as quasistatic in comparison to the rest of the terms in Eq. (60). The largest in magnitude term on the right hand side is the total reaction term, for which this assumption implies:

$$
\frac{1}{|J(t, z, E)|}\frac{\partial}{\partial t}\,|J(t, z, E)| \ll V_n(E)\,\Sigma_t(z, E)\,.
\tag{66}
$$

For a (very low) $1\,\text{cm}^{-1}$ total cross section, and a (very slow) thermal neutron ($V_n(E) = 2200\,\text{m\,s}^{-1}$), the collision frequency per neutron $V_n(E)\,\Sigma_t(z,E)$ is $2.2 \times 10^5\,\text{s}^{-1}$. Therefore, for this assumption to be invalid, the current density has to vary by about a factor of $100\,000$ in one second, or faster. This is almost never the case in a reactor, and so this assumption is generally very good. It leads to the following simplification:

$$\frac{1}{V_n(E)}\frac{\partial}{\partial t}\varphi_1(t,z,E) \cong 0. \tag{67}$$

It is important to note that this assumption does not imply that the reactor is at steady state, as the time derivative term of Eq. (58a) may still be nonzero — only that the variation in current density does not look like a shock front travelling through a region in a reactor.

2. The external source is isotropic. This is normally a very good assumption for external sources encountered in a reactor: they tend to be photoneutron sources, which, like prompt and delayed sources, emit neutrons isotropically. This leads to the following simplification:

$$s_{ex,1}(t,z,E) \cong 0. \tag{68}$$

The following notation will now be used for the 0th moment of the external source, for convenience:

$$s_{ex}(t,z,E) = s_{ex,0}(t,z,E) = \int_{-1}^{1} d\mu\, s_{ex}(t,z,E,\mu). \tag{69}$$

With these assumptions, Eq. (60) reduces as follows:

$$0 = -\frac{1}{3}\frac{\partial}{\partial z}\varphi_0(t,z,E) - \Sigma_t(z,E)\,\varphi_1(t,z,E) + \sum_{j=1}^{J}\int_0^\infty dE'\Sigma_{s^*,1}^j(z,E' \to E)\,\varphi_1(t,z,E'). \tag{70}$$

Rearranging Eq. (70) yields a formal expression for the energy-dependent diffusion coefficient $D(z,E)$, by solving for $\varphi_1(t,z,E)$, and using Eq. (61):

$$D(z,E) = \frac{1}{3\left[\Sigma_t(z,E) - \dfrac{1}{\varphi_1(t,z,E)}\displaystyle\sum_{j=1}^{J}\int_0^\infty dE'\Sigma_{s^*,1}^j(z,E' \to E)\,\varphi_1(t,z,E')\right]}. \tag{71}$$

Equation (71) clearly shows, that while the diffusion approximation is often thought of as an approximation of the streaming term only, it also accounts for anisotropic (1st Legendre moment) scattering, which may be significant. This is sometimes neglected when constructing $D(z,E)$, as shown below.

Before proceeding to construct a usable form of $D(z,E)$, we will summarize the construction of the Legendre moments of the double differential scattering cross section. The double differential (cone-to-cone) scattering cross section $\Sigma_{s^*}^j(z,E' \to E,\mu_0)$, used in the

construction of the Legendre moments, is fundamentally given by:

$$\Sigma_{s*}^j(z, E' \to E, \mu_0) = \Sigma_{s_{el}}^j(z, E') \, f_{s_{el}}^j(E' \to E, \mu_0) +$$

$$+ \sum_{i=1}^{I_j} \Sigma_{s_{in,i}}^j(z, E') \, f_{s_{in,i}}^j(E' \to E, \mu_0) + \Sigma_{s_{in,c}}^j(z, E') \, f_{s_{in,c}}^j(E' \to E, \mu_0) \,. \tag{72}$$

Here, $\Sigma_{s_{el}}^j(z, E')$ and $f_{s_{el}}^j(E' \to E, \mu_0)$ are the elastic scattering cross section and the double differential elastic scattering probability density, respectively. $\Sigma_{s_{in,i}}^j(z, E')$ is the discrete level i inelastic scattering cross section, $f_{s_{in,i}}^j(E' \to E, \mu_0)$ is the corresponding double differential probability density. $\Sigma_{s_{in,c}}^j(z, E')$ and $f_{s_{in,c}}^j(E' \to E, \mu_0)$ are the continuum inelastic scattering cross section and double differential probability density, respectively.

These quantities are discussed in more detail in section 8. For now, it is sufficient to note the following:

- All double differential scattering probability densities normalize as follows:

$$\int_0^\infty dE \int_{-1}^1 d\mu_0 f_{s_{el}}^j(E' \to E, \mu_0) =$$

$$= \int_0^\infty dE \int_{-1}^1 d\mu_0 f_{s_{in,i}}^j(E' \to E, \mu_0) = \tag{73}$$

$$= \int_0^\infty dE \int_{-1}^1 d\mu_0 f_{s_{in,c}}^j(E' \to E, \mu_0) = 1.$$

- A double differential scattering probability density (any of them) can be written as:

$$f_s^j(E' \to E, \mu_0) = f_{s,E}^j(E' \to E) \, f_{s,\mu_0}^j(E' \to E, \mu_0) \,, \tag{74}$$

in which $f_{s,E}^j(E' \to E)$ is the scattering probability density in target energy, and $f_{s,\mu_0}^j(E' \to E, \mu_0)$ is the scattering probability density in scattering angle cosine. In general, $f_{s,\mu_0}^j(E' \to E, \mu_0)$ is a function of both source and target energies, as well as the scattering angle cosine. Both of these scattering probability densities normalize as follows:

$$\int_0^\infty dE f_{s,E}^j(E' \to E) = \int_{-1}^1 d\mu_0 f_{s,\mu_0}^j(E' \to E, \mu_0) = 1. \tag{75}$$

- The scattering cross section consists of the sum of the elastic and "total inelastic" scattering cross sections:

$$\Sigma_s^j(z, E') = \Sigma_{s_{el}}^j(z, E') + \Sigma_{s_{in}}^j(z, E') \,, \tag{76}$$

in which the "total inelastic" scattering cross section $\Sigma_{s_{in}}^j(z, E')$, the combination of all discrete inelastic and continuum inelastic scattering cross sections, is given by:

$$\Sigma_{s_{in}}^j(z, E') = \sum_{i=1}^{I_j} \Sigma_{s_{in,i}}^j(z, E') + \Sigma_{s_{in,c}}^j(z, E') \,. \tag{77}$$

17

$\Sigma^j_{s_{in}}(z, E')$ is only nonzero at high energies, and is almost always significantly smaller than $\Sigma^j_{s_{el}}(z, E')$ even at those energies.

- Using Eqs. (72), (74), (76) and (77), the full effective probability densities can be determined:

$$f^j_{s,E}(E' \to E) = \left[\Sigma^j_{s_{el}}(z, E') f^j_{s_{el},E}(E' \to E) + \right.$$
$$+ \sum_{i=1}^{I_j} \Sigma^j_{s_{in,i}}(z, E') f^j_{s_{in,i},E}(E' \to E) + \tag{78}$$
$$\left. + \Sigma^j_{s_{in,c}}(z, E') f^j_{s_{in,c},E}(E' \to E) \right] \bigg/ \Sigma^j_s(z, E'),$$

$$f^j_{s,\mu_0}(E' \to E, \mu_0) = \frac{\Sigma^j_{s*}(z, E' \to E, \mu_0)}{\Sigma^j_s(z, E') f^j_{s,E}(E' \to E)}, \tag{79}$$

which lets us express the double differential scattering cross section as:

$$\Sigma^j_{s*}(z, E' \to E, \mu_0) = \Sigma^j_s(z, E') f^j_{s,E}(E' \to E) f^j_{s,\mu_0}(E' \to E, \mu_0). \tag{80}$$

It can be shown that the full effective probability densities still normalize to 1.

- Inelastic scattering only occurs at high energies, and primarily for heavy isotopes. Some lighter isotopes are capable of it as well, but heavier isotopes are much more prone to it. It tends to be close to isotropic in μ_0, although not perfectly so.

We can now construct the Legendre scattering moments. The 0th Legendre scattering moment is given by:

$$\Sigma^j_{s*,0}(z, E' \to E) = \int_{-1}^1 d\mu_0 \Sigma^j_{s*}(z, E' \to E, \mu_0) =$$
$$= \Sigma^j_s(z, E') f^j_{s,E}(E' \to E) = \Sigma^j_s(z, E' \to E). \tag{81}$$

which is simply the single differential (in target energy) scattering cross section. The 1st Legendre scattering moment is given by:

$$\Sigma^j_{s*,1}(z, E' \to E) = \int_{-1}^1 d\mu_0 \mu_0 \Sigma^j_{s*}(z, E' \to E, \mu_0) =$$
$$= \Sigma^j_s(z, E') f^j_{s,E}(E' \to E) \int_{-1}^1 d\mu_0 \mu_0 f^j_{s,\mu_0}(E' \to E, \mu_0) = \tag{82}$$
$$= \Sigma^j_s(z, E' \to E) \overline{\mu}^j_0(E' \to E).$$

Here $\overline{\mu}^j_0(E' \to E)$ is the average scattering angle through which the scatter off isotope j from energy E' to E occurs, given by the second integral term in Eq. (82). As shown above, the reason there may be several scattering angles for a given energy pair is because an energy may be reachable from more than one discrete inelastic scattering energy level,

or, potentially, the continuum inelastic scattering as well. If inelastic scattering is neglected, then the term becomes a function of E'/E, and corresponds to the only possible scattering angle cosine for elastic scattering from energy E' to E.

Integrals of Legendre scattering moments over all target energies also have physical meaning. Denoting such integral for n^{th} Legendre scattering moment as $\Sigma_{s*,n}^j(z, E')$, and evaluating them for $n = 0$ and 1 yields (using Eqs. (75), (81) and (82)) the following:

$$\Sigma_{s*,0}^j(z, E') = \int_0^\infty dE \Sigma_{s*,0}^j(z, E' \to E) = \Sigma_s^j(z, E'),$$ (83)

$$\Sigma_{s*,1}^j(z, E') = \int_0^\infty dE \Sigma_{s*,1}^j(z, E' \to E) = \overline{\mu}_0^j(E') \Sigma_s^j(z, E'),$$ (84)

in which $\overline{\mu}_0^j(E')$ is the average scattering angle cosine for scattering from isotope j at energy E', given by:[1]

$$\overline{\mu}_0^j(E') = \frac{\int_0^\infty dE \overline{\mu}_0^j(E' \to E) \Sigma_s^j(z, E' \to E)}{\int_0^\infty dE \Sigma_s^j(z, E' \to E)} = \frac{\int_0^\infty dE \Sigma_{s*,1}^j(z, E' \to E)}{\Sigma_s^j(z, E')}.$$ (85)

$\overline{\mu}_0^j(E')$ is not position-dependent because the position-dependent quantity in Eq. (85), the number density of isotope j, cancels out.

To summarize: the 0th Legendre scattering moment is the single differential (in target energy) scattering cross section, and the 1st Legendre scattering moment is the product of the single differential scattering cross section and the average scattering angle for a given source/target energy pair. The integrals of these moments over all target energies are the scattering cross section and the product of the average scattering angle cosine and the scattering cross section, respectively. We may now proceed to construct $D(z, E)$.

Equation (71) is formal because it depends on $\varphi_1(t, z, E)$ — an unknown quantity. However, $\varphi_1(t, z, E)$ only plays the role of a weighting quantity here, and so various approximations for it may be used. Several different approximations, all of which lead to a practically usable $D(z, E)$, are presented below.

