

Chapter 2

Multigroup Equations

Consider the neutron transport equation that we derived in the previous chapter:

$$\begin{aligned} \left(\frac{1}{v} \frac{\partial}{\partial t} + \hat{\Omega} \cdot \nabla + \Sigma_t \right) \psi(\mathbf{x}, \hat{\Omega}, E, t) = \\ \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int_0^{\infty} dE' \Sigma_s(\mathbf{x}, E', t) K_l(E' \rightarrow E) \phi_{lm}(\mathbf{x}, E', t) + \\ \frac{1}{4\pi} \chi(\mathbf{x}, E) \int_0^{\infty} dE' \bar{\nu} \Sigma_f(\mathbf{x}, E') \phi(\mathbf{x}, E') + q(\mathbf{x}, \hat{\Omega}, E, t). \quad (2.1) \end{aligned}$$

We will now try to discretize this equation in energy. First, we define an energy grid that spans a finite range $E \in [0, E_0]$, where E_0 is the upper cutoff in energy. We will divide this range into G energy bins that are called *energy groups*. They are numbered so that group g spans the range $E \in [E_g, E_{g-1}]$ and $g = 1, 2, \dots, G$. This numbering is backward in some sense as the highest energy group is group 1 and the lowest energy group is group G .

We will define the integrated angular flux over a group as ψ_g and call this the angular flux for group g . It is defined by

$$\psi_g(\mathbf{x}, \hat{\Omega}, t) = \int_{E_g}^{E_{g-1}} dE \psi(\mathbf{x}, \hat{\Omega}, E, t). \quad (2.2)$$

Group-integrated moments are similarly defined:

$$\phi_{lmg}(\mathbf{x}, t) = \int_{E_g}^{E_{g-1}} dE \phi_{lm}(\mathbf{x}, E, t). \quad (2.3)$$

Additionally, we can define a group source, q_g as

$$q_g(\mathbf{x}, \hat{\Omega}, t) = \int_{E_g}^{E_{g-1}} dE q(\mathbf{x}, \hat{\Omega}, E, t). \quad (2.4)$$

Upon integrating Eq. (2.1) over a group, some of the terms simplify, and we

get

$$\begin{aligned} \hat{\Omega} \cdot \nabla \psi_g + \int_{E_g}^{E_{g-1}} dE \left(\frac{1}{v} \frac{\partial}{\partial t} + \Sigma_t \right) \psi(\mathbf{x}, \hat{\Omega}, E, t) = \\ \int_{E_g}^{E_{g-1}} dE \left[\sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int_0^{\infty} dE' \Sigma_s(\mathbf{x}, E', t) K_l(E' \rightarrow E) \phi_{lm}(\mathbf{x}, E', t) + \right. \\ \left. \frac{1}{4\pi} \chi(\mathbf{x}, E) \int_0^{\infty} dE' \bar{\nu} \Sigma_f(\mathbf{x}, E') \phi(\mathbf{x}, E') \right] + q_g. \quad (2.5) \end{aligned}$$

To simplify this equation we will make some definitions. The group-averaged total macroscopic cross-section is

$$\Sigma_{tg}(\mathbf{x}, \hat{\Omega}, t) = \frac{1}{\psi_g} \int_{E_g}^{E_{g-1}} dE \Sigma_t(\mathbf{x}, E, t) \psi(\mathbf{x}, \hat{\Omega}, E, t). \quad (2.6)$$

Note that although the original cross-section was not dependent on $\hat{\Omega}$, the weighting we used in the integral is dependent on angle so the group-averaged cross-section now depends on angle. We will discuss this further below. We also need to define a group-averaged speed for the neutrons as

$$\frac{1}{v_g(\mathbf{x}, \hat{\Omega}, t)} = \frac{1}{\psi_g} \int_{E_g}^{E_{g-1}} dE \frac{1}{v(E)} \psi(\mathbf{x}, \hat{\Omega}, E, t). \quad (2.7)$$

As in the definition of Σ_{tg} , we have introduced dependencies into v_g that were not present prior to averaging.