Approximation 1. A net current $\varphi_1(t, z, E)$ is assumed, based on a transport calculation. Such calculations are frequently conducted prior to a full core (diffusion theory-based) analysis, and their primary purpose is the evaluation of multigroup parameters (discussed in section 5), including the diffusion coefficient. This transport calculation has to make certain simplifying assumptions by itself, unless it is run for a full core (which is almost always prohibitively expensive). Only the shape in energy of $\varphi_1(t, z, E)$ (i.e., "current spectrum") has to be known to construct $D(z, E)$: the scale does not matter. The shape is typically assumed to be nearly constant, which allows the diffusion coefficient to be time-invariant; otherwise, $D(t, z, E)$ is used. The closer the assumed net current is to the physical net current, the more accurate the diffusion model will be.

---

[1]In Approximation 3 below, scattering angle and target energy are decoupled, so a slightly different expression for $\overline{\mu}_0^j(E')$ is used.

Approximation 2. The net current $\varphi_1(t, z, E)$ is assumed to have the same approximate shape in energy as the approximate scalar flux energy spectrum $\psi(z, E)$ — a known quantity, discussed in greater detail in section 5. This allows the approximation of the diffusion coefficient as follows:

$$D(z, E) \cong \frac{1}{3 \left[\Sigma_t(z, E) - \dfrac{1}{\psi(z, E)} \displaystyle\sum_{j=1}^{J} \int_0^\infty dE' \Sigma_{s^*,1}^j(z, E' \to E) \, \psi(z, E') \right]}. \tag{86}$$

Both Approximations 1 and 2 require rather detailed information to be available to construct the diffusion coefficient; this is often not possible. For this reason, Approximations 3 and 4 are often used instead, at least for initial analysis.

Approximation 3. It is assumed that there is no energy change due to anisotropic scattering. Effectively, this allows us to approximate $\Sigma_{s^*,1}^j(z, E' \to E)$ as follows:

$$\Sigma_{s^*,1}^j(z, E' \to E) \cong \Sigma_s^j(z, E') \, \delta(E' - E) \int_{-1}^{1} d\mu_0 \mu_0 f_{s,\mu_0}^j(E', \mu_0), \tag{87}$$

where $f_{s,\mu_0}^j(E' \to E, \mu_0)$ was replaced with $f_{s,\mu_0}^j(E', \mu_0)$. The two functions are related as follows: $f_{s,\mu_0}^j(E' \to E, \mu_0)$ is the probability density characterizing all possible scattering angle cosines for the (E', E) source/target pair, while $f_{s,\mu_0}^j(E', \mu_0)$ is the probability density characterizing all possible scattering angle cosines regardless of the target energy. Both are probability densities in μ_0, but $f_{s,\mu_0}^j(E', \mu_0)$ here is used to account for the range of reachable scattering angle cosines that the approximation of $f_{s,E}^j(E' \to E) = \delta(E' - E)$ otherwise neglected. This therefore yields the following 1$^{\text{st}}$ Legendre scattering moment:

$$\Sigma_{s^*,1}^j(z, E' \to E) \cong \overline{\mu}_0^j(E') \, \Sigma_s^j(z, E') \, \delta(E' - E), \tag{88}$$

which, substituted into Eq. (71), yields the desired approximation of the diffusion coefficient:

$$D(z, E) \cong \frac{1}{3 \left[\Sigma_t(z, E) - \displaystyle\sum_{j=1}^{J} \overline{\mu}_0^j(E) \, \Sigma_s^j(z, E) \right]} \tag{89}$$

Here, because the scattering angle cosine and target energy were decoupled, $\overline{\mu}_0^j(E')$ was found through:

$$\overline{\mu}_0^j(E') = \int_{-1}^{1} d\mu_0 \mu_0 f_{s,\mu_0}^j(E', \mu_0). \tag{90}$$

This approximation is clearly very convenient, because it requires no prior knowledge of the current or scalar flux spectrum. The assumption that lead to it, however, is questionable. It works best for heavy isotopes. The reason is the following: an inspection of the scattering probability densities of such isotopes reveals, that at high energies, their elastic scattering angular probability densities are very forward-biased (in μ_0), and so, combined with the very

high nucleus to neutron mass ratio, no appreciable energy loss occurs. At lower energies, their elastic scattering angular probability densities are nearly isotropic (in μ_0, which for heavy isotopes is very close to μ_{CM}), which means $\overline{\mu}_0^j(E') \cong 0$, and so the inscattering term cancels out. Significant downscattering may be occuring — but it is isotropic, and for $D(z, E)$, we are only interested in anisotropic scattering.

Inelastic scattering, which, as noted above, occurs for heavy isotopes at high energies, is nearly isotropic in μ_0, and so does not strongly violate the above approximation.

It is important to note (for comparision with the next approximation), that with Approximation 3, there is no limit on the strength of absorption. In fact, diffusion theory can be shown to work perfectly in a uniform homogeneous absorber.

Approximation 3 works much worse for light water, because Hydrogen-1 acts as a moderator, and therefore clearly slows down neutrons with almost every collision. The mean scattering angle cosine for Hydrogen-1 is 2/3, and so most scattering is clearly anisotropic for it. Fortunately, the next approximation allows the construction of $D(z, E)$ for hydrogenous environments.

Approximation 4.[2] It is assumed that the anisotropic inscattering and outscattering rates are balanced. This assumption is justified by analyzing the net slowing-down density, as shown below.

Let $q^{\downarrow}(t, z, E, \mu)$ be the angular slowing-down density: the rate density in space and zenith angle cosine of neutrons slowing down (downscattering) past E. It is given by:

$$q^{\downarrow}(t, z, E, \mu) = \sum_{j=1}^{J} \int_{E}^{\infty} dE' \int_{0}^{E} dE'' \int_{-1}^{1} d\mu' \Sigma_{s*}^{j}(z, E' \to E'', \mu_0) \, \varphi(t, z, E', \mu') \,. \qquad (91)$$

Similarly, let $q^{\uparrow}(t, z, E, \mu)$ be the accelerating density:[3] the rate density in space and zenith angle cosine of neutrons accelerating (upscattering) past E. It is given by:

$$q^{\uparrow}(t, z, E, \mu) = \sum_{j=1}^{J} \int_{0}^{E} dE' \int_{E}^{\infty} dE'' \int_{-1}^{1} d\mu' \Sigma_{s*}^{j}(z, E' \to E'', \mu_0) \, \varphi(t, z, E', \mu') \,. \qquad (92)$$

Multiplying both Eq. (91) and (92) by $P_n(\mu)$, integrating over $\mu \in [-1, 1]$ and making use of Eqs. (49)–(51) to greatly simplify the resulting expressions yields the nth Legendre moments of the slowing-down and accelerating densities:

$$q_n^{\downarrow}(t, z, E) = \sum_{j=1}^{J} \int_{E}^{\infty} dE' \int_{0}^{E} dE'' \Sigma_{s*,n}^{j}(z, E' \to E'') \, \varphi_n(t, z, E') \,, \qquad (93)$$

$$q_n^{\uparrow}(t, z, E) = \sum_{j=1}^{J} \int_{0}^{E} dE' \int_{E}^{\infty} dE'' \Sigma_{s*,n}^{j}(z, E' \to E'') \, \varphi_n(t, z, E') \,. \qquad (94)$$

---

[2]Most books do not show this approximation.
[3]Not a commonly used term; $q^{\uparrow}(t, z, E, \mu)$ is almost always neglected in this type of treatment.

Next, we differentiate Eqs. (93) and (94) using the Leibniz integral rule and the second fundamental theorem of calculus, and obtain:

$$\frac{\partial}{\partial E}q_n^\downarrow(t,z,E) = \sum_{j=1}^J \left[-\int_0^E dE'' \Sigma_{s^*,n}^j(z,E\rightarrow E'')\,\varphi_n(t,z,E) + \right.$$
$$\left. +\int_E^\infty dE' \Sigma_{s^*,n}^j(z,E'\rightarrow E)\,\varphi_n(t,z,E') \right], \tag{95}$$

$$\frac{\partial}{\partial E}q_n^\uparrow(t,z,E) = \sum_{j=1}^J \left[\int_E^\infty dE'' \Sigma_{s^*,n}^j(z,E\rightarrow E'')\,\varphi_n(t,z,E) - \right.$$
$$\left. -\int_0^E dE' \Sigma_{s^*,n}^j(z,E'\rightarrow E)\,\varphi_n(t,z,E') \right]. \tag{96}$$

Subtracting Eq. (94) from Eq. (93) yields $q_n^\Downarrow(t,z,E)$, the nth Legendre moment of the net slowing-down density. Similarly, subtracting Eq. (96) from Eq. (95) yields the energy derivative of $q_n^\Downarrow(t,z,E)$, which can be simplified:

$$\frac{\partial}{\partial E}q_n^\Downarrow(t,z,E) = \frac{\partial}{\partial E}q_n^\downarrow(t,z,E) - \frac{\partial}{\partial E}q_n^\uparrow(t,z,E) =$$
$$= \sum_{j=1}^J \left[\int_0^\infty dE' \Sigma_{s^*,n}^j(z,E'\rightarrow E)\,\varphi_n(t,z,E') - \left(\int_0^\infty dE'' \Sigma_{s^*,n}^j(z,E\rightarrow E'') \right)\varphi_n(t,z,E) \right] =$$
$$= \sum_{j=1}^J \left[\int_0^\infty dE' \Sigma_{s^*,n}^j(z,E'\rightarrow E)\,\varphi_n(t,z,E') \right] - \sum_{j=1}^J \Sigma_{s^*,n}^j(z,E)\,\varphi_n(t,z,E)$$
$$\tag{97}$$

We are interested in Eq. (97) for $n=1$. This quantity classifies the variation in energy of the anisotropic net slowing-down density. This quantity may vary in energy only due to absorption or leakage. Assuming a very low-absorption (i.e., hydrogenous) and homogeneous environment, away from boundaries (therefore, with weak spatial variation), we can make the following approximation:

$$\frac{\partial}{\partial E}q_1^\Downarrow(t,z,E) \cong 0. \tag{98}$$

With this approximation, Eq. (97) for $n=1$ can be rearranged to yield:

$$\sum_{j=1}^J \left[\int_0^\infty dE' \Sigma_{s^*,1}^j(z,E'\rightarrow E)\,\varphi_1(t,z,E') \right] = \sum_{j=1}^J \Sigma_{s^*,1}^j(z,E)\,\varphi_1(t,z,E). \tag{99}$$

Equation (99) is a statement of anisotropic inscattering and outscattering rate balance, as stated above. The assumptions of negligible absorption and negligible spatial variation in scalar flux were necessary to justify it. The left hand side is exactly the same as the

22

inscattering part of Eq. (71), so subsituting Eq. (99) into Eq. (71), and utilizing Eq. (84) yields the desired approximation of the diffusion coefficient:

$$D(z, E) \cong \frac{1}{3 \left[\Sigma_t(z, E) - \sum_{j=1}^{J} \overline{\mu}_0^j(E) \, \Sigma_s^j(z, E) \right]}. \tag{100}$$

Equations (89) and (100) are identical. This indicates that both Approximations 3 and 4, despite very different physical assumptions that went into them, can be used simultaneously, yielding the same diffusion coefficient.

It is important to recognize that both approximations still fail in a number of practical situations. Homogenizing a light water reactor assembly, for example, yields a medium filled with both a strong anisotropic moderator (Hydrogen-1), which violates Approximation 3, and a strong absorber (actinides), which violates Approximation 4. Homogenization is necessary, however, because without it flux is far too anisotropic in angle to be adequately approximated as linearly anisotropic.

For this reason, Approximations 1 and 2 (the more practical one) are generally preferable to Approximations 3 and 4. Approximations 3 and 4 are still very useful as initial estimates.

Approximation 5. Scattering is assumed to be fully isotropic in the lab coordinate system. This can be stated as:

$$\overline{\mu}_0^j(E' \to E) \cong 0, \tag{101}$$

which instantly eliminates $\Sigma_{s*,1}^j(z, E' \to E)$, which greatly simplifies Eq. (71) to yield:

$$D(z, E) \cong \frac{1}{3\Sigma_t(z, E)}. \tag{102}$$

This approximation is the simplest one of the ones presented here, and by far the least accurate. For it to be adequate, only heavy isotopes must be present, with spectrum dominated by energies at which scattering is, for these isotopes, isotropic in the CMCS. Prompt fission neutrons are not born at these energies, and so the approximation can be considered extremely coarse at best. It should be avoided whenever possible.

Other approximations for $D(z, E)$ exist, based on more complicated approximations for $\frac{\partial}{\partial E} q_1^{\Downarrow}(t, z, E)$. The see limited use, because Approximations 1 and 2 are still significantly more accurate, and using a nonzero $\frac{\partial}{\partial E} q_1^{\Downarrow}(t, z, E)$ tends not to justify the resultant complexity.

To summarize: five approximations for $D(z, E)$ were presented above. Regardless of which one is used, $D(z, E)$ becomes a known quantity. We can now complete the 1D continuous energy neutron diffusion equation.

Differentiating Eq. (65) with respect to z yields:

$$\frac{\partial}{\partial z} \varphi_1(t, z, E) = -\frac{\partial}{\partial z} D(z, E) \frac{\partial}{\partial z} \varphi_0(t, z, E), \tag{103}$$

substituting which into Eq. (58a) and using Eqs. (53), (69) and (81) yields the 1D continuous

energy neutron diffusion equation:

$$\frac{1}{V_n(E)}\frac{\partial}{\partial t}\phi(t,z,E) = \frac{\partial}{\partial z}D(z,E)\frac{\partial}{\partial z}\phi(t,z,E) - \Sigma_t(z,E)\,\phi(t,z,E) +$$

$$+ \sum_{j=1}^{J}\int_0^\infty dE'\Sigma_s^j(z,E'\to E)\,\phi(t,z,E') +$$

$$+ \int_0^\infty dE'\left[\sum_{j_f=1}^{J_f}\chi_p^{j_f}(E',E)\,\nu_p^{j_f}(E')\,\Sigma_f^{j_f}(z,E')\right]\phi(t,z,E') +$$

$$+ \sum_{m=1}^{M}\chi_{d,m}(E)\,\lambda_m c_m(t,z) + s_{ex}(t,z,E)\,. \tag{104}$$

The 1D DNPE in the form to support Eq. (104) is obtained by simply substituting Eq. (53) into Eq. (59):

$$\frac{\partial}{\partial t}c_m(t,z) = \int_0^\infty dE'\left[\sum_{j_f=1}^{J_f}\nu_{d,m}^{j_f}(E')\,\Sigma_f^{j_f}(z,E')\right]\phi(t,z,E') -$$

$$- \lambda_m c_m(t,z) \quad \forall m \in [1,\dots,M]\,. \tag{105}$$

This concludes the derivation of the 1D continuous energy NDE and the related DNPE. We can now proceed to the multigroup discretization.

5   Multigroup 1D NDE Discretization

The energy limits in Eqs. (104) and (105) are from $E = 0$ to $E = \infty$, however, in practice, the maximum energy of a neutron in a nuclear reactor is bounded. Therefore, without any loss of accuracy, we can assume that all energies of interest are in a finite interval:

$$E \in \left[0, E_0\right]. \tag{106}$$

Multigroup energy discretization is based on grouping the neutron energies in the finite interval in Eq. (106) into G energy groups. This discretization is shown in Figure 3.

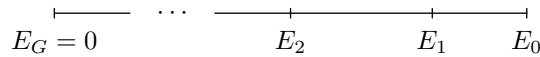$$E_G = 0 \qquad \cdots \qquad E_2 \qquad E_1 \qquad E_0$$

Figure 3: Energy Spectrum Discretization

The energy group boundaries $\{E_g\}$ are chosen prior to multigroup discretization. The set of energy group boundaries chosen for a problem is called the "energy group structure," or simply the "group structure." The group structure is almost always fixed throughout the

domain. Group g is bounded by $[E_g, E_{g-1}]$; the groups are not necessarily equal in energy width.

Multigroup discretization of the 1D NTE starts by integrating Eq. (104) over energy group g. To construct the group quantities, we assume that the intragroup flux densities, also known as in-group spectrum functions, are known. The following serious approximation is made: the intragroup spectra are assumed to be uniform and time-invariant within individual regions. This is a good approximation because the diffusion approximation only applies for homogenized reactors anyway — over which the spectrum is homogenized along with macroscopic properties. The intragroup g spectrum function within region r is denoted $\psi_g^r(E)$. The macroscopic properties are still shown as spatially-dependent; this is for completeness only, because there exist forms of homogenization which allow smoothly spatially varying properties while maintaining a uniform spectrum. Such region r is normally a fuel assembly, or a subsection of one.

The group quantities generally become less sensitive to the intragroup spectra as the groups become smaller. If the groups are taken sufficiently small that a constant in energy (or in lethargy) flux can be assumed, intragroup spectra stop being a source of error. For coarse groups, however, the quality of the solution is highly sensitive to the accuracy of the intragroup spectra.

The derivation below assumes the spectra to be uniform within individual regions, but derivations with position-dependent spectra are also demonstrated, to illustrate why they are much more difficult to treat.

Intragroup spectra for full core analysis typically come from lattice codes, which tend to use much finer group structures than full core analyses. For the purposes of this paper, spectra can be assumed known. They are normalized as follows:

$$\int_{E_g}^{E_{g-1}} dE \psi_g^r(E) = 1. \tag{107}$$

The intragroup g flux spectra therefore control the energy shape of the flux and current within group g, respectively. They are region-dependent, but are densities in energy only. The magnitude of the flux within group g is controlled by the group g flux $\phi_g(t, z)$, as follows:

$$\phi(t, z, E) = \phi_g(t, z)\, \psi_g^r(E) \text{ if } E \in [E_g, E_{g-1}], \tag{108}$$

integrating which over group g, and using the normalization from Eq. (107) also yields:

$$\int_{E_g}^{E_{g-1}} dE \phi(t, z, E) = \phi_g(t, z). \tag{109}$$

As stated above, $\left\{\psi_g^r(E)\right\}$ are known quantities; the group fluxes $\left\{\phi_g(t, z)\right\}$ are the unknowns.

To construct the 1D multigroup NDE in terms of $\phi_g(t, z)$, we substitute Eq. (108) into Eq. (104), and integrate over group g, therefore discretizing the equation in energy. The terms are treated individually below.

The region r group g speed V_{ng}^r is defined through the following:

$$\frac{1}{V_{ng}^r} = \frac{\int_{E_g}^{E_{g-1}} dE \frac{1}{V_n(E)} \frac{\partial}{\partial t} \phi(t, z, E)}{\int_{E_g}^{E_{g-1}} dE \frac{\partial}{\partial t} \phi(t, z, E)} = \frac{\int_{E_g}^{E_{g-1}} dE \frac{1}{V_n(E)} \left(\frac{\partial}{\partial t} \phi_g(t, z) \psi_g^r(E) \right)}{\int_{E_g}^{E_{g-1}} dE \left(\frac{\partial}{\partial t} \phi_g(t, z) \psi_g^r(E) \right)} =$$

$$= \frac{\frac{\partial}{\partial t} \phi_g(t, z) \int_{E_g}^{E_{g-1}} dE \frac{1}{V_n(E)} \psi_g^r(E)}{\frac{\partial}{\partial t} \phi_g(t, z) \int_{E_g}^{E_{g-1}} dE \psi_g^r(E)} = \int_{E_g}^{E_{g-1}} dE \frac{1}{V_n(E)} \psi_g^r(E) \,. \tag{110}$$

Note, how in the above integral, the normalization of $\psi_g^r(E)$ was used to remove the division by the group flux. In all similar integrals below, the intragroup spectra will be used directly, where appropriate. The resulting expressions would normally be more complicated, but they are simplified due to Eq. (107).

Equation (110) also illustrates another very important point: when the group quantities are condensed, the quantities that are normally not dependent on certain independent variables (such as the neutron speed, which is normally only a function of energy) may become dependent on them, due to the weighting flux used to construct the group quantity. In this case, the group neutron speeds may differ between regions, if the corresponding intragroup spectra are different between these regions. This will be seen with all spectrum-weighted quantities below; to avoid this growth of dependence, more restrictive approximations may be placed on $\psi_g^r(E)$, such as making it uniform throughout the reactor. Such approximations clearly introduce inaccuracies, and will be avoided in this paper until section 6.

Integrating the time derivative term in Eq. (104) over group g, and substituting in Eq. (110) yields the group g time derivative term:

$$\int_{E_g}^{E_{g-1}} dE \frac{1}{V_n(E)} \frac{\partial}{\partial t} \phi(t, z, E) = \frac{1}{V_{ng}^r(z)} \frac{\partial}{\partial t} \phi_g(t, z) \,. \tag{111}$$

Note, that if we assumed a time- and position-varying spectrum, this term would be significantly more complicated:

$$\int_{E_g}^{E_{g-1}} dE \frac{1}{V_n(E)} \frac{\partial}{\partial t} \phi(t, z, E) = \frac{\partial}{\partial t} \left[\int_{E_g}^{E_{g-1}} dE \frac{1}{V_n(E)} \phi(t, z, E) \right] =$$

$$= \frac{\partial}{\partial t} \left[\left(\int_{E_g}^{E_{g-1}} dE \frac{1}{V_n(E)} \psi_g^r(t, z, E) \right) \phi_g(t, z) \right] = \frac{\partial}{\partial t} \left[\frac{1}{V_{ng}^r(t, z)} \phi_g(t, z) \right] = \tag{112}$$

$$= \frac{1}{V_{ng}^r(t, z)} \frac{\partial}{\partial t} \phi_g(t, z) + \left[\frac{\partial}{\partial t} \left(\frac{1}{V_{ng}^r(t, z)} \right) \right] \phi_g(t, z) \,.$$

The first term in Eq. (112) is clearly the same as Eq. (111), and the second term is zero if the spectrum is assumed to be time-invariant. It accounts for the variation in the group g

neutron balance due to a transient change in neutron spectrum, which may occur even if the group flux stays constant (i.e., $\frac{\partial}{\partial t}\phi_g(t,z) = 0$). This is one of the reasons why the spectrum is typically assumed time-invariant; fortunately, it is a good assumption if sufficiently fine groups are used, and there is no thermal feedback.

To treat the diffusion term, we must construct the group g diffusion coefficient. Group diffusion coefficient construction is discussed in more detail in section 7; below, $D(z,E)$ is treated as an exactly known quantity, within the accuracy of the approximation used to build it (see section 4 for a discussion of the approximations).