The scattering term requires two indices to describe because we will be dealing with neutrons moving from one group to another. We define a group to

group scattering cross-section for moment l as

$$\Sigma_{slm,g' \rightarrow g}(\mathbf{x}, t) = \frac{1}{\phi_{lm}g'} \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \Sigma_s(\mathbf{x}, E', t) K_l(E' \rightarrow E) \phi_{lm}(\mathbf{x}, E', t) \quad (2.8)$$

To treat the fission term we will need to define an average $\bar{\nu}\Sigma_f$ for a group; this is defined in a similar manner as the total cross-section

$$\bar{\nu}\Sigma_{fg}(\mathbf{x}, \hat{\Omega}, t) = \frac{1}{\psi_g} \int_{E_g}^{E_{g-1}} dE \bar{\nu}\Sigma_f(\mathbf{x}, E, t) \psi(\mathbf{x}, \hat{\Omega}, E, t). \quad (2.9)$$

We also need to integrate the fission spectrum over a group to define χ_g as

$$\chi_g(\mathbf{x}, t) = \int_{E_g}^{E_{g-1}} dE \chi(\mathbf{x}, E, t). \quad (2.10)$$

Note that

$$\sum_{g=1}^G \chi_g = 1.$$

Using all of these definitions allows us to write Eq. (2.5) as

$$\begin{aligned} \left(\frac{1}{v} \frac{\partial}{\partial t} + \hat{\Omega} \cdot \nabla + \Sigma_{tg}(\mathbf{x}, \hat{\Omega}, t) \right) \psi_g(\mathbf{x}, \hat{\Omega}, t) = \\ \left[\sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \sum_{g'=1}^G \Sigma_{slm,g' \rightarrow g}(\mathbf{x}, t) \phi_{lm}(\mathbf{x}, t) + \right. \\ \left. \frac{1}{4\pi} \chi_g(\mathbf{x}) \sum_{g'=1}^G \bar{\nu}\Sigma_{fg'}(\mathbf{x}, \hat{\Omega}) \phi_g(\mathbf{x}, t) \right] + q_g. \quad (2.11) \end{aligned}$$

In deriving this equation we have written the integrals over E' using sums over

the groups as:

$$\int_0^\infty dE' = \sum_{g'=1}^G.$$

2.1 Angle-Independent Cross-sections

The total and fission cross-sections, as well as the neutron speed, in Eq. (2.11) depend on $\hat{\Omega}$ because they were weighted against angular flux. In practice, however, we generally replace these cross-sections with averages based on the scalar flux as

$$\Sigma_{tg}(\mathbf{x}, t) \approx \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE \Sigma_t(\mathbf{x}, E, t) \phi(\mathbf{x}, \hat{\Omega}, E, t), \quad (2.12)$$

where we have written the group-integrated scalar flux as

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

We say that this is an approximation because the original quantity that we need to replace is the integral over the group of $\Sigma_t \psi$. Similarly, we can write the average for $\bar{\nu} \Sigma_f$ as

$$\bar{\nu} \Sigma_{fg}(\mathbf{x}, t) \approx \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE \bar{\nu} \Sigma_f(\mathbf{x}, E, t) \phi(\mathbf{x}, \hat{\Omega}, E, t). \quad (2.13)$$

Additionally, the scattering cross-sections have a dependence on m because they have been weighted by a spherical harmonics moment of the angular flux. These

are replaced by averages using the $m = 0$ moments:

$$\Sigma_{sl,g' \rightarrow g}(\mathbf{x}, t) = \frac{1}{\phi_{l0g'}} \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \Sigma_s(\mathbf{x}, E', t) K_l(E' \rightarrow E) \phi_{l0}(\mathbf{x}, E', t). \quad (2.14)$$

We can justify these choices by making the assumption that the angular flux is separable in energy in each group. That means we can write the angular flux as

$$\psi(\mathbf{x}, \hat{\Omega}, E, t) = \aleph_g(E) F_g(\mathbf{x}, \hat{\Omega}, t) \quad \text{for } E \in [E_g, E_{g-1}], g = 1, \dots, G, \quad (2.15)$$

where $\aleph_g(E)$ gives the energy dependence in group G , and $F_g(\mathbf{x}, \hat{\Omega}, t)$ is the dependence in space, angle, and time in the group. The implication of this assumption is that the dependence of the angular flux in space, angle, and time is the same inside each group. Obviously, the validity of this approximation depends on the width of the groups: if a group is narrow then we can expect that the dependence in space, angle, and time will be constant for each energy in the group. Regardless, this assumption introduces some error that is hard to quantify in general.