The group g region r diffusion coefficient is defined as follows:

$$D_g^r(z) = \int_{E_g}^{E_{g-1}} dE D(z,E)\,\psi_g^r(E)\,. \tag{113}$$

Integrating the diffusion term in Eq. (104) over group g, and substituting in Eq. (113) yields the group g diffusion term:

$$\int_{E_g}^{E_{g-1}} dE \frac{\partial}{\partial z} D(z,E) \frac{\partial}{\partial z}\phi(t,z,E) = \frac{\partial}{\partial z} D_g^r(z) \frac{\partial}{\partial z}\phi_g(t,z)\,. \tag{114}$$

A time dependence of the spectrum does not introduce complications for this term, but the position dependence does:

$$\int_{E_g}^{E_{g-1}} \frac{\partial}{\partial z}D(z,E) \frac{\partial}{\partial z}\phi(t,z,E) = \frac{\partial}{\partial z}\left\{ \int_{E_g}^{E_{g-1}} dE D(z,E) \frac{\partial}{\partial z}\left[\phi_g(t,z)\,\psi_g^r(t,z,E)\right]\right\} =$$

$$= \frac{\partial}{\partial z}\int_{E_g}^{E_{g-1}} dE\left(D(z,E)\,\psi_g^r(E) \right)\left(\frac{\partial}{\partial z}\phi_g(t,z) \right) +$$

$$+ \frac{\partial}{\partial z}\int_{E_g}^{E_{g-1}} dE\left(D(z,E) \frac{\partial}{\partial z}\psi_g^r(t,z,E) \right)\left(\phi_g(t,z) \right) =$$

$$= \frac{\partial}{\partial z}\left[D_g^r(t,z) \frac{\partial}{\partial z}\phi_g(t,z)\right] + \frac{\partial}{\partial z}\left[D_g^{*r}(t,z)\,\phi_g(t,z)\right]\,, \tag{115}$$

with $D_g^{*r}(t,z)$ given by:

$$D_g^{*r}(t,z) = \int_{E_g}^{E_{g-1}} dE D(z,E) \frac{\partial}{\partial z}\psi_g^r(t,z,E)\,. \tag{116}$$

The first term in Eq. (115) is clearly the same as Eq. (114), and the second term is zero if the spectrum is assumed to be uniform within region r (it may still be time-dependent). The group diffusion coefficient $D_g^{*r}(t,z)$ of this second term can be thought of as being weighted by the spatial derivative of the intragroup spectrum, instead of by the spectrum itself. This second diffusion term accounts for diffusion that may occur in group g due to

spatial variation of the spectrum, even if there is no spatial variation in the group scalar flux itself (i.e. $\frac{\partial}{\partial z}\phi_g(t, z) = 0$). As stated above, homogenization is usually done in such a way that the spectrum within a region is uniform, and so this term is not present. Without homogenization, the assumption of the uniform spectrum in a region is not adequate.

The group g region r total cross section is constructed trivially:

$$\Sigma^r_{tg}(z) = \int_{E_g}^{E_{g-1}} dE \Sigma_t(z, E)\, \psi^r_g(E)\,. \tag{117}$$

Integrating the total reaction term in Eq. (104) over group g, and substituting in Eq. (117) yields the group g total reaction term:

$$\int_{E_g}^{E_{g-1}} dE \Sigma_t(z, E)\, \phi(t, z, E) = \Sigma^r_{tg}(z)\, \phi_g(t, z)\,. \tag{118}$$

To construct the group g' to g scattering cross section (sometimes referred to as the group-to-group constant), we first recognize that the integral over all source energies can be discretized, without any approximations, as follows:

$$\int_0^\infty dE' \Sigma^j_s(z, E' \to E)\, \phi(t, z, E') = \sum_{g'=1}^G \int_{E_{g'}}^{E_{g'-1}} dE' \Sigma^j_s(z, E' \to E)\, \phi(t, z, E')\,. \tag{119}$$

The region r group g' to g scattering cross section for isotope j is then given by:

$$\Sigma^{r,j}_{sgg'}(z) = \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \Sigma^j_s(z, E' \to E)\, \psi^r_{g'}(E')\,. \tag{120}$$

At this point, the isotope-specific group-to-group scattering cross sections can finally be easily combined, because they are all now functions of z only. We did not do so until now to emphasize that all isotopes have drastically different scattering probability distribution functions $f^j_{s,E}(E' \to E)$. At this point, each isotope simply has a scattering kernel $\{\Sigma^{r,j}_{sgg'}(z)\}$, which at any location z is a nearly lower triangular matrix ($\Sigma^{r,j}_{sgg'}(z)$ is the row g, column g' element). It is almost lower triangular because, except at very low energies, there is no upscattering.

The isotope-specific group-to-group scattering cross sections combine as follows:

$$\Sigma^r_{sgg'}(z) = \sum_{j=1}^J \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \Sigma^j_s(z, E' \to E)\, \psi^r_{g'}(E') = \sum_{j=1}^J \Sigma^{r,j}_{sgg'}(z)\,. \tag{121}$$

Integrating the inscattering term in Eq. (104) over group g, and substituting in Eq. (121) yields the group g inscattering term:

$$\int_{E_g}^{E_{g-1}} dE \sum_{j=1}^J \int_0^\infty dE' \Sigma^j_s(z, E' \to E)\, \phi(t, z, E') = \sum_{g'=1}^G \Sigma^r_{sgg'}(z)\, \phi_{g'}(t, z)\,. \tag{122}$$

28

The prompt fission source term is treated similarly to the inscattering term. The integral over source energies is split over groups:

$$\int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E', E) \, \nu_p^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \phi(t, z, E') =$$
$$= \sum_{g'=1}^G \int_{E_{g'}}^{E_{g'-1}} dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E', E) \, \nu_p^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \phi(t, z, E'), \tag{123}$$

and the combined region r group g' to g prompt neutron production cross section is defined similarly to the group-to-group combined scattering cross section:

$$\chi_p \nu_p \Sigma_{fgg'}^r(z) = \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E', E) \, \nu_p^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \psi_{g'}^r(E'). \tag{124}$$

Note, that here, $\chi_p \nu_p \Sigma_{fgg'}^r(z)$ is actually one quantity, which is a function of z, and accounts for the prompt neutrons generated in group g from fissions in group g'. Typically, this quantity is given as $(1 - \beta) \, \nu \Sigma_{fgg'}^r(z)$, which is due to the prompt spectrum being assumed to be fission neutron energy (E')-independent — a reasonable assumption in most reactors, and β being used to denote the delayed neutron fraction (DNF, also assumed to be fission neutron energy-independent). $\nu_p(E')$ is used here instead because it is the quantity actually given in nuclear databases. The target energy-independent treatment of this term, which is a very common simplification, is provided in section 6.

It is also important to note that, because $\chi_p^{j_f}(E', E)$ is a density in E, and normalizes to 1 when integrated over all energies, the group prompt neutron production cross sections must normalize as well:

$$\nu_p \Sigma_{fg'}^{j_f,r}(z) = \sum_{g=1}^G \chi_p \nu_p \Sigma_{fgg'}^{j_f,r}(z) = \int_{E_{g'}}^{E_{g'-1}} dE' \nu_p^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \, \psi_{g'}^r(E'). \tag{125}$$

Integrating the prompt fission source term in Eq. (104) over group g, and substituting in Eq. (124) yields the group g prompt fission source term:

$$\int_{E_g}^{E_{g-1}} dE \int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E', E) \, \nu_p^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \phi(t, z, E') =$$
$$= \sum_{g'=1}^G \chi_p \nu_p \Sigma_{fgg'}^r(z) \, \phi_{g'}(t, z). \tag{126}$$

The total reaction, inscattering and prompt fission source terms would not be significantly complicated by a time- and position-dependent spectrum — the group cross sections would

simply become time-dependent. The total reaction term would change as follows:

$$\int_{E_g}^{E_{g-1}} dE\Sigma_t(z,E)\,\phi(t,z,E) = \int_{E_g}^{E_{g-1}} dE\Sigma_t(z,E)\,\phi_g(t,z)\,\psi_g^r(t,z,E) = \Sigma_{tg}^r(t,z)\,\phi_g(t,z)\,,$$
(127)

and the inscattering and prompt fission terms would, similarly, become:

$$\int_{E_g}^{E_{g-1}} dE \sum_{j=1}^{J} \int_0^\infty dE'\Sigma_s^j(z,E'\to E)\,\phi(t,z,E') =$$

$$= \int_{E_g}^{E_{g-1}} dE \sum_{j=1}^{J} \int_0^\infty dE'\Sigma_s^j(z,E'\to E)\,\phi_{g'}(t,z)\,\psi_{g'}^r(t,z,E') = \sum_{g'=1}^{G} \Sigma_{sgg'}^r(t,z)\,\phi_{g'}(t,z)\,,$$
(128)

and

$$\int_{E_g}^{E_{g-1}} dE \int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E',E)\,\nu_p^{j_f}(E')\,\Sigma_f^{j_f}(z,E') \right]\phi(t,z,E') =$$

$$= \int_{E_g}^{E_{g-1}} dE \int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \chi_p^{j_f}(E',E)\,\nu_p^{j_f}(E')\,\Sigma_f^{j_f}(z,E') \right]\phi_{g'}(t,z)\,\psi_{g'}^r(t,z,E') = \quad (129)$$

$$= \sum_{g'=1}^{G} \chi_p\nu_p\Sigma_{fgg'}^r(t,z)\,\phi_{g'}(t,z)\,.$$

While there is a single vector of length G of total group cross sections (as well as diffusion coefficients, neutron speeds and external sources) at any location z at time t, there are $G \times G$ group-to-group scattering and $G \times G$ group-to-group prompt fission production cross sections. For this reason, while it is conceptually simple to construct time-dependent total cross sections, it is computationally expensive to have the scattering kernel and prompt fission source matrix be time-dependent as well. This is another reason why intragroup spectra are usually assumed to be time-invariant (unless thermal feedback is present).

Lastly, we treat the flux-independent terms: the delayed neutron and the external sources. Defining the group g precursor family m delayed yield spectral fraction as:

$$\chi_{dg,m} = \int_{E_g}^{E_{g-1}} dE\chi_{d,m}(E)\,,$$
(130)

integrating the delayed neutron source term in Eq. (104) and substituting in Eq. (130) yields the group g delayed neutron source:

$$\int_{E_g}^{E_{g-1}} dE \sum_{m=1}^{M} \chi_{d,m}(E)\,\lambda_m c_m(t,z) = \sum_{m=1}^{M} \chi_{dg,m}\lambda_m c_m(t,z)\,.$$
(131)

30

The group g external source term is constructed similarly:

$$s_{exg}(t, z) = \int_{E_g}^{E_{g-1}} dE \, s_{ex}(t, z, E) \,. \tag{132}$$

The delayed neutron and the external source terms do not depend on the flux, and so are unaffected if time- or position-dependent intragroup spectra are used.

Combining the terms from Eqs. (111), (114), (118), (122), (126), (131) and (132) yields the set of G 1D multigroup neutron diffusion equations:

$$\frac{1}{V_{ng}^r(z)} \frac{\partial}{\partial t} \phi_g(t, z) = \frac{\partial}{\partial z} D_g^r(z) \frac{\partial}{\partial z} \phi_g(t, z) - \Sigma_{tg}^r(z) \, \phi_g(t, z) + \sum_{g'=1}^{G} \Sigma_{sgg'}^r(z) \, \phi_{g'}(t, z) + \\
+ \sum_{g'=1}^{G} \chi_p \nu_p \Sigma_{fgg'}^r(z) \, \phi_{g'}(t, z) + \sum_{m=1}^{M} \chi_{dg,m} \lambda_m c_m(t, z) + s_{exg}(t, z) \quad \forall g \in [1, \ldots, G] \,. \tag{133}$$

To discretize the 1D DNPE (Eq. (105)) in energy, we need to convert its precursor source term into a multigroup form. To do so, we simply split the integral over groups:

$$\int_0^\infty dE' \left[\sum_{j_f=1}^{J_f} \nu_{d,m}^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \phi(t, z, E') = \\
= \sum_{g'=1}^{G} \int_{E_{g'}}^{E_{g'-1}} dE' \left[\sum_{j_f=1}^{J_f} \nu_{d,m}^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \phi(t, z, E') \,, \tag{134}$$

define the group g' region r delayed neutron source term:

$$\nu_d \Sigma_{fg',m}^r(z) = \int_{E_{g'}}^{E_{g'-1}} dE' \left[\sum_{j_f=1}^{J_f} \nu_{d,m}^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \psi_{g'}^r(E') \,, \tag{135}$$

and substitute Eqs. (134) and (135) back into Eq. (105) to yield the 1D multigroup DNPE:

$$\frac{\partial}{\partial t} c_m(t, z) = \sum_{g'=1}^{G} \nu_d \Sigma_{fg',m}^r(z) \, \phi_{g'}(t, z) - \lambda_m c_m(t, z) \quad \forall m \in [1, \ldots, M] \,. \tag{136}$$

Intragroup spectrum would only have a minor effect on the delayed neutron source term:

$$\nu_d \Sigma_{fg',m}^r(t, z) = \int_{E_{g'}}^{E_{g'-1}} dE' \left[\sum_{j_f=1}^{J_f} \nu_{d,m}^{j_f}(E') \, \Sigma_f^{j_f}(z, E') \right] \psi_{g'}^r(t, z, E') \,. \tag{137}$$

Equations (133) and (136) are based on uniform, steady state intra group spectra. The 1D multigroup NDE with transient, position-dependent spectra is obtained by replacing the

31

corresponding terms in Eq. (133) with Eqs. (112), (115), (127), (128) and (129), which yields:

$$\frac{1}{V_{ng}^r(t,z)}\frac{\partial}{\partial t}\phi_g(t,z) + \left[\frac{\partial}{\partial t}\left(\frac{1}{V_{ng}^r(t,z)}\right)\right]\phi_g(t,z) = \frac{\partial}{\partial z}\left[D_g^r(t,z)\frac{\partial}{\partial z}\phi_g(t,z)\right] +$$

$$+ \frac{\partial}{\partial z}\left[D_g^{*r}(t,z)\,\phi_g(t,z)\right] - \Sigma_{tg}^r(t,z)\,\phi_g(t,z) + \sum_{g'=1}^{G}\Sigma_{sgg'}^r(t,z)\,\phi_{g'}(t,z) +$$

$$+ \sum_{g'=1}^{G}\chi_p\nu_p\Sigma_{fgg'}^r(t,z)\,\phi_{g'}(t,z) + \sum_{m=1}^{M}\chi_{dg,m}\lambda_m c_m(t,z) + s_{exg}(t,z) \quad \forall g \in [1,\ldots,G].$$

$$(138)$$

Similarly, the 1D multigroup DNPE with transient, position-dependent spectra is obtained by replacing the precursor source term in Eq. (136) with Eq. (137):

$$\frac{\partial}{\partial t}c_m(t,z) = \sum_{g'=1}^{G}\nu_d\Sigma_{fg',m}^r(t,z)\,\phi_{g'}(t,z) - \lambda_m c_m(t,z) \quad \forall m \in [1,\ldots,M]. \qquad (139)$$

Equations (138) and (139) are clearly more complicated than Eqs. (133) and (136). For reasons discussed throughout this chapter, the uniform, steady state intragroup spectra approximation is sufficient for most transient diffusion analysis, and so Eqs. (133) and (136) are used much more often. Spatial variation of the spectrum frequently arizes from excessively coarse homogenization (i.e., the regions r are too large), and the separation of the spatial domain into more regions usually is enough to allow for spectrum uniformity. For the spectrum to be strongly time-dependent, temperature feedback is typically required, which primarily affects the absorption (radiative capture) term — which, as discussed above, is relatively easy to make time-dependent, because it does not require the recomputation of a $G \times G$ scattering/fission source kernel.

Lastly, it is worth noting that Eq. (133) is frequently given in a different form:

$$\frac{1}{V_{ng}^r(z)}\frac{\partial}{\partial t}\phi_g(t,z) = \frac{\partial}{\partial z}D_g^r(z)\frac{\partial}{\partial z}\phi_g(t,z) - \Sigma_{Rg}^r(z)\,\phi_g(t,z) + \sum_{g'\neq g}^{G}\Sigma_{sgg'}^r(z)\,\phi_{g'}(t,z) +$$

$$+ \sum_{g'=1}^{G}\chi_p\nu_p\Sigma_{fgg'}^r(z)\,\phi_{g'}(t,z) + \sum_{m=1}^{M}\chi_{dg,m}\lambda_m c_m(t,z) + s_{exg}(t,z) \quad \forall g \in [1,\ldots,G],$$

$$(140)$$

with the group g region r removal cross section given by:

$$\Sigma_{Rg}^r(z) = \Sigma_{tg}^r(z) - \Sigma_{sgg}^r(z). \qquad (141)$$

Here $\sum_{g'\neq g}^{G}$ denotes the sum over all groups g' except g. Sometimes the removal cross section term is further split as follows:

$$\Sigma_{Rg}^r(z) = \Sigma_{tg}^r(z) - \Sigma_{sgg}^r(z) = \Sigma_{ag}^r(z) + \sum_{g'\neq g}^{G}\Sigma_{sgg'}^r(z). \qquad (142)$$

The formulations of Eqs. (133) and (140) (with either Eq. (141) or (142)) are completely equivalent; they differ only in notation. Equation (142) is particularly commonly used for describing two-group diffusion problems with no upscattering.

This concludes the derivation of the multigroup 1D neutron diffusion equation, which was the primary purpose of this document. It resulted in a very general formulation, that does not make any of the approximations typically made in literature when deriving these equations. Section 6 discusses the simplifications made to reduce the multigroup 1D NDE and DNPE into more conventional, much simpler forms.

Sections 7 and 8 discuss several details of constructing the corresponding condensed terms based on available nuclear data, they can be very easily skipped without **any** loss of understanding of any of the derivations so far.

6   Further Simplifications

The simplifications to Eqs. (133) and (136) can be roughly separated into three groups: the eigenvalue simplification, the small simplifications that are commonly made without a significant reduction in accuracy for most problems, and the coarse simplifications that should be avoided in most analyses, because they significantly impact accuracy.

In many of the simplifications below, a modified form of prompt fission and delayed neutron source terms can be used; it was described in detail in the *Neutron Transport Equation Derivation* document, and is quickly summarized below.

The total average number neutrons per fission $\nu^{j_f}(E')$ is frequently used in combination with delayed neutron fractions, instead of using $\nu_p^{j_f}(E')$ and $\nu_{d,m}^{j_f}(E')$. $\nu^{j_f}(E')$ is defined by:

$$\nu^{j_f}(E') = \nu_p^{j_f}(E') + \sum_{m=1}^{M} \nu_{d,m}^{j_f}(E'). \tag{143}$$

There are two ways define the isotope- and precursor family-specific delayed neutron fractions: as fission energy-dependent quantities, and as one-group averages. These definitions are given by Eqs. (144) and (145), respectively.

$$\beta_m^{j_f}(E') = \frac{\nu_{d,m}^{j_f}(E')}{\nu^{j_f}(E')}, \tag{144}$$

$$\beta_m^{j_f}(t, z) = \frac{\displaystyle\int_0^{\infty} dE' \nu_{d,m}^{j_f}(E') \Sigma_f^{j_f}(z, E') \phi(t, z, E')}{\displaystyle\int_0^{\infty} dE' \nu^{j_f}(E') \Sigma_f^{j_f}(z, E') \phi(t, z, E')}. \tag{145}$$

These equations illustrate that $\beta_m^{j_f}(E')$ is a tabulated property of a fissionable isotope, while $\beta_m^{j_f}(t, z)$ is a calculated parameter, controlled by the reactor's composition and spectrum. $\beta_m^{j_f}(t, z)$ can be thought of as a **modified** one-group approximation of $\beta_m^{j_f}(E')$. $\beta_m^{j_f}(E)$

33

was only given here for completeness: it is just another way of treating $\nu_{d,m}^{j_f}(E')$, and so is almost never seen. $\beta_m^{j_f}(t,z)$ is the more insightful parameter: it is the effective ratio (fraction) of delayed (precursor family m) to total neutrons produced by fissions of isotope j_f at a given location. $\beta_m^{j_f}(t,z)$ can also be collapsed into a total isotope-specific delayed neutron fraction $\beta^{j_f}(t,z)$:

$$\beta^{j_f}(t,z) = \sum_{m=1}^{M} \beta_m^{j_f}(t,z).\tag{146}$$

Note, that $\beta_m^{j_f}(t,z)$ actually depends on $\phi(t,z,E')$, which is an unknown parameter. In practice, however, only a very rough estimate of the flux spectrum is necessary, because $\beta_m^{j_f}(E')$ is very weakly dependent on E'; it drops at very high energies, due to a threshold rise in $\nu_p^{j_f}(E')$, but remains nearly a constant throughout the rest of the spectrum. It also does not exhibit resonances. For these reasons, a very rough approximation of the spectrum (necessary to take the integrals in Eq. (145)) is enough for a very good estimate of $\beta_m^{j_f}(t,z)$.

The multigroup precursor-specific delayed neutron fraction is given by defining a group production cross section, the multigroup form of $\nu^{j_f}(E')\,\Sigma_f^{j_f}(z,E')$:

$$\nu\Sigma_{fg'}^{j_f,r}(z) = \nu_p\Sigma_{fg'}^{j_f,r}(z) + \sum_{m=1}^{M} \nu_d\Sigma_{fg',m}^{j_f,r}(z),\tag{147}$$

and substituting it, along with other multigroup quantities, into Eq. (145), as follows:

$$\beta_m^{j_f,r}(t,z) = \frac{\displaystyle\sum_{g'=1}^{G} \nu_d\Sigma_{fg',m}^{j_f,r}(z)\,\phi_{g'}(t,z)}{\displaystyle\sum_{g'=1}^{G} \nu\Sigma_{fg'}^{j_f,r}(z)\,\phi_{g'}(t,z)}.\tag{148}$$

We can also define an isotope-independent combined group production cross section, the multigroup form of $\nu(E')\,\Sigma_f(z,E')$, as follows:

$$\nu\Sigma_{fg'}^{r}(z) = \sum_{j_f=1}^{J_f} \nu\Sigma_{fg'}^{j_f,r}(z).\tag{149}$$

$\left\{\beta_m^{j_f,r}(t,z)\right\}$ remain dependent on the coarse spectrum $\{\phi_g(t,z)\}$, which is computed by solving the NDEs. Using approximate, assumed coarse spectra to estimate $\left\{\beta_m^{j_f,r}(t,z)\right\}$, and by extension, $\beta^{j_f,r}(t,z)$, can be useful when constructing the fission source matrices, because it allows specifying "effective" (isotope-averaged) prompt and delayed fission yield spectrum functions. They are constructed below.

As with the multigroup quantities construction in section 5, the coarse spectrum $\{\phi_g(t,z)\}$ used for calculating $\left\{\beta_m^{j_f,r}(t,z)\right\}$ is usually assumed to be time-invariant. As stated above,

this is a good assumption because the dependence of DNFs on the spectrum is weak: only the difference between fast and thermal spectrum matters, which does not tend to change significantly in reactors (i.e., reactors don't go from fast to thermal and vice versa during a transient). For this reason, below all DNFs and effective spectra are time-invariant as well, based on an assumed coarse spectrum $\{\phi_g(z)\}$.

Note, that, effectively, $\left\{\beta_m^{j_f,r}(z)\right\}$ and $\{\beta^{j_f,r}(z)\}$ are weighted averages of the delayed neutron fraction across all fission energies, but are still isotope-specific.