Upon making the separability assumption, the will be no angular dependence in the cross-sections. The group-integrated angular flux can be written as

$$\psi_g(\mathbf{x}, \hat{\Omega}, t) = \int_{E_g}^{E_{g-1}} dE \psi(\mathbf{x}, \hat{\Omega}, E, t) = F_g(\mathbf{x}, \hat{\Omega}, t) \int_{E_g}^{E_{g-1}} dE \aleph_g(E) = C F_g(\mathbf{x}, \hat{\Omega}, t) \quad (2.16)$$

Then we use this in the original definition of Σ_{tg} , Eq. (2.6), to get

$$\Sigma_{tg}(\mathbf{x}, t) = \frac{1}{C} \int_{E_g}^{E_{g-1}} dE \Sigma_t(\mathbf{x}, E, t) \aleph_g(E). \quad (2.17)$$

Therefore, if the group structure is fine enough that the separability assumption is reasonable, we can use scalar-flux-weighted cross-sections in our multigroup equations.

2.2 Extended Legendre and P_1 Consistent Multi-group Equations

In the case where the groups structure is not fine, the separability assumption is not warranted and we would like to improve our method without resorting to angle-dependent cross-sections. We will derive these improvements for the 1-D slab, steady-state equations. We choose this framework for several reasons 1) it does not have the complication of requiring a spherical harmonics expansion of the angular flux, 2) most multigroup data sets do not have $m \neq 0$ moments of the scattering cross-section, and 3) we will make assumptions that will only be reasonable in steady-state. In slab geometry, the neutron transport equation can be written as

$$\begin{aligned} & \left(\mu \frac{\partial}{\partial z} + \Sigma_t(z, E) \right) \psi(z, \mu, E) = \\ & \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\hat{\Omega}) \int_0^{\infty} dE' \Sigma_s(z, E') K_l(E' \rightarrow E) \phi_l(z, E') + \\ & \frac{\chi_g(z)}{2} \int_0^{\infty} dE' \bar{\nu} \Sigma_f(z, E') \phi(z, E') + q(z, \hat{\Omega}, E), \quad (2.18) \end{aligned}$$

where the angular flux has been assumed to only vary in the z direction and have no dependence on the azimuthal angle, φ . The lack of azimuthal dependence means that multiplied both sides of the equation by 2π , which is the same as integrating over φ .

In slab geometry the moments are Legendre polynomial moments and are given by

$$\phi_l(z, E) = \int_{-1}^1 d\mu \psi(z, \mu, E) P_l(\mu). \quad (2.19)$$

Also, these moments allow us to write the slab-geometry angular flux as

$$\psi(z, \mu, E) = \sum_{l=0}^{\infty} \frac{2l+1}{2} \phi_l(z, E) P_l(\mu). \quad (2.20)$$

We will integrate Eq. (2.18) over a group to get

$$\begin{aligned} \mu \frac{\partial \psi_g}{\partial z} = & \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\hat{\Omega}) \sum_{g'=1}^G [\Sigma_{sl,g' \rightarrow g}(z) - \delta_{gg'} \Sigma_{tlg'}] \phi_{lg'}(z) + \\ & \frac{\chi_g(z)}{2} \sum_{g'=1}^G \bar{\nu} \Sigma_{fg'}(z) \phi_{g'}(z) + q_g(z, \hat{\Omega}), \end{aligned} \quad (2.21)$$

where $\delta_{gg'}$ is the

$$\phi_{lg}(z) = \int_{E_g}^{E_{g-1}} dE \phi_l(z, E), \quad (2.22)$$

and

$$\Sigma_{sl,g' \rightarrow g}(z) = \frac{1}{\phi_{g'}} \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \Sigma_s(z, E') K_l(E' \rightarrow E) \phi_l(z, E'). \quad (2.23)$$

$$\Sigma_{tlg}(z) = \frac{1}{\phi_{g'}} \int_{E_g}^{E_{g-1}} dE \Sigma_t(z, E) \phi_l(z, E'). \quad (2.24)$$