The fissionable isotope-averaged delayed neutron fractions are therefore weighted averages across all fission energies and fissionable isotopes. The precursor family-specific DNF and the combined one are given by Eqs. (150) and (151), respectively:

$$\beta_m(z) = \frac{\sum_{j_f=1}^{J_f}\left[\beta_m^{j_f}(z)\int_0^\infty dE'\nu^{j_f}(E)\,\Sigma_f^{j_f}(z,E')\,\phi(z,E')\right]}{\sum_{j_f=1}^{J_f}\left[\int_0^\infty dE'\nu^{j_f}(E)\,\Sigma_f^{j_f}(z,E')\,\phi(z,E')\right]}, \tag{150}$$

$$\beta(z) = \sum_{m=1}^{M}\beta_m(z). \tag{151}$$

Converting Eq. (150) to multigroup form yields:

$$\beta_m^r(z) = \frac{\sum_{j_f=1}^{J_f}\left[\beta_m^{j_f,r}(z)\sum_{g'=1}^{G}\nu\Sigma_{fg'}^{j_f,r}(z)\,\phi_{g'}(z)\right]}{\sum_{j_f=1}^{J_f}\left[\sum_{g'=1}^{G}\nu\Sigma_{fg'}^{j_f,r}(z)\,\phi_{g'}(z)\right]}. \tag{152}$$

Besides the delayed neutron fractions, combined (across fissionable isotopes) prompt and delayed yield spectra may also be defined, by Eqs. (153) and (154), respectively:

$$\chi_p(z,E) = \frac{\sum_{j_f=1}^{J_f}\left[\left(1-\beta^{j_f}(z)\right)\int_0^\infty dE'\chi_p^{j_f}(E',E)\,\nu^{j_f}(E')\,\Sigma_f^{j_f}(z,E')\,\phi(z,E')\right]}{\left(1-\beta(z)\right)\sum_{j_f=1}^{J_f}\left[\int_0^\infty dE'\nu^{j_f}(E')\,\Sigma_f^{j_f}(z,E')\,\phi(z,E')\right]}, \tag{153}$$

$$\chi_{d,m}(z,E) = \frac{\chi_{d,m}(E)\sum_{j_f=1}^{J_f}\left[\beta_m^{j_f}(z)\int_0^\infty dE'\nu^{j_f}(E')\,\Sigma_f^{j_f}(z,E')\,\phi(z,E')\right]}{\beta_m(z)\sum_{j_f=1}^{J_f}\left[\int_0^\infty dE'\nu^{j_f}(E')\,\Sigma_f^{j_f}(z,E')\,\phi(z,E')\right]}. \tag{154}$$

Equations (153) and (154) show that the combined yield spectra are essentially combinations' of the individual isotopes' yield spectra, weighted by the corresponding isotopes' total neutron production rates at the position.

The multigroup versions of Eqs. (153) and (154) are given by Eqs. (155) and (156):

$$
\chi_{pg}^r(z) = \frac{\displaystyle\sum_{j_f=1}^{J_f}\left[\sum_{g'=1}^{G}\chi_p \nu_p \Sigma_{fgg'}^{j_f,r}(z)\,\phi_{g'}(z)\right]}{\left(1-\beta^r(z)\right)\displaystyle\sum_{j_f=1}^{J_f}\left[\sum_{g'=1}^{G}\nu\Sigma_{fg'}^{j_f,r}(z)\,\phi_{g'}(z)\right]}, \tag{155}
$$

$$
\chi_{dg,m}^r(z) = \frac{\chi_{dg,m}\displaystyle\sum_{j_f=1}^{J_f}\left[\beta_m^{j_f,r}(z)\sum_{g'=1}^{G}\nu\Sigma_{fg'}^{j_f,r}(z)\,\phi_{g'}(z)\right]}{\beta_m^r(z)\displaystyle\sum_{j_f=1}^{J_f}\left[\sum_{g'=1}^{G}\nu\Sigma_{fg'}^{j_f,r}(z)\,\phi_{g'}(z)\right]}. \tag{156}
$$

Note, that unlike the numerator in Eq. (153), the numerator in Eq. (155) contains only a term with ν_p, and cannot be replaced with some form of $\nu\Sigma_{g'}^r(z)$. This is due to the dependence of $\chi_p(E',E)$ on E'. A simplification later in this section resolves this issue.

The eigenvalue simplification is, by definition, used to study the reactivity impacts of certain modifications to the core (temperature, burnup, control and regulating rod/blade movement, boron injection, etc.) without analyzing the resulting transients. It is also used to find the steady state power profiles (i.e., $\{\phi_g(z)\}$), and other steady state analysis. Because it is a form of steady state analysis, the time dependence is dropped from all terms.

The eigenvalue simplification consists of four modifications to Eq. (133):

a. The time derivative is made zero, because the eigenvalue problem is steady state.

b. The external source is removed, because otherwise the steady state problem would be a fixed source problem, which does not use an eigenvalue. Eigenvalue problems are necessarily homogeneous (in that they cannot contain external source vectors).

c. An eigenvalue k_{eff} is added to the problem — without it, the steady state homogeneous problem would not be solvable. k_{eff} modifies the fission neutron sources by dividing all of the production cross sections by k_{eff}.

d. The precursor densities are assumed to be in equilibrium with the eigenfunction flux; this means that the precursor densities do not change in time. This yields the following simplification for $c_m(z)$, by rearranging the steady state version of Eq. (136):

$$
c_m(z) = \frac{1}{\lambda_m k_{eff}}\sum_{g'=1}^{G}\nu_d\Sigma_{fg',m}^r(z)\,\phi_{g'}(z). \tag{157}
$$

Substituting $c_m(z)$ into the steady state version of Eq. (131), adding it to Eq. (126), yields the group g steady state fission neutron source term, which accounts for both

the prompt and delayed neutrons:

$$\frac{1}{k_{\text{eff}}} \sum_{g'=1}^{G} \chi_p \nu_p \Sigma_{fgg'}^r(z)\, \phi_{g'}(z) + \sum_{m=1}^{M} \chi_{dg,m} \lambda_m c_m(z) =$$

$$= \frac{1}{k_{\text{eff}}} \sum_{g'=1}^{G} \left\{ \left[\chi_p \nu_p \Sigma_{fgg'}^r(z) + \sum_{m=1}^{M} \chi_{dg,m} \nu_d \Sigma_{fg',m}^r(z) \right] \phi_{g'}(z) \right\}. \tag{158}$$

With these four modifications, the 1D multigroup NDE (Eq. (104)) becomes an eigenvalue problem:

$$-\frac{\partial}{\partial z} D_g^r(z) \frac{\partial}{\partial z} \phi_g(z) + \Sigma_{tg}^r(z)\, \phi_g(z) - \sum_{g'=1}^{G} \Sigma_{sgg'}^r(z)\, \phi_{g'}(z) =$$

$$= \frac{1}{k_{\text{eff}}} \sum_{g'=1}^{G} \left\{ \left[\chi_p \nu_p \Sigma_{fgg'}^r(z) + \sum_{m=1}^{M} \chi_{dg,m} \nu_d \Sigma_{fg',m}^r(z) \right] \phi_{g'}(z) \right\}. \tag{159}$$

Using the delayed neutron fractions instead, we can obtain a more intuitive expression for the "steady-state yield spectrum" — the yield spectrum function that accounts for both the prompt and delayed neutrons:

$$\chi(z, E) = \left[1 - \beta(z) \right] \chi_p(z, E) + \sum_{m=1}^{M} \beta_m(z)\, \chi_{d,m}(z, E), \tag{160}$$

integrating which over energy group g and substituting in multigroup DNFs yields the multigroup steady-state yield spectrum:

$$\chi_g^r(z) = \left[1 - \beta^r(z) \right] \chi_{pg}^r(z) + \sum_{m=1}^{M} \beta_m^r(z)\, \chi_{dg,m}^r(z). \tag{161}$$

With this spectrum, Eq. (159) can be simplified into Eq. (162). It is important to note, that because an approximate steady coarse spectrum was used to construct the DNFs, Eq. (162) is only an approximation of Eq. (159):

$$-\frac{\partial}{\partial z} D_g^r(z) \frac{\partial}{\partial z} \phi_g(z) + \Sigma_{tg}^r(z)\, \phi_g(z) - \sum_{g'=1}^{G} \Sigma_{sgg'}^r(z)\, \phi_{g'}(z) = \frac{1}{k_{\text{eff}}} \chi_g^r(z) \sum_{g'=1}^{G} \nu \Sigma_{fg'}^r(z)\, \phi_{g'}(z). \tag{162}$$

This concludes the eigenvalue simplification summary. The next group are the common simplifications that do not impact accuracy significantly, but do so enough to be not be made in most production codes. They are listed below.

1. The prompt fission yield spectrum $\chi_p^{jf}(E', E)$, which is a density in target energy E, is frequently assumed to be independent of the source energy. This is generally a very

good assumption: yield spectra vary very little as functions of fission energy. This assumption is particularly good for LWRs, in which a thermal E' may be immediately assumed (with some loss of accuracy).

This simplification modifies the prompt neutron source term. The $\chi_p \nu_p \Sigma_{fgg'}^{j_f,r}(z)$ quantity now becomes unnecessary, and is separated into the spectral yield fraction $\chi_{pg}^{j_f}$ and the prompt neutron production cross section $\nu_p \Sigma_{fg'}^{j_f,r}(z)$. $\chi_{pg}^{j_f}$ is now given by:

$$\chi_{pg}^{j_f} = \int_{E_g}^{E_{g-1}} dE \chi_p^{j_f}(E) \,, \tag{163}$$

which, together with Eq. (125), therefore leads to:

$$\chi_p \nu_p \Sigma_{fgg'}^{r}(z) \cong \chi_{pg}^{j_f} \cdot \nu_p \Sigma_{fg'}^{j_f,r}(z) \,. \tag{164}$$

This simplification has an important consequence: it now requires G (prompt neutron production) group cross sections per location, instead of $G \times G$ that was required by $\chi_p^{j_f}(E', E)$. Equation (155) can now be rewritten in terms of only $\nu \Sigma_{fg'}^{j_f,r}(z)$:

$$\chi_{pg}^{r}(z) = \frac{\displaystyle\sum_{j_f=1}^{J_f} \chi_{pg}^{j_f} \left(1 - \beta^{j_f,r}(z)\right) \left[\sum_{g'=1}^{G} \nu \Sigma_{fg'}^{j_f,r}(z)\, \phi_{g'}(z)\right]}{\left(1 - \beta^r(z)\right) \displaystyle\sum_{j_f=1}^{J_f} \left[\sum_{g'=1}^{G} \nu \Sigma_{fg'}^{j_f,r}(z)\, \phi_{g'}(z)\right]}. \tag{165}$$

The advantage of using Eq. (165) over (155) to build $\chi_g^r(z)$ is clear: now all coefficients in $\chi_g^r(z)$ depend either on g or on g', but never on both — and so the storage requirements for the construction of the fission source vector at a location z drop from being $\mathcal{O}(G^2)$ to $\mathcal{O}(G)$, which for a dense kernel is very helpful. Additionally, many legacy solvers only allow a vertical vector to characterize the spectrum yield, instead of the $G \times G$ matrix, and this small simplification allows us to use the presented model with those solvers.

2. The properties are assumed to be uniform within region r. This assumption is acceptable because, as stated above, diffusion only works for homogenized systems anyway (and so the z-dependence was retained only to support certain homogenization schemes that allow for weak spatial variation in properties, but not in intragroup spectra). Small regions may be required to model such problem more accurately.

3. No upscattering is assumed, that is, with $g' < g$, $\Sigma_{sgg'}^r = 0$. This assumption is completely physical except at very low energies; with a small number of groups G, such as a two-group model, there will not be upscattering, and so this assumption holds.

4. A single fissionable isotope is assumed. In most LWRs this assumption is decent at the beginning of core life, when most fissions come from Uranium-235; later in the

38

cycle this assumption stops working, because much of the power comes from fissioning Plutonium that was bred through neutron captures by Uranium-238. Assuming $J_f = 1$ significantly reduces the DNF calculations, and also justifies using the next assumption.

5. An approximate one-group spectrum (usually, a standard fast or thermal spectrum, depending on the reactor) is chosen specifically for computing the delayed neutron fractions. Doing so results in known (and weakly, if at all, varying, if Assumption 2 holds) delayed neutron fractions, and therefore known effective prompt and delayed neutron spectra. The advantages of doing so are outlined above.

With the above simplifications, implementing the steady state yield spectrum, the eigenvalue problem becomes:

$$- D_g^r \frac{\partial^2}{\partial z^2} \phi_g(z) + \Sigma_{tg}^r \phi_g(z) - \sum_{g'=1}^{G} \Sigma_{sgg'}^r \phi_{g'}(z) = \frac{1}{k_{eff}} \chi_g^r \sum_{g'=1}^{G} \nu \Sigma_{fg'}^r \phi_{g'}(z) \,. \qquad (166)$$

The last group are the questionable simplifications that are still sometimes shown in literature. It is best to avoid them, except for special cases, and possibly scoping studies.

1. Delayed neutron source's modification of the spectrum is neglected entirely: all neutrons are assumed to be born into the prompt fission neutron yield spectrum. This is equivalent to enforcing $\beta = 0$. It prevents the user from having to choose a weighting one-group flux to build the DNFs and essentially replaces χ_g^r with χ_{pg}^r. This assumption may work to judge the criticality of the core in the middle of a short transient (i.e., prior to the precursors having had time to catch up), but should be avoided in most other cases.

2. G is limited to 1 group for an LWR, or less than 25 groups for a fast reactor. The resulting model **will** produce a qualitatively appropriate result — but will not be able to adequately model either reactor types' performance. One-group parameters chosen based on an already executed solution of the same problem with more groups (i.e., *a posteriori* cross section condensation) may perform adequately, but ones built based on a different problem (even for the same reactor) most likely will not.

3. The diffusion coefficient is assumed zero — that is, the problem is now an infinite homogeneous medium. This method clearly has no application past some algorithm testing.

4. Another variation on the above approximation — the entire reactor is assumed uniform and homogenized (that is, region r comprises the full reactor). This is generally never an appropriate model.

As stated previously, this third group of simplifications should be avoided. Equation (166) is a clear example of a significantly simplified model, that should be used when simpler versions of NDEs are desired.

This concludes the simplifications usually made to the multigroup NDE. The next section discusses the construction and evaluation of the $D_g^r(z)$ coefficient. Sections 7 and 8 are absolutely **not** necessary for understanding the multigroup diffusion principles.

7 Group Diffusion Coefficient Treatment

In section 5, $D(z, E)$ was treated as a known quantity, and its multigroup discretization was constructed accordingly. As was shown in section 4, however, $D(z, E)$ is actually a derived quantity, using one of several approximations. These approximations in turn impact how the group g diffusion coefficient in region r, $D_g^r(z)$, is constructed, and are individually discussed below.

Approximations 3–5 are handled trivially, because they do not rely on a known current or flux spectrum. As such, the group diffusion coefficients they result in are constructed exactly the same way as $D_g^r(z)$ was in section 5, with no additional complications.

Approximations 1 and 2 assume a known current $\varphi_1(t, z, E)$ and flux $\psi(z, E)$ spectrum, respectively. Current spectrum weighting will be used below, with all the same arguments applying to flux spectrum weighting as well. The current spectrum will be denoted $J(z, E)$. Section 4 summarizes how these allow the user to construct a fully known $D(z, E)$.

However, in practice, when assuming a known spectrum, a piecewise (groupwise) spectrum $\{J_{\overline{g}}^r(z)\}$ is usually what is assumed, together with a spectrum group structure. It is important to note that here, the groups $\overline{g}$ do not have to be the same as the groups g in section 5, because groups $\overline{g}$ are only used to construct $D(z, E)$. Similarly to the group fluxes in section 5, $\{J_{\overline{g}}^r(z)\}$ has associated intragroup spectra $\{\Psi_{\overline{g}}^r(E)\}$, which are combined similarly to Eq. (108):

$$J(z, E) = J_{\overline{g}}^r(z)\, \Psi_{\overline{g}}^r(E) \ \text{ if } E \in [E_{\overline{g}}, E_{\overline{g}-1}]. \tag{167}$$

The intragroup spectra each normalize to 1. These can be used to construct the group-to-group anisotropic scattering moments, similarly to Eq. (119):

$$\Sigma_{s^*\overline{g}\overline{g}',1}^{r,j}(z) = \int_{E_{\overline{g}}}^{E_{\overline{g}-1}} dE \int_{E_{\overline{g}'}}^{E_{\overline{g}'-1}} dE' \Sigma_{s^*,1}^j(z, E' \to E)\, \Psi_{\overline{g}'}^r(E'), \tag{168}$$

which can be summed over all scattering isotopes to yield:

$$\Sigma_{s^*\overline{g}\overline{g}',1}^r(z) = \sum_{j=1}^J \Sigma_{s^*\overline{g}\overline{g}',1}^{r,j}(z). \tag{169}$$

Rewriting $D(z, E)$ in terms of $\{J_{\overline{g}}(z)\}$ and $\left\{\Sigma_{s^*\overline{g}\overline{g}',1}^r(z)\right\}$ yields:

$$D(z, E) = \cfrac{1}{3\left[\Sigma_t(z, E) - \cfrac{1}{J_{\overline{g}}^r(z)\, \Psi_{\overline{g}}^r(E)} \displaystyle\sum_{\overline{g}=1}^{\overline{G}} \Sigma_{s^*\overline{g}\overline{g}',1}^r(z)\, J_{\overline{g}'}^r(z)\right]} \ \text{ if } E \in [E_{\overline{g}}, E_{\overline{g}-1}]. \tag{170}$$

Equation (170) illustrates an important issue. All group quantities in section 5 relied on the spectra only for weighted averaging of the energy-dependent quantities, and were

not explicitly a function of the spectrum. $D(z, E)$, however, is, and so even if very accurate intragroup coarse spectra $\left\{\psi_g^r(E)\right\}$ are chosen (used in Eq. (113)), $D_g^r(z)$ may still be inaccurate, due to its dependence on $\left\{J_{\overline{g}}^r(z)\right\}$ and $\left\{\Psi_{\overline{g}}^r(E)\right\}$.

This issue frequently results in significant errors in group diffusion coefficient calculations by lattice and Monte Carlo codes, if they use the same group structure g for $\left\{J_g^r(z)\right\}$ and $\left\{\Psi_g^r(E)\right\}$ as they do for the coarse group structure in section 5. The best way to avoid these errors is to use a finer group spectrum for constructing $D(z, E)$, such that $\overline{G} \gg G$. If a sufficiently high $\overline{G}$ is used, the current spectrum $J(z, E)$ can be replaced with the flux spectrum $\psi(z, E)$; this is because only the shape of the weighting spectrum in energy matters, and the current and scalar flux generally have similar spectra. This amounts to using Approximation 2 instead of Approximation 1. It is also a much simpler procedure numerically, because while the flux cannot be zero in a reactor, net current at many locations frequently is, which requires an implementation of division-by-zero checks into the code (due to Eq. (170)), and slows down the construction of $D_g^r(z)$.

The group diffusion coefficient construction is guided by Eq. (113); once $D(z, E)$ has been constructed, the rest of the procedure is similar to the other group quantities.

Finally, we mention the following alternative form of group diffusion coefficient weighting, frequently seen in literature. Assuming a known scalar flux $\phi(t, z, E)$, we may simply construct the group diffusion coefficient as:

$$D_g(t, z) = \frac{\int_{E_g}^{E_{g-1}} dE D(z, E) \frac{\partial}{\partial z} \phi(t, z, E)}{\int_{E_g}^{E_{g-1}} dE \frac{\partial}{\partial z} \phi(t, z, E)}. \tag{171}$$

This expression is exact, but it is also formal, because it requires knowing not only the shape in energy, but also the group magnitude of the scalar flux, in order to evaluate the spatial derivative. It can be viewed as a weighting of the diffusion coefficient by the spatial derivative of the flux, as opposed to by the flux or current spectrum. Equation (171) still requires an expression for $D(z, E)$, and so is normally impractical to use, compared to Eq. (113) and the construction of $D(z, E)$ as described above in this section.

This concludes the discussion of issues associated with group diffusion coefficient calculation.

8 Double Differential Scattering Cross Section Treatment

Equation (72) gives the full expression for the double differential cone-to-cone scattering cross section. In this section the construction of the double differential scattering probability distribution functions is summarized, with the intention of relating the desired expressions (see sections 4 and 5) to the data formats given in ENDF/B-VII and similar databases. Upscattering is neglected in this section, but inelastic scattering is not.

We begin by expanding $f_{s_{el}}^j(E' \to E, \mu_0)$, the double differential elastic scattering probability density function, using Eq. (74):

$$f_{s_{el}}^j(E' \to E, \mu_0) = f_{s_{el},E}^j(E' \to E)\, f_{s_{el},\mu_0}^j(E' \to E, \mu_0)\,, \tag{172}$$

in which $f_{s_{el},E}^j(E' \to E)$ and $f_{s_{el},\mu_0}^j(E' \to E, \mu_0)$ are the single differential elastic scattering probability densities in energy and scattering angle cosine (for a given target energy), respectively.

Let μ_0 and and μ_{cm} denote the scattering angle cosines in lab (LCS) and center of mass (CMCS) coordinate systems, respectively. Let A_j be the ratio of the mass of the scattering nucleus to the mass of the neutron (very close to the isotope's mass number), and α_j be given by:

$$\alpha_j = \left(\frac{A_j - 1}{A_j + 1}\right)^2. \tag{173}$$

ENDF/B-VII specifies $f_{s_{el},\mu_{cm}}^j(E', \mu_{cm})$, the elastic scattering probability density in scattering angle cosine in the CMCS. To relate $f_{s_{el},\mu_{cm}}^j(E', \mu_{cm})$ to $f_{s_{el},E}^j(E' \to E)$, which is used in the expansion in Eq. (172), we use:

$$f_{s_{el},E}^j(E' \to E)\, dE = f_{s_{el},\mu_{cm}}^j(E', \mu_{cm})\, d\mu_{cm}, \tag{174}$$

rearranging which yields:

$$f_{s_{el},E}^j(E' \to E) = f_{s_{el},\mu_{cm}}^j(E', \mu_{cm})\, \frac{d\mu_{cm}}{dE}. \tag{175}$$

For elastic scattering, the scattering angle cosine μ_{cm} and the source/target energy pair $(E' \to E)$ are rigidly tied together through the following (derived through conservation of energy and momentum):

$$\frac{E}{E'} = \frac{A_j^2 + 2A_j\mu_{cm} + 1}{(A_j + 1)^2} = \frac{1 + \alpha_j}{2} + \frac{1 - \alpha_j}{2}\mu_{cm}, \tag{176}$$

rearranging which yields:

$$\mu_{cm}(E/E') = \frac{2}{1 - \alpha_j}\frac{E}{E'} - \frac{1 + \alpha_j}{1 - \alpha_j}. \tag{177}$$

The scattering angle cosine is bounded as $-1 \leq \mu_{cm} \leq 1$. Substituting these values into Eq. (176) demonstrates that E is similarly bounded for elastic scattering, as $\alpha_j E' \leq E \leq E'$. Elastic scattering is not possible for target energies outside this interval.

Differentiating Eq. (177) with respect to E yields $d\mu_{cm}/dE$:

$$\frac{d\mu_{cm}}{dE} = \frac{2}{(1 - \alpha_j)\, E'}, \tag{178}$$

which we can substitute back into Eq. (175) to obtain $f^j_{s_{el},E}(E' \to E)$:

$$f^j_{s_{el},E}(E' \to E) = \begin{cases} f^j_{s_{el},\mu_{cm}}(E', \mu_{cm}(E/E')) \dfrac{2}{(1-\alpha_j)\,E'} & \text{if } \alpha_j E' \le E \le E', \\ 0 & \text{otherwise.} \end{cases} \quad (179)$$

$f^j_{s_{el},E}(E' \to E)$ is piecewise, because, as noted above, reachable target energies are limited for elastic scattering.