We then add $\Sigma_{tg}(z)\psi_g(z, \hat{\Omega})$ to each side of Eq. (2.21), where $\Sigma_{tg}(z)$ has yet to be defined. This gives

$$\begin{aligned} \mu \frac{\partial \psi_g}{\partial z} + \Sigma_{tg}(z)\psi(z, \hat{\Omega}) = & \\ & \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\hat{\Omega}) \sum_{g'=1}^G [\Sigma_{sl,g' \rightarrow g}(z) + \delta_{gg'} (\Sigma_{tg'}(z) - \Sigma_{tlg'}(z))] \phi_{lg'}(z) + \\ & \frac{\chi_g(z)}{2} \sum_{g'=1}^G \bar{\nu} \Sigma_{fg'}(z) \phi_{g'}(z) + q_g(z, \hat{\Omega}). \end{aligned} \quad (2.25)$$

We now have a choice to make for Σ_{tg} . If we use $\Sigma_{tg} = \Sigma_{t0g}$, then we call this the P_1 -consistent form of the multigroup equations because it is consistent with the multigroup form of the P_1 approximation to the transport equation, as we will see later. We can write this form in shorthand as

$$\begin{aligned} \mu \frac{\partial \psi_g}{\partial z} + \Sigma_{t0g}(z) \psi(z, \hat{\Omega}) &= \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\hat{\Omega}) \sum_{g'=1}^G \Sigma_{sl^*, g' \rightarrow g}(z) \phi_{lg'}(z) + \\ &\quad \frac{\chi_g(z)}{2} \sum_{g'=1}^G \bar{\nu} \Sigma_{fg'}(z) \phi_{g'}(z) + q_g(z, \hat{\Omega}), \end{aligned} \quad (2.26)$$

where the scattering cross-section has been defined to contain the correction:

$$\Sigma_{sl^*, g' \rightarrow g}(z) = \Sigma_{sl, g' \rightarrow g}(z) + \delta_{gg'} (\Sigma_{t0g'}(z) - \Sigma_{tlg'}). \quad (2.27)$$

There is a different choice we could make for Σ_{tg} called the extended transport approximation. To do this, we realize that in numerical calculations, the Legendre moments will be truncated at some level that we call L . We will use this truncation to motivate our choice for Σ_{tg} . With a truncated Legendre expansion, Eq. (2.25) becomes

$$\begin{aligned} \mu \frac{\partial \psi_g}{\partial z} + \Sigma_{tg}(z) \psi(z, \hat{\Omega}) &= \\ \sum_{l=0}^L \frac{2l+1}{2} P_l(\hat{\Omega}) \sum_{g'=1}^G &[\Sigma_{sl, g' \rightarrow g}(z) + \delta_{gg'} (\Sigma_{tg'}(z) - \Sigma_{tlg'}(z))] \phi_{lg'}(z) + \\ &\quad \frac{\chi_g(z)}{2} \sum_{g'=1}^G \bar{\nu} \Sigma_{fg'}(z) \phi_{g'}(z) + q_g(z, \hat{\Omega}). \end{aligned} \quad (2.28)$$

There will be an In particular we want to minimize the magnitude of the first neglected term. This means we want to satisfy the equation

$$\sum_{g'=1}^G [\Sigma_{sL+1, g' \rightarrow g} + \delta_{gg'} (\Sigma_{tg'} - \Sigma_{tL+1, g'})] \phi_{L+1, g'} = 0, \quad (2.29)$$

where for simplicity we have dropped the z dependence. In many reactor problems the scattering out of a group is the same as the scattering into a group.

We make this approximation by setting

$$\sum_{g'=1}^G \Sigma_{sL+1,g' \rightarrow g} \phi_{L+1,g'} = \sum_{g=1}^G \Sigma_{sL+1,g \rightarrow g'} \phi_{L+1,g},$$

and substituting this relation into Eq. (2.29) gives

$$\Sigma_{tg} = \Sigma_{tL+1,g} - \sum_{g=1}^G \Sigma_{sL+1,g \rightarrow g'}. \quad (2.30)$$

This value of Σ_{tg} is known as the extended transport approximation. If we use the form of Eq. (2.26), the value of $\Sigma_{sl^*,g' \rightarrow g}$ becomes

$$\Sigma_{sl^*,g' \rightarrow g} = \Sigma_{sl,g' \rightarrow g}(z) + \delta_{gg'} \left(\Sigma_{tL+1,g} - \sum_{g=1}^G \Sigma_{sL+1,g \rightarrow g'} - \Sigma_{tlg'} \right). \quad (2.31)$$

The upshot of all this is that we can get multigroup equations without angular dependence by defining the total cross-section and the scattering cross-sections to handle the angular piece with either the P_1 or extended transport approximation.

2.3 Wait, where do we get group fluxes?

In this entire discussion we have neglected this fundamental point: to compute the multigroup cross-sections (and speeds) we need to know the group-integrated scalar flux and flux moments. These are precisely the quantities we are seeking. Therefore, we have spun ourselves in circles, so to speak. To resolve this we will need an auxiliary calculation to give us an approximation to the group fluxes.

The general procedure used in practice to compute these group fluxes is to perform calculations with a fine group structure (that is many groups) and coarse spatial resolution. The resulting fine group fluxes are then used to collapse to a coarse group structure and then a fine spatial resolution calculation is performed. Oftentimes, there are three steps in this process:

1. A fine group, coarse space calculation (e.g., thousands of groups and infinite lattice in space),
2. A medium-resolution group and space calculation (e.g., 100s of groups and a single assembly), and

3. A coarse group and fine space calculation (e.g., less than 10 groups and entire reactor core).

Below we will sketch some of the ways that the fine group problem can be solved and how coarse group fluxes can be computed. The transition from the medium-resolution to coarse groups will be covered when we discuss homogenization later.

2.3.1 Flat-group flux approximation

If one uses the finest cross-section data available, it may be possible to assume that the flux moments are constant inside each group. Consider a that we have point-wise measurements of cross-section data. Call a generic measurement point $E_{g-1/2}$. We then define the group boundaries as

$$E_g = \frac{E_{g-1/2} - E_{g+1/2}}{2}, \quad E_{g-1} = \frac{E_{g-3/2} - E_{g-1/2}}{2}. \quad (2.32)$$

We then say that the flux moments are constant in the group, $\phi_{lg} = C$. Therefore, we say that the cross-sections for a generic reaction, ℓ , are given by

$$\sigma_{g\ell}^{\text{flat}} = \sigma_\ell(E_{g-1/2}), \quad (2.33)$$

and the neutron speeds are

$$\left(\frac{1}{v}\right)_g^{\text{flat}} = \frac{1}{v(E_{g-1/2})} \quad (2.34)$$

This approximation is typically only justified when only the finest group structures are used.

2.3.2 Analytic flux approximation

A better approximation than the flat-flux approximation for thermal nuclear reactors is to use reactor theory considerations to give the flux shape in each energy group. To do this we split the energy spectrum into 3 regions: fission, slowing-down, and thermal region. For more detail on these regions and the flux shapes in each, see Stacey's monograph [2].

For the fission region, i.e., the region where fission neutrons are born, one

can show that a reasonable approximation to the scalar flux is given by

$$\phi(E) \propto \frac{\chi(E)}{\Sigma_t(E)}, \quad E \in [50\text{keV}, 10\text{MeV}]. \quad (2.35)$$

For the fission spectrum, we use the Watt fission spectrum [3] which writes for ^{235}U as

$$\chi(E) = -0.483941 \sinh(\sqrt{2E}) e^{-E} \text{ MeV}^{-1}. \quad (2.36)$$

For the slowing down region, the scalar flux is approximated by

$$\phi(E) \propto \frac{1}{\bar{\xi} \Sigma_t(E) E}, \quad E \in [1\text{eV}, 50\text{keV}]. \quad (2.37)$$

This formula can be derived via Fermi age theory [2]. The quantity $\bar{\xi}$ is the average logarithmic energy loss by scattering. For a given moderating nucleus of mass number A , $\bar{\xi}$ is given by

$$\bar{\xi} = 1 - \frac{(A-1)^2}{2A} \ln \left(\frac{A+1}{A-1} \right). \quad (2.38)$$

For a mixture of moderating atoms, one can calculate an effective value as

$$\bar{\xi}^{\text{mix}} \Sigma_s(E) = \sum_i N_i \bar{\xi}_i \sigma_s(E). \quad (2.39)$$

Note the effective value is energy dependent.