For many isotopes, at many energies except the higher end of the spectrum, elastic scattering is nearly isotropic in CMCS. For such isotopes, $f^j_{s_{el},\mu_{cm}}(E', \mu_{cm}(E/E')) = 1/2$, and Eq. (179) simplifies to:

$$f^j_{s_{el},E}(E' \to E) = \begin{cases} \dfrac{1}{(1-\alpha_j)\,E'} & \text{if } \alpha_j E' \le E \le E', \\ 0 & \text{otherwise.} \end{cases} \quad (180)$$

We now need to find the expression for $f^j_{s_{el},\mu_0}(E' \to E, \mu_0)$, the elastic scattering probability density in scattering angle cosine (in LCS) for a given source/target energy pair. Equation (177) effectively shows that a given source/target energy pair $(E' \to E)$ can only be obtained through a single scattering angle cosine in CMCS, which that equation specifies. Conservation of momentum and energy also yields the relation between μ_0 and μ_{cm}:

$$\mu_0 = \frac{A_j \mu_{cm} + 1}{\sqrt{A_j^2 + 2A_j \mu_{cm} + 1}}, \quad (181)$$

which illustrates that μ_0 and μ_{cm} also have a one-to-one relation. This means that specifying the source/target energy pair $(E' \to E)$ restricts μ_0 to a single possible value, which means that $f^j_{s_{el},\mu_0}(E' \to E, \mu_0)$ must be a Dirac delta function centered about that value. To find this value, we substitute $\mu_{cm}(E/E')$ from Eq. (177) into Eq. (181):

$$\mu_0(E/E') = \frac{A_j \mu_{cm}(E/E') + 1}{\sqrt{A_j^2 + 2A_j \mu_{cm}(E/E') + 1}}. \quad (182)$$

$f^j_{s_{el},\mu_0}(E' \to E, \mu_0)$ is a Dirac delta function centered about $\mu_0(E/E')$:

$$f^j_{s_{el},\mu_0}(E' \to E, \mu_0) = \delta(\mu_0 - \mu_0(E/E')). \quad (183)$$

Substituting Eqs. (179) and (183) into Eq. (172) yields the double differential elastic scattering probability function in terms of quantities given in ENDF/B-VII:

$$f^j_{s_{el}}(E' \to E, \mu_0) = \begin{cases} f^j_{s_{el},\mu_{cm}}(E', \mu_{cm}(E/E')) \times \\ \qquad \times \dfrac{2}{(1-\alpha_j)\,E'}\delta(\mu_0 - \mu_0(E/E')) & \text{if } \alpha_j E' \le E \le E', \\ 0 & \text{otherwise,} \end{cases} \quad (184)$$

and the relevant single differential probability densities used in section 4 were given in Eqs. (179) and (183). $\mu_{cm}(E/E')$ and $\mu_0(E/E')$ are given by Eqs. (177) and (182), respectively.

Discrete inelastic scattering works the same way as elastic scattering, but some of the energy is used to excite the scattering nucleus, instead of fully remaining in the form of kinetic energy of the neutron and the scatterer. Let this excitation energy, which is different for every discrete scattering level i, be denoted Q_i^j; it is sometimes referred to as the level i Q-factor. It is a known, tabulated quantity in ENDF/B-VII, together with the discrete inelastic scattering cross sections. The total energy available to be divided as kinetic energy between the scatterer and the neutron after the inelastic scattering event is therefore:

$$E_i'' = E' - Q_i^j. \tag{185}$$

Elastic scattering can be viewed as a form of discrete inelastic scattering with $Q_i^j = 0$.

The double differential discrete inelastic scattering probability density function is split the same way as the elastic scattering probability density (Eq. (172)):

$$f_{s_{in,i}}^j(E' \to E, \mu_0) = f_{s_{in,i},E}^j(E' \to E)\, f_{s_{in,i},\mu_0}^j(E' \to E, \mu_0)\,, \tag{186}$$

in which $f_{s_{in,i},E}^j(E' \to E)$ and $f_{s_{in,i},\mu_0}^j(E' \to E, \mu_0)$ are the single differential discrete inelastic level i scattering probability densities in energy and scattering angle cosine (for a given target energy), respectively.

Similarly to elastic scattering, ENDF/B-VII also specifies $f_{s_{in,i},\mu_{cm}}^j(E', \mu_{cm})$, the discrete inelastic level i scattering probability density in scattering angle cosine in the CMCS. We therefore can use a very similar procedure to elastic scattering (but accounting for E_i'' instead of E') to find the single differential discrete inelastic scattering probability densities. The source/target energy ratios are now the available kinetic/total energy ratios, which modifies the scattering angle cosine functions:

$$\mu_{cm}(E/E_i'') = \frac{2}{1-\alpha_j}\frac{E}{E_i''} - \frac{1+\alpha_j}{1-\alpha_j}, \tag{187}$$

and

$$\mu_0(E/E_i'') = \frac{A_j\mu_{cm}(E/E_i'') + 1}{\sqrt{A_j^2 + 2A_j\mu_{cm}(E/E_i'') + 1}}. \tag{188}$$

Equation (187) illustrates that the target energy is now bounded as $\alpha_j E_i'' \le E \le E_i''$. $d\mu_{cm}/dE$ is also affected:

$$\frac{d\mu_{cm}}{dE} = \frac{2}{(1-\alpha_j)\,E_i''}. \tag{189}$$

Using Eqs. (187)–(189) to replace the appropriate terms in Eq. (179), recognizing the new scattering interval bounds, and replacing $f_{s_{el},\mu_{cm}}^j(E', \mu_{cm})$ with $f_{s_{in,i},\mu_{cm}}^j(E', \mu_{cm})$ yields

$f^j_{s_{in,i},E}(E' \to E)$:

$$f^j_{s_{in,i},E}(E' \to E) = \begin{cases} f^j_{s_{in,i},\mu_{cm}}\Big(E',\mu_{cm}\big(E/E''_i(E')\big)\Big) \times \\ \qquad \times \dfrac{2}{(1-\alpha_j)\,E''_i(E')} & \text{if } \alpha_j E''_i(E') \leq E \leq E''_i(E'), \\[2mm] 0 & \text{otherwise,} \end{cases} \tag{190}$$

in which $E''_i(E')$ is given by Eq. (185).

Equation (188) converts Eq. (183) trivially:

$$f^j_{s_{in,i},\mu_0}(E' \to E, \mu_0) = \delta\Big(\mu_0 - \mu_0\big(E/E''_i(E')\big)\Big). \tag{191}$$

Substituting Eqs. (190) and (191) into Eq. (186) yields the double differential discrete inelastic scattering probability function in terms of quantities given in ENDF/B-VII:

$$f^j_{s_{in,i}}(E' \to E, \mu_0) = $$
$$= \begin{cases} f^j_{s_{in,i},\mu_{cm}}\Big(E',\mu_{cm}\big(E/E''_i(E')\big)\Big) \times \\ \qquad \times \dfrac{2}{(1-\alpha_j)\,E''_i(E')}\delta\Big(\mu_0 - \mu_0\big(E/E''_i(E')\big)\Big) & \text{if } \alpha_j E''_i(E') \leq E \leq E''_i(E'), \\[2mm] 0 & \text{otherwise,} \end{cases} \tag{192}$$

with the relevant single differential probability densities used in section 4 given by Eqs. (190) and (191). $E''_i(E')$, $\mu_{cm}(E/E''_i)$ and $\mu_0(E/E''_i)$ are given by Eqs. (185), (187) and (188), respectively.

Continuum inelastic scattering is treated differently from elastic and discrete inelastic scattering, because in it the source/target energy ratios and scattering angle cosines are not rigidly related. For this reason, ENDF/B-VII lists the double differential continuum inelastic scattering distribution function $f^j_{s_{in,c}}(E' \to E, \mu_{cm})$ directly, as a function of two variables for a given E'. In comparison, $f^j_{s_{el},\mu_{cm}}(E',\mu_{cm})$ and $f^j_{s_{in,i},\mu_{cm}}(E',\mu_{cm})$ are given as functions of one variable, μ_{cm}, for a given E'. To convert the scattering angle cosine dependence from CMCS to LCS, we first recognize that:

$$f^j_{s_{in,c}}(E' \to E, \mu_0)\, d\mu_0 = f^j_{s_{in,c}}(E' \to E, \mu_{cm})\, d\mu_{cm}, \tag{193}$$

rearranging which yields:

$$f^j_{s_{in,c}}(E' \to E, \mu_0) = f^j_{s_{in,c}}(E' \to E, \mu_{cm})\frac{d\mu_{cm}}{d\mu_0}. \tag{194}$$

Solving Eq. (181) for μ_{cm} yields:

$$\mu_{cm} = \frac{\mu_0^2 + \mu_0\sqrt{A_j^2 + \mu_0^2 - 1} - 1}{A_j}, \tag{195}$$

differentiating which gives $d\mu_{cm}/d\mu_0$, the desired derivative:

$$\frac{d\mu_{cm}}{d\mu_0} = \frac{\left(\mu_0 + \sqrt{A_j^2 + \mu_0^2 - 1}\right)^2}{A_j\sqrt{A_j^2 + \mu_0^2 - 1}}. \tag{196}$$

Substituting Eq. (196) back into Eq. (194) yields the double differential continuum inelastic scattering probability function in terms of quantities given in ENDF/B-VII:

$$f_{s_{in,c}}^j(E' \to E, \mu_0) = f_{s_{in,c}}^j(E' \to E, \mu_{cm}(\mu_0)) \frac{\left(\mu_0 + \sqrt{A_j^2 + \mu_0^2 - 1}\right)^2}{A_j\sqrt{A_j^2 + \mu_0^2 - 1}}, \tag{197}$$

in which $\mu_{cm}(\mu_0)$ is given by Eq. (195).

It is still necessary to construct the single differential continuum scattering probability densities, for use in expressions in section 4. The split through Eq. (74) still holds:

$$f_{s_{in,c}}^j(E' \to E, \mu_0) = f_{s_{in,c},E}^j(E' \to E) \, f_{s_{in,c},\mu_0}^j(E' \to E, \mu_0), \tag{198}$$

and each single differential probability density still normalizes according to Eq. (75). Therefore, to obtain $f_{s_{in,c},\mu_0}^j(E' \to E, \mu_0)$, we simply integrate Eq. (197) over all scattering angle cosines:

$$\begin{aligned}
f_{s_{in,c},E}^j(E' \to E) &= \int_{-1}^{1} d\mu_0 f_{s_{in,c}}^j(E' \to E, \mu_0) = \\
&= \int_{-1}^{1} d\mu_0 f_{s_{in,c}}^j(E' \to E, \mu_{cm}(\mu_0)) \frac{d\mu_{cm}}{d\mu_0} = \int_{-1}^{1} d\mu_{cm} f_{s_{in,c}}^j(E' \to E, \mu_{cm}).
\end{aligned} \tag{199}$$

$f_{s_{in,c},\mu_0}^j(E' \to E, \mu_0)$ is obtained by dividing Eq. (197) by Eq. (199):

$$\begin{aligned}
f_{s_{in,c},\mu_0}^j(E' \to E, \mu_0) &= \frac{f_{s_{in,c}}^j(E' \to E, \mu_0)}{f_{s_{in,c},E}^j(E' \to E)} = \\
&= \frac{f_{s_{in,c}}^j(E' \to E, \mu_{cm}(\mu_0))}{\displaystyle\int_{-1}^{1} d\mu_{cm} f_{s_{in,c}}^j(E' \to E, \mu_{cm})} \frac{\left(\mu_0 + \sqrt{A_j^2 + \mu_0^2 - 1}\right)^2}{A_j\sqrt{A_j^2 + \mu_0^2 - 1}}.
\end{aligned} \tag{200}$$

This concludes the summary of double differential scattering probability function construction for elastic, discrete inelastic and continuum inelastic scattering without upscattering.