Finally, in the thermal energy range, we assume a Maxwellian with a hardened temperature as

$$\phi(E) \propto \frac{E}{(kT_n)^2} e^{-E/kT_n}, \quad (2.40)$$

where k is the Boltzmann constant. T_n is the neutron temperature

$$T_n = \left(1 + \frac{C \Sigma_a^{\text{thermal}}}{\bar{\xi} \Sigma_s^{\text{thermal}}} \right), \quad (2.41)$$

where C is a constant depending on the system and the absorption and scattering cross-sections are an average over the thermal range.

An example spectrum from this type of flux spectrum is shown in Fig. 2.1. In this figure the reactor is a combination of graphite (as pure ^{12}C) and enriched uranium. The fission region is above 0.1 MeV, the slowing-down range is from 0.5 eV to 0.1 MeV, and the thermal region is below 0.5 eV in this example. The reactor is operating at room temperature and we have assumed the neutron temperature is the same as the reactor temperature.

Also in this example, the flux is constrained so that it is continuous at the energy region boundaries. The flux profile is fairly sensitive to how the cutoffs between regions are set, so this approach is best for taking a fine group structure to a medium group structure that does not overlap the region boundaries.

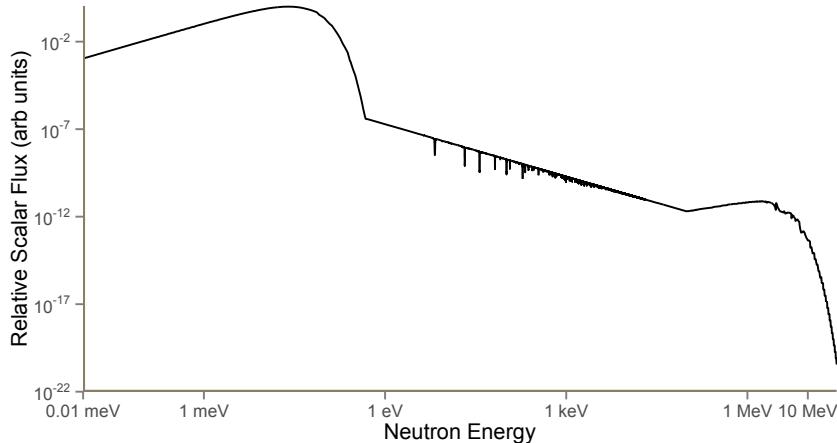


Figure 2.1: The spectrum for a homogeneous reactor comprised of 10% enriched uranium and graphite using the analytic flux method. The ratio of graphite atoms to ^{238}U atoms is 1000:5.

2.3.3 Infinite Medium Calculations

In an infinite medium problem, the streaming term in the transport equation will be zero. Additionally, given that the scattering is azimuthally independent, we can write a k-eigenvalue problem form of Eq. (2.26) as

$$\Sigma_{tg}\phi = \sum_{g'=1}^G \Sigma_{s0^*, g' \rightarrow g}\phi_{g'} + \frac{\chi}{k} \sum_{g'=1}^G \bar{\nu} \Sigma_{fg'}\phi_{g'}, \quad (2.42a)$$

$$\Sigma_{\text{tt}g}\phi_l = \sum_{g'=1}^G \Sigma_{\text{s}l^*, g' \rightarrow g} \phi_{lg'}, \quad l > 1. \quad (2.42\text{b})$$

Given that we are only interested in the scalar flux up to a constant we can set the fission source term divided by k to be unity so that Eq. (2.43) becomes

$$\Sigma_{\text{tg}}\phi = \sum_{g'=1}^G \Sigma_{\text{s}0^*, g' \rightarrow g} \phi_{g'} + \chi. \quad (2.43)$$

We could solve these equations using the flat-flux approximation and then compute medium-resolution group approximations using the formula

$$\Sigma_{\ell\hat{g}} = \frac{\sum_{g \in \hat{g}} \phi_g \Sigma_{\ell g}}{\sum_{g \in \hat{g}} \phi_g}, \quad (2.44)$$

where \hat{g} denotes a group in the medium-resolution group-set. This has the benefit of not assuming a flux shape for the collapse, rather it relies on the actual cross-section data